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**DEVELOPMENT AND VALIDATION OF ATMOSPHERIC
DISPERSION MODELS
FOR IDEAL GASES AND HYDROGEN FLUORIDE**

PART I : TECHNICAL REFERENCE MANUAL

by

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The Industry Cooperative HF Mitigation/Assessment Program
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PREFACE

This report is one of several work products generated by the Industry Cooperative HF Mitigation/Assessment Program. This ad hoc industry program was begun in late 1987 to study and test techniques for mitigating accidental releases of hydrogen fluoride (HF) and alkylation unit acid and to better estimate ambient impacts from such releases.

The hazards of HF have long been recognized, and operating practices have been aimed at minimizing the possibility of a release and mitigating the effects of a release should it occur. These practices have been continually monitored and improved to maximize safety protection based on the available technical data. This recent program has been aimed at further improvements based on new technical data.

This program has been sponsored and funded by twenty companies from the chemical and petroleum industries. These include Allied-Signal, Amoco, Ashland, Chevron, Conoco/Dupont, Dow, Elf Aquitaine, Exxon, Kerr-McGee, Marathon, Mobil, Phillips, Saras, Shell International, Sohio, Sun, Tenneco, Texaco, Unocal, and 3M.

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EXECUTIVE SUMMARY

Program Overview

The thermodynamic behavior of hydrogen fluoride when diluted with air, particularly moist air, is very different from that of a simple ideal gas. In particular, the gas-air mixture can, depending on conditions, be denser than ambient air or substantially less dense than air. This behavior of an HF cloud would have a major influence on the dispersion behavior of HF in the atmosphere if it were released accidentally. Experience has shown that for gases such as LNG thermodynamic effects must be included in dispersion models in order to accurately simulate such releases. Because of the unique thermodynamic properties of HF, it was felt that those properties would be important in accurately simulating an HF release.

In 1986, it was decided that, because of the special properties of this gas, data on its dispersion were needed. A series of six atmospheric releases of superheated anhydrous hydrofluoric acid (HF) was performed at the Frenchman Flat spill test facility in Nevada by Amoco Oil Company and Lawrence Livermore National Laboratory. These experiments are known as the Goldfish Test Series (Blewitt et al., 1987a, b, and c). They provided a data base against which existing dispersion models were tested. The existing models did not take account of the changes in molecular weight and temperature in HF/H₂O/air mixtures, and model comparisons with three of the Goldfish releases (Blewitt et al., 1987b) indicated that the models generally under-predicted the observed plume centerline concentration data by as much as a factor of two.

As a result of the modeling difficulties associated with HF, and the difficulties in extrapolating the results from the desert setting where the Goldfish experiments were conducted to an industrialized or urban environment where an accidental release might occur, a program to improve HF model prediction was undertaken as part of a cooperative effort to develop assessment and mitigation techniques related to HF. This program was sponsored and funded by 20 companies from the chemical and petroleum industries all of which are either users or producers of HF. This HF

user/producer group is called the Industry Cooperative HF Mitigation Assessment Group. A sub-committee of this group, called the Ambient Assessment Group (AAG), was charged to direct this model improvement program.

This program identified three major areas in which substantial uncertainties existed in previous models: 1) the modeling of the complex thermodynamics of HF/H₂O/Air mixtures (including aerosol effects on cloud density); 2) the treatment of a wide range of surface roughness conditions (including possible multiple surface roughness conditions) and 3) jet flow and air entrainment for pressurized releases of HF, followed by transition to ground-based dense gas dispersion.

The major objectives of this study were to develop and validate computer-based models to calculate the release properties in addition to simulating jet and plume behavior downwind of an accidental release of HF. The AAG felt that it was important to provide enough detail in the near field or jet region, as well as the far field, so that reliable predictions of cloud properties could be estimated at the entrance to a mitigation device such as a water spray as well as estimating the distance or extent of the hazard zone. In addition, in order to address the effectiveness of mitigation systems, dispersion calculations should be able to commence downwind of the mitigation device so that the reduction in the hazard zone can be determined. Thus, it was decided that the models to be developed should have the following attributes:

- 1) the ability to account for the HF/H₂O/air thermodynamics and cloud aerosol effects on cloud density (both positive and negative effects);
- 2) the ability to model both pressurized (jet release, at any angle of release) and non-pressurized (evaporating pool) releases;
- 3) the ability to predict concentrations over a wide range of surface roughness conditions (possibly multiple roughness conditions);

- 4) the ability to predict concentrations at specific locations for user-specified averaging periods which are consistent with release duration;
- 5) the ability to consider steady state, time varying and finite duration releases and, for some cases, time varying releases and,
- 6) the ability to compute crosswind and vertical concentration profiles.

In developing such a model the AAG felt that it should use as the starting point an existing public domain model (defined as a model for which the computer source code is available for a nominal fee).

Following a review of existing models and proposals from model developers, the AAG selected the proposal of Shell Research Ltd. to develop a system of programs, based around the HEGADAS dense gas dispersion model, that would provide all the required capabilities previously listed. The resulting models have been incorporated into a software package entitled HGSYSTEM. It is important to stress that while the focus of this program has been to simulate the behavior and dispersion of HF clouds, the models contained within HGSYSTEM are models that are capable of simulating other chemicals in addition to HF.

The development of the models and their incorporation into the HGSYSTEM package was conducted in two phases. In Phase I, the HEGADAS model was modified to meet the objectives outlined above. The HFPLUME model was developed and tested to simulate jet flows from pressurised releases, dispersing initially as an elevated HF plume. The touchdown and slumping of an initially-elevated dense HF plume were also modelled in HFPLUME, with a link into HEGADAS to complete the modelling of the transition from an elevated to grounded dense gas cloud. In Phase II, a source estimation model, a pool evaporation model, and a far-field Gaussian model (linked to HFPLUME) were added to provide a more complete source and dispersion modeling package.

The HGSYSTEM software package runs on an IBM or equivalent PC. It contains an interactive program that provides a straightforward means of either running a single model, or of performing a linked series of model calculations.

Models Contained Within HGSYSTEM

Figure 1 provides a flow chart of the models contained in HGSYSTEM. These models are stand-alone computer programs which can be run separately or can be linked together to simulate all of the aspects of an accidental release of material into the atmosphere.

HFSPILL calculates the time dependent rate of release of HF, vapor or liquid, from a storage vessel during depressurization. A liquid release may either create a liquid pool on the ground, or if flashing occurs, form a jet composed of vapor and small droplets. If a pool is formed, the model EVAP can be used to predict steady or time-dependent evaporation. Otherwise, HFPLUME is used for the jet/plume dispersion calculations including touchdown and early spreading on the ground if the gas remains denser than air. Transition is then made to the dense-gas dispersion model HEGADAS-5. Conversely, if the plume remains buoyant, far-field passive dispersion calculations are performed by PGPLUME. There is also a version of the HFPLUME model to be used for ideal-gas releases; this is called PLUME.

HEGADAS 5 can simulate continuous (steady state) or time varying releases. Time-dependent input can be provided by EVAP, or from the steady state HFPLUME calculations with a known finite duration. The facility is provided to allow for changing surface roughness downwind. Post-processors allow the easy extraction of output parameters or profiles for automated plotting of results.

When two of the models are linked, e.g., HFPLUME and HEGADAS, the first model calculates some of the parameters required as input by the following model. The first model checks against criteria to decide when

calculation should be stopped and the next model started. Relevant parameters are then written to a file which is used as input to the next model. This file has the same form as the normal input files. The user can initially check the results of the upstream models before allowing the models to run automatically in sequence.

A user interface guides the user in the choice of models and standard input files to be edited; this automates the model execution and their linking.

Major Program Findings and Conclusions

The objective of the Impact Assessment Component was to develop a PC-based computer model which would estimate the downwind hazard zone from an accidental release of HF. In addition, these programs may be used to aid in the analysis of the reduction in the hazard zone as the result of implementing mitigation systems.

This program identified three major areas in which substantial uncertainties existed in previous models. (1) The modeling of the complex thermodynamics of HF/H₂O/Air mixtures (including aerosol effects on cloud density), (2) the treatment of a wide range of surface roughness conditions (including possible multiple surface roughness conditions) and (3) jet flow and air entrainment for pressurized releases of HF, followed by transition to ground-based dense gas dispersion.

As a result of this program a model has now been developed and independently evaluated which can accurately simulate HF dispersion over a wide range of conditions.

As a result of this program the following findings have been made:

- 1) Comparison between the HGSYSTEM models HFPLUME and HEGADAS and the Goldfish experiments gives good agreement between observed and predicted concentrations and temperatures.

- 2) With the inclusion of HF thermodynamics into the models, significant effects on plume dispersion result from changes in the water vapor content of the atmosphere.
- 3) The analysis of wind-tunnel data has resulted in a revised and more realistic gravity-spreading relationship in HEGADAS.
- 4) Following the inclusion of the improved gravity-spreading relation, the existing entrainment formulation in the model was found to be replicate experimental data over a very wide range of surface roughness without alteration.
- 5) For finite duration releases, the formulation for dispersion in the along-wind direction has been improved. This accounts for wind-shear, (i.e. the increase in wind speed with height) which is a function of atmospheric stability. In addition, for finite duration releases, the model has been improved to enable integration of the plume in order to account for the transient nature of the plume.

Comparison of HGSYSTEM With Goldfish Experiments

The first three Goldfish experiments were conducted to examine the dispersion properties of an HF cloud. These have been used to verify the HGSYSTEM models.

In these experiments, HF concentrations were measured at three downwind locations: 300, 1000 and 3000 meters. At each of these downwind distances, an array of samplers was located perpendicular to the plume. At a majority of these locations concentration measurements were made at 1, 3 and 8 meters above the ground. By employing a sampling array in this manner, it was possible to describe the cross section of the plume. The averaging time of the HF measurements was approximately 60 seconds.

In examining the results from HGSYSTEM, it is important to keep in mind how the physics or fundamentals of the models were formulated. The models in HGSYSTEM were developed using experimental laboratory data.

Parameters which quantify a particular physical process have been determined, where possible, from laboratory experiments which study that process in isolation. The models were then evaluated against independent field data to ensure that they correctly describe the effect of these various physical processes in combination. Thus an independence is maintained between the model formulation and the data which is used to evaluate the models (i.e. the models were not tuned or calibrated to any particular field data set). By using this approach, greater confidence can be given to the predictions from the model when it is applied to the simulation of an accidental release.

In simulating the Goldfish field experiments, HFPLUME was run to simulate the near field cloud properties. When the transition criteria were satisfied the cloud properties from HFPLUME were transferred to HEGADAS.

For Goldfish test number 1 the release duration was 2 minutes; therefore, once the plume traveled much further than 700 meters, a steady state model could not be used with confidence since the travel time of the plume exceeds the release duration. Thus, for the 3000 and possibly the 1000 meter sensors, the use of a steady state model could overstate the observed concentrations. The further downwind the simulation is conducted the greater the deviation between steady state and finite release duration calculations. The remaining two tests, Goldfish 2 and 3, had a release duration of 6 minutes, which permitted steady state calculations out to the final sensor arc at 3000 meters from the release point.

Comparison with the Goldfish experiments was performed in two ways. First, the model-predicted plume centerline concentrations were compared to observed centerline concentrations. This comparison is shown in Figures 2, 3 and 4 which are graphs of observed versus predicted plume centerline concentrations for Goldfish 1, 2 and 3. It should be noted that for the Goldfish 2, the plume centerline was not observed at a downwind distance of 3000 meters because of a shift in the wind direction. Second, a comparison of predicted and observed concentrations on a point-by-point basis was made for each downwind sampling distance. Thus, in this second method, a comparison is presented of the predicted and observed plume cross

section. This is shown in Figure 5, which is a comparison of the crosswind plume for Goldfish 1 at a downwind distance of 300 meters and a height of 1 meter. Figure 6 presents crosswind plume information for Goldfish 2 at a distance of 1000 meters and elevations of 1 meter. Figure 7 presents the comparison of the crosswind data for Goldfish 3 at 3000 meters downwind. Examination of these figures indicates that the model is predicting both the centerline (peak) concentration and the width of the cloud correctly.

Summary of Technical Developments

The following summarizes the technical developments which have been incorporated into the HGSYSTEM models.

HF Thermodynamics

HF-specific thermodynamic calculations have been incorporated in the models, since the thermodynamic properties of mixtures of HF and moist air can have a very strong influence on the dispersion of an HF cloud. Upon release into the atmosphere HF forms polymers up to $(\text{HF})_8$ which has a molecular weight of 160 g/g-Mole. As more air is entrained into the cloud, the HF depolymerizes which reduces the mean molecular weight. This process is endothermic and results in a cooling of the cloud. As water vapor is entrained into the cloud through mixing there is a strong exothermic reaction. Thus, there are competing mechanisms which influence cloud temperature and cloud density.

The thermodynamics sub-model used in HGSYSTEM is essentially the model first proposed and later revised by Schotte (1987, 1988). This sub-model determines the equilibrium concentrations of an ideal gas mixture containing air, water vapor, HF monomer, dimer $(\text{HF})_2$, hexamer $(\text{HF})_6$, octamer $(\text{HF})_8$, the complex $\text{H}_2\text{O}=\text{HF}$, and the possible existence of liquid HF/water aerosol.

Figure 8 illustrates the effect of ambient humidity on plume centerline concentrations. After about 100 meters relative humidity has a pronounced effect on predicted concentration. These trends are a result of

the thermodynamic reactions which alter the cloud density. For relative humidity around 50%, this reduces the gravity spreading in the early stages of dispersion, resulting in a plume which then dilutes more slowly than for a relative humidity of 10%. At higher relative humidities, this effect is counteracted by the enhanced vertical mixing resulting from the persisting additional buoyancy.

Figure 9 presents plume trajectories from HFPLUME for varying relative humidities. For this example, the computer model was run simulating a plume being released at a height of 10 meters in a horizontal direction. At low relative humidities the plume becomes dense and falls to the ground. However, at humidities above 70 percent, the plume is initially dense, but as more heat is released by reaction between HF and water, the plume becomes buoyant. This buoyant effect will result in substantially lower ground level concentrations.

Jet/plume modelling

HFPLUME has been based on a careful analysis of the difference between plume and undisturbed atmosphere, and the assignment of appropriate plume coordinates following the plume center of mass. The three regions of airborne, touchdown, and slumped plume are represented by circular, circular section, and semi-elliptic cross sections. They permit the description within a single formalism of descent to ground, ground-impact and subsequent gravity-spreading of a dense-gas plume. This approach is also applied to buoyant plumes. Jet entrainment, passive dispersion, momentum/buoyance effects and plume/ground impact are represented in each plume region.

Gravity Spreading

As part of this study, comparisons were made between predictions of HEGADAS and an extensive set of wind-tunnel simulations of dense-gas plumes (Peterson and Ratcliff, 1988). One finding from this analysis was that the well-defined gravity-current head at the edge of such a plume can be destroyed by boundary-layer turbulence much sooner than had previously been thought. After the collapse, the velocity of lateral spread is

typically reduced by an order of magnitude. Such a phenomenon had been studied in the laboratory by Linden and Simpson (1986, 1988). Using the wind-tunnel data and the work of Linden and Simpson, a criterion for this collapse was developed and implemented in HEGADAS-5. The findings of Linden and Simpson, and the success of the gravity-current-collapse condition in explaining data from a low-wind propane release and the Goldfish releases, indicate that the observations were not just an artifact of the wind-tunnel simulation. The HEGADAS-5 model was changed to successfully simulate this effect.

Surface Roughness Effects

Previous evaluations of HEGADAS and other dense gas dispersion models have been made using field experiments in which the surface roughness was small (0.03 to 0.00006 meters). An application of practical concern is a release in an industrial complex where the surface roughness is on the order of 0.5 meters or larger, followed by dispersion in a rural (0.03 meters) or urban (0.5 meters) environment. The assumptions, particularly relating to boundary layer profiles and turbulence, made in the development of HEGADAS are not strictly valid for a cloud whose height is comparable with the height of the obstacles on the surface. However, it was desirable to know whether, empirically, the model predictions relate to observations of dispersion at high roughness length. Therefore, HEGADAS predictions were compared with data collected in a boundary layer wind tunnel by Petersen and Ratcliff (1988).

As stated in the previous gravity spreading section, the wind tunnel data analysis resulted in changes to the gravity spreading algorithms. However, no change to the vertical entrainment formulation in HEGADAS was found necessary as a result of this study.

Surface roughness and gravity spreading are closely interrelated, the effect of high roughness length can be seen in Figure 10 which shows the effect of changing the gravity spreading relationship in HEGADAS. This figure presents model predictions from HEGADAS, the previous version of HEGADAS (Version 4) and two of the Petersen, Ratcliff experiments. As indicated in this figure, the revised model replicates the observed

centerline concentration and the cloud width better than the previous version of the model.

Figure 11 illustrates the effect of increased surface roughness above the valves observed for the Goldfish experiments. As indicated by this figure, there is almost an order of magnitude difference in the concentrations between the concentrations observed during the Goldfish experiments and the dispersion predictions in an urban environment.

Documentation

Documentation of the HGSYSTEM models is contained in three volumes:-

- 1) A Technical Reference Manual;
- 2) A User's Guide for the HGSYSTEM models; and
- 3) A systems manual.

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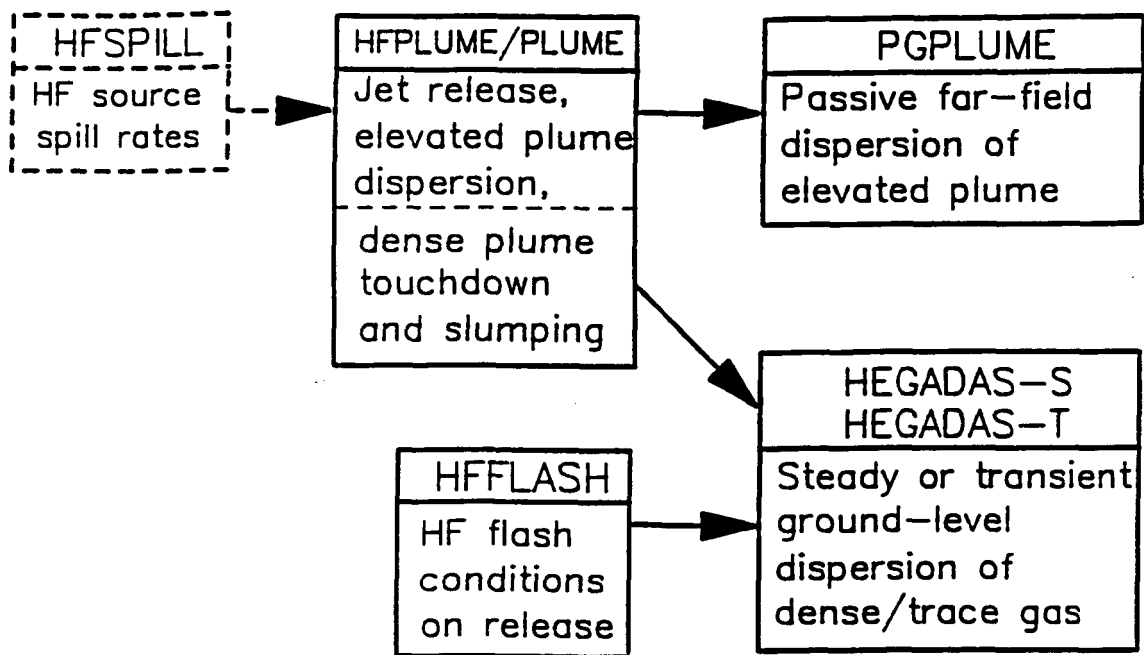
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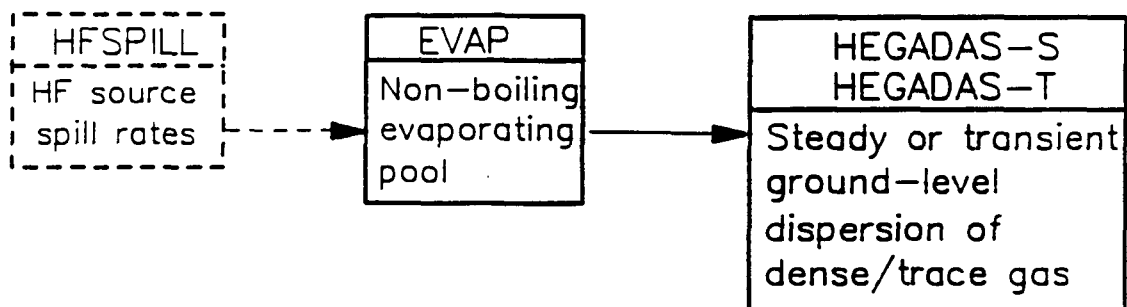
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(a)



(b)

Fig. 1. HGSYSTEM models for simulation of spillage, evaporation and dispersion of HF or of non-reactive gas; the programs HFSPILL, HFPLUME and HFFLASH are applicable to HF only

- (a) pressurised release [a transition is made from HFPLUME/PLUME to either PGPLUME (elevated dispersion) or HEGADAS (ground-level dispersion)]
- (b) unpressurised release

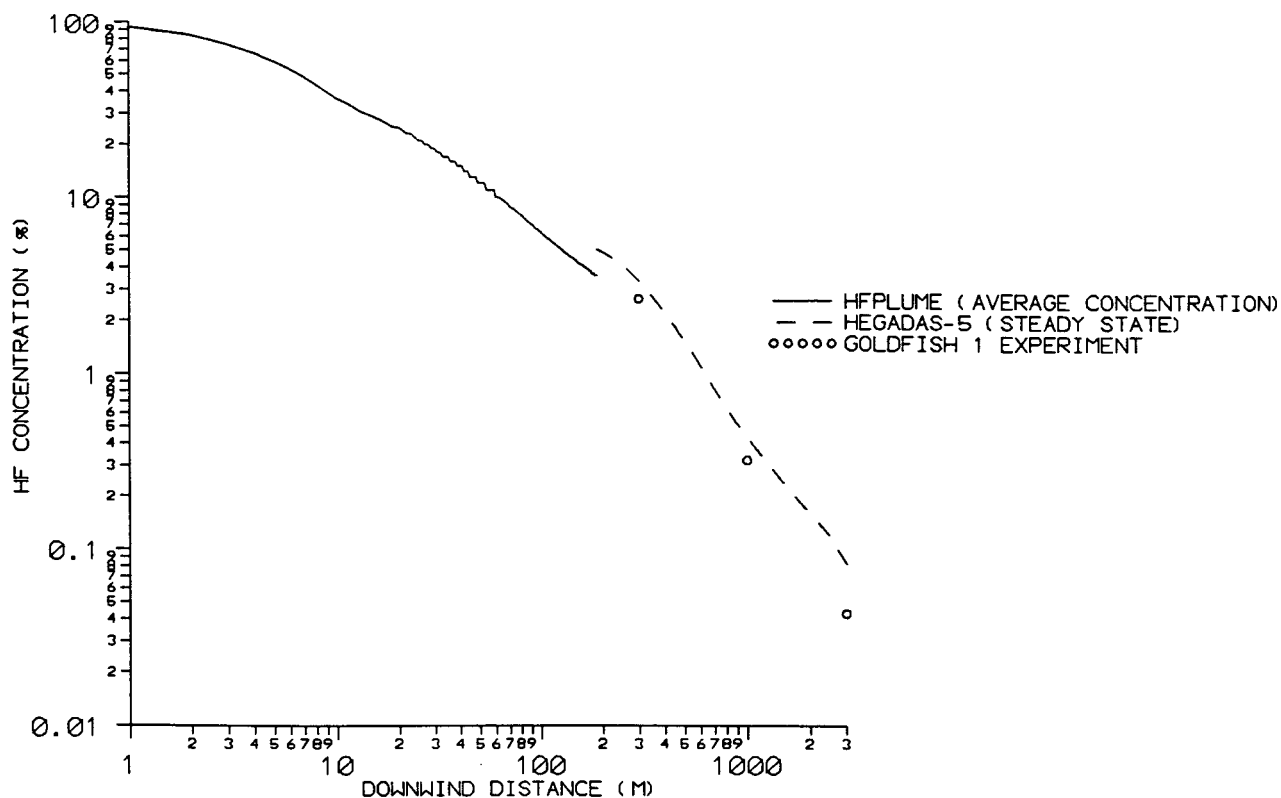


FIGURE 2. COMPARISON OF OBSERVED AND PREDICTED PLUME CENTERLINE CONCENTRATIONS FOR HFPLUME/HEGADAS-5 (STEADY STATE) FOR GOLDFISH 1

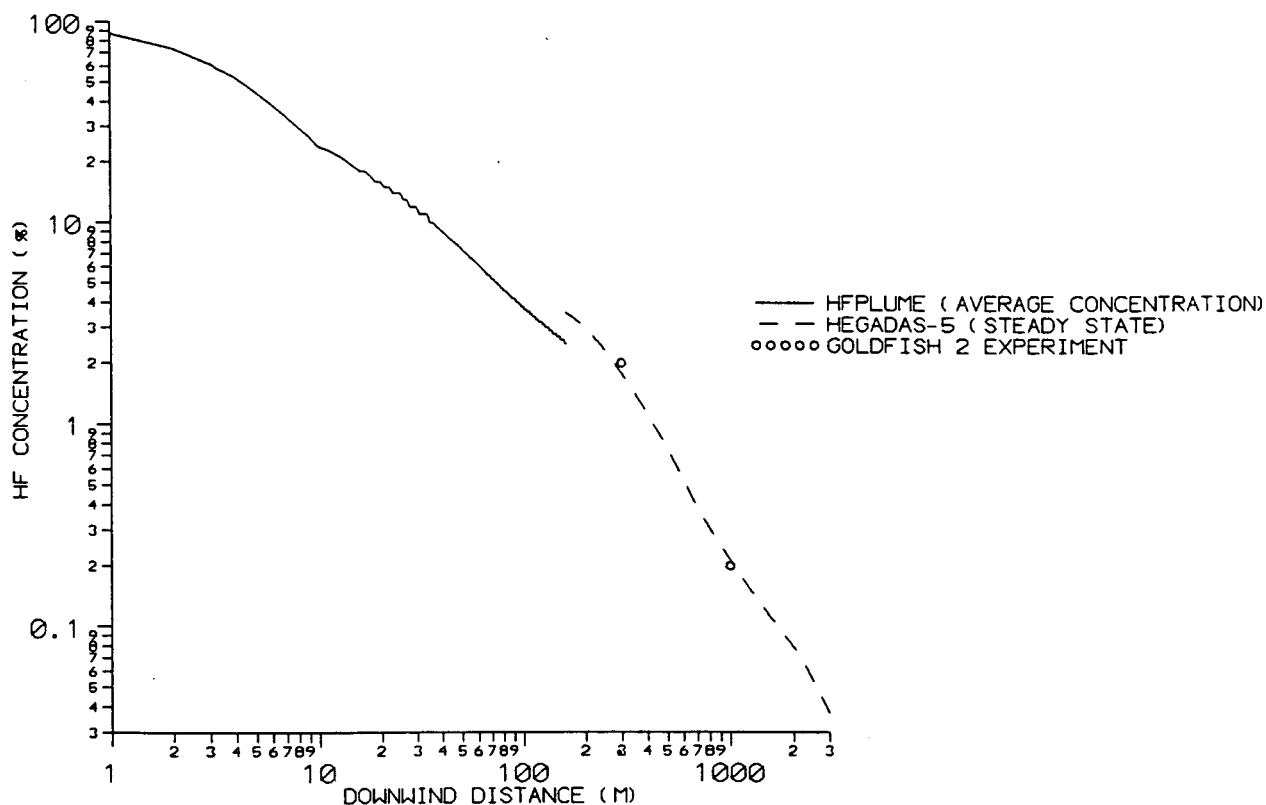


FIGURE 3. COMPARISON OF OBSERVED AND PREDICTED PLUME CENTERLINE CONCENTRATIONS FOR HFPLUME/HEGADAS-5 (STEADY STATE) FOR GOLDFISH 2

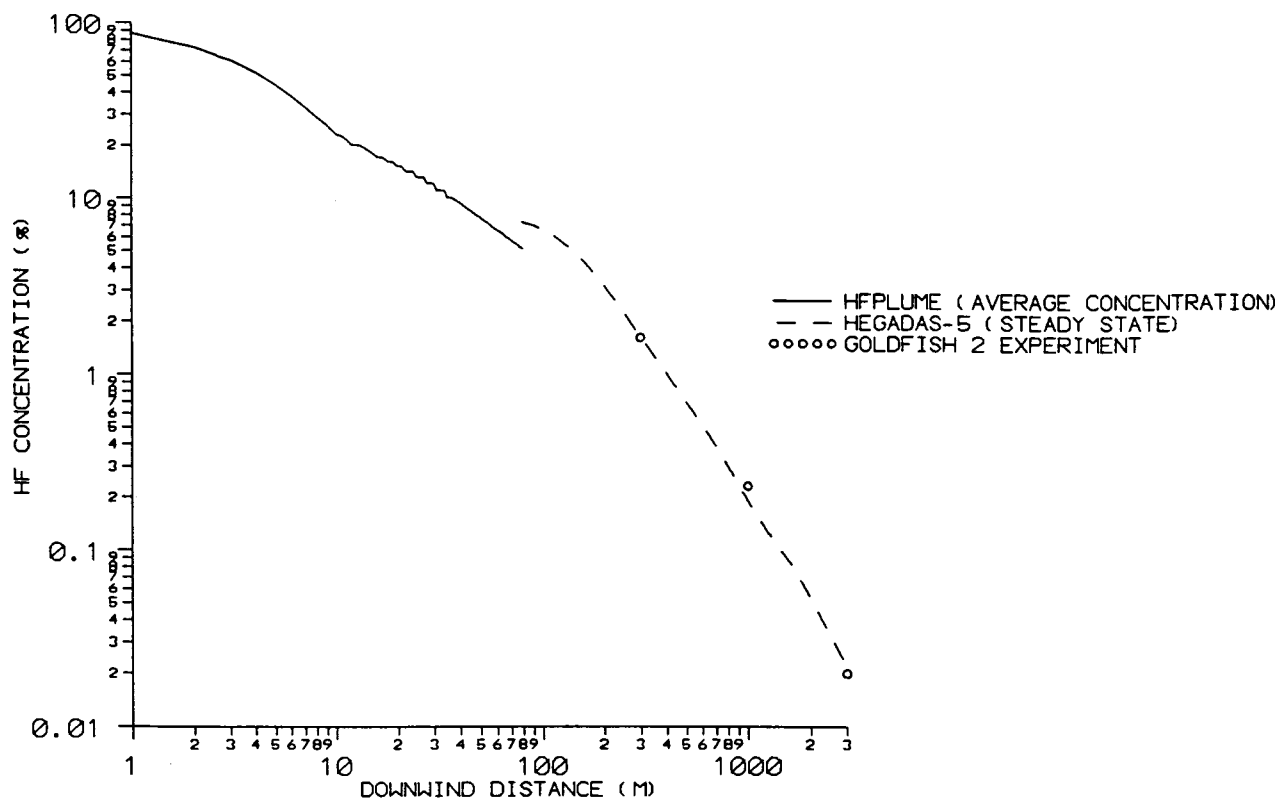


FIGURE 4. COMPARISON OF OBSERVED AND PREDICTED PLUME CENTERLINE CONCENTRATIONS FOR HFPLUME/HEGADAS-5 (STEADY STATE) FOR GOLDFISH 3

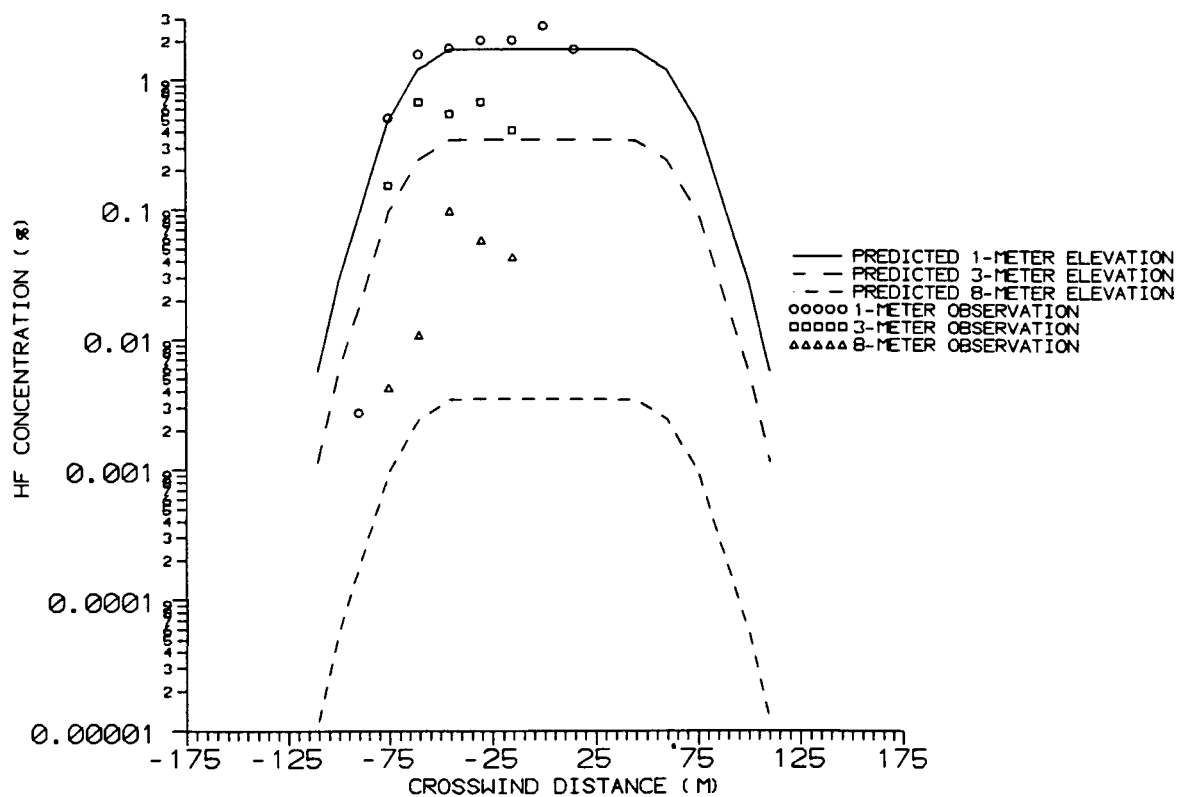


FIGURE 5. COMPARISON OF OBSERVED AND PREDICTED PLUME CROSS SECTION FOR GOLDFISH 1 AT A DOWNWIND DISTANCE OF 300 METERS

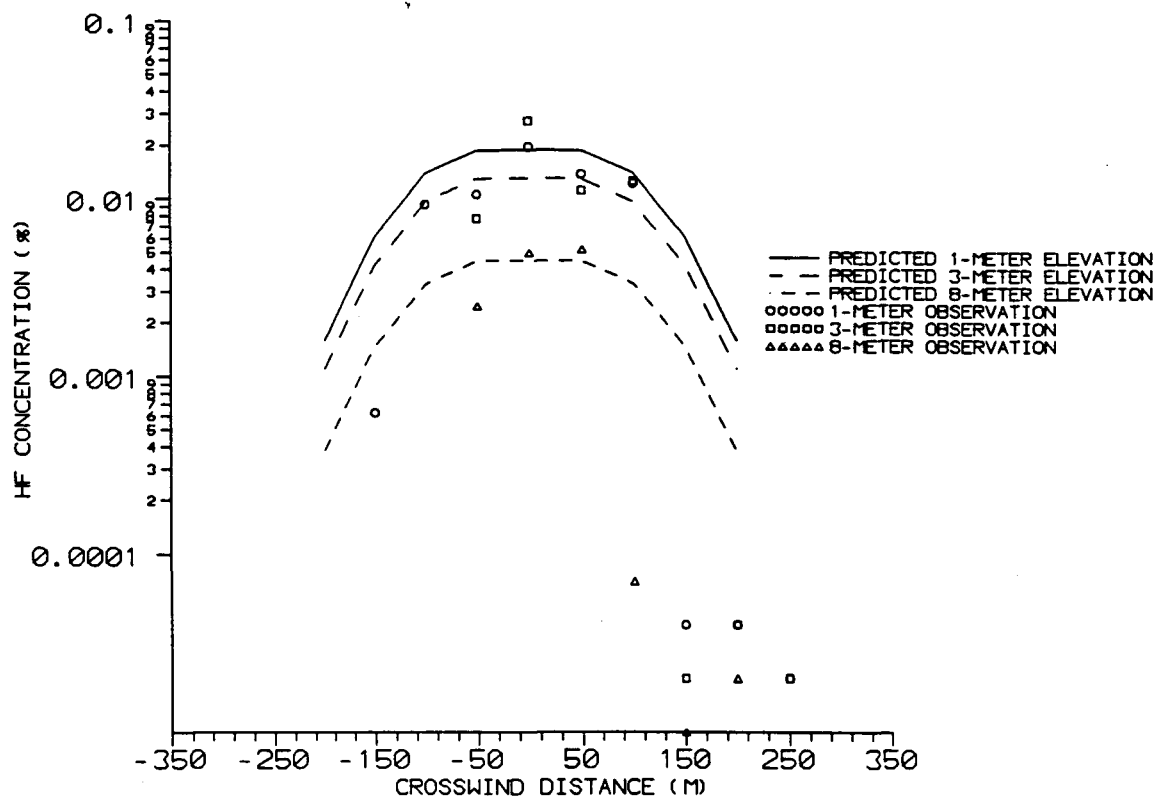


FIGURE 6. COMPARISON OF OBSERVED AND PREDICTED PLUME CROSS SECTION FOR GOLDFISH 2 AT A DOWNWIND DISTANCE OF 1000 METERS

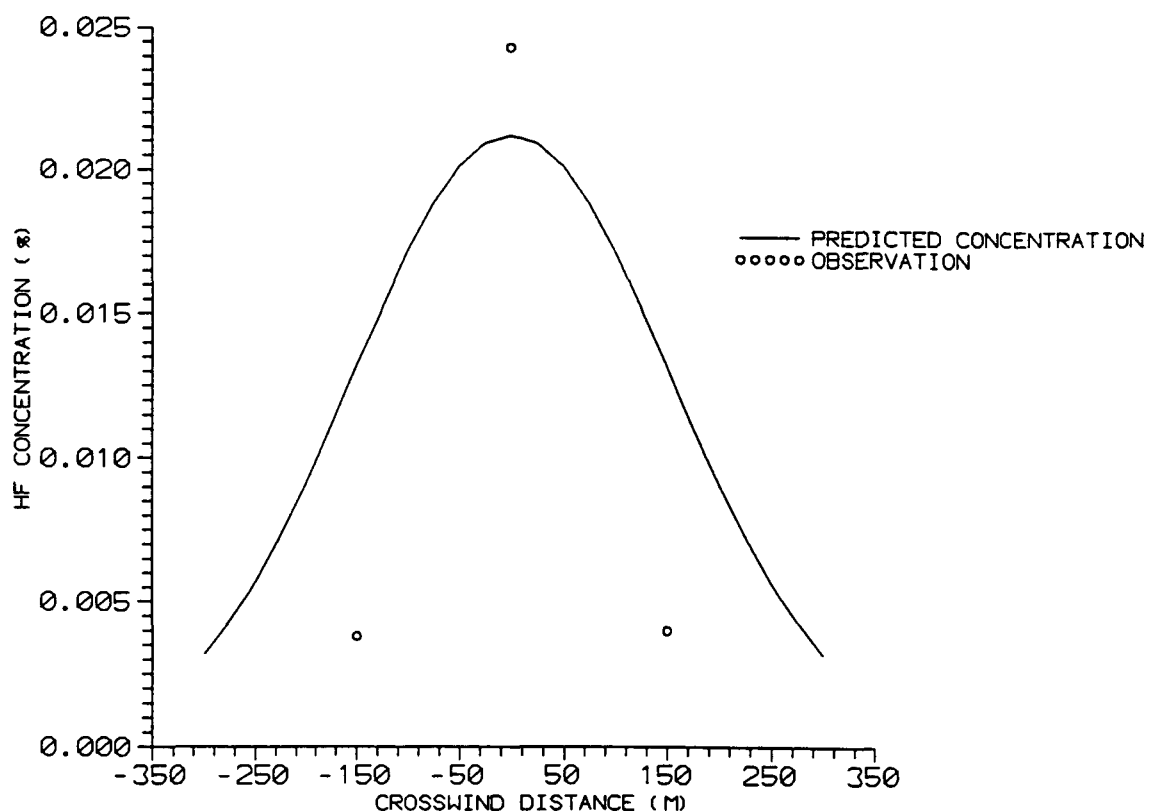


FIGURE 7. COMPARISON OF OBSERVED AND PREDICTED PLUME CROSS SECTION FOR GOLDFISH 3 AT A DOWNWIND DISTANCE OF 3000 METERS

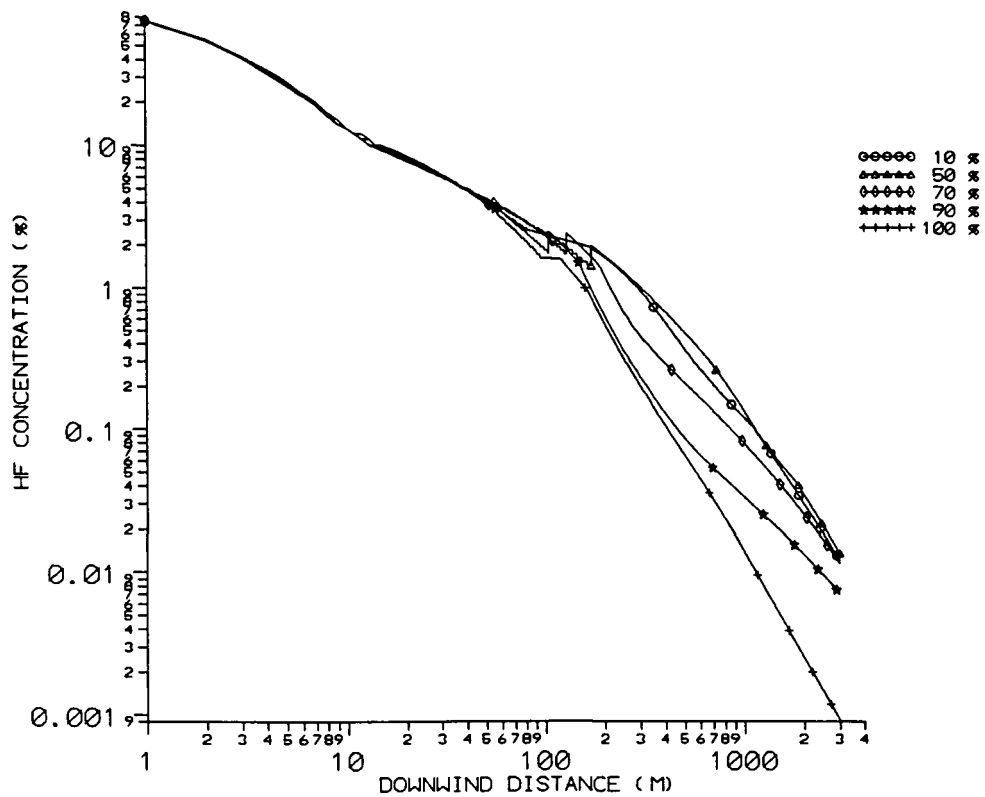


FIGURE 8. EFFECT OF RELATIVE HUMIDITY ON HFPLUME/HEGADAS-5 CONCENTRATION PREDICTIONS.

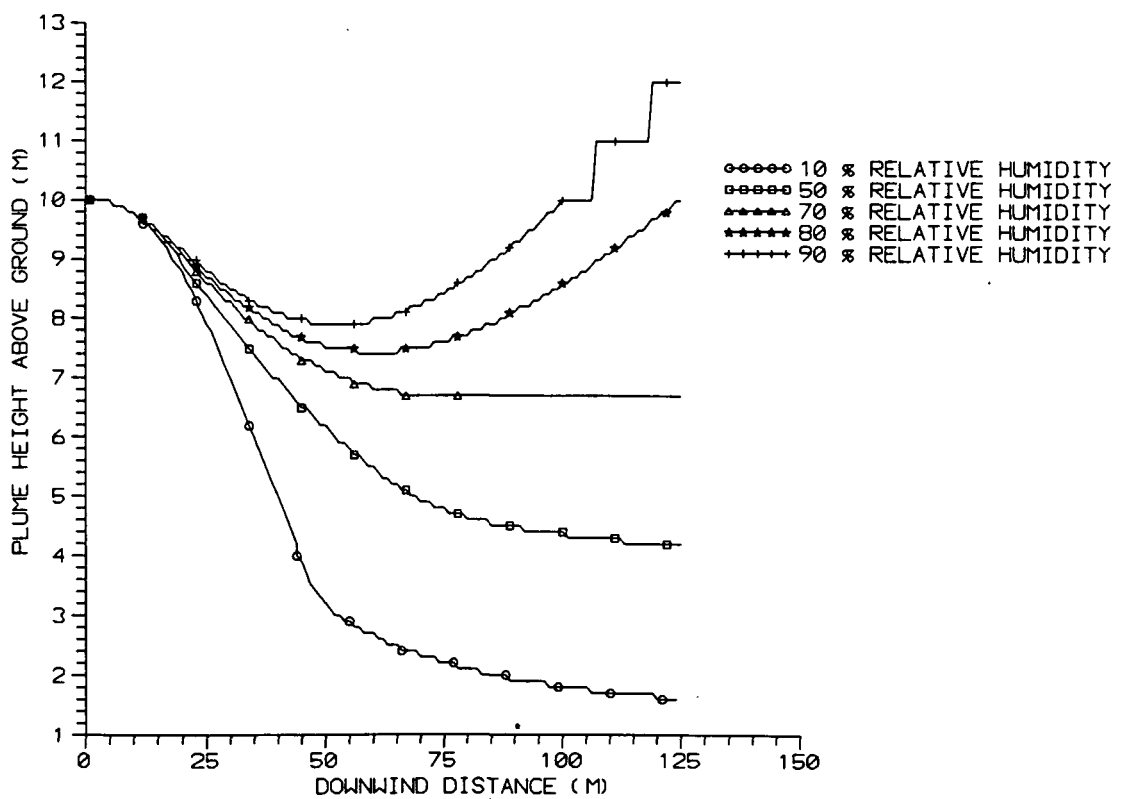


FIGURE 9. EFFECT OF RELATIVE HUMIDITY ON PLUME TRAJECTORY FOR JET RELEASES

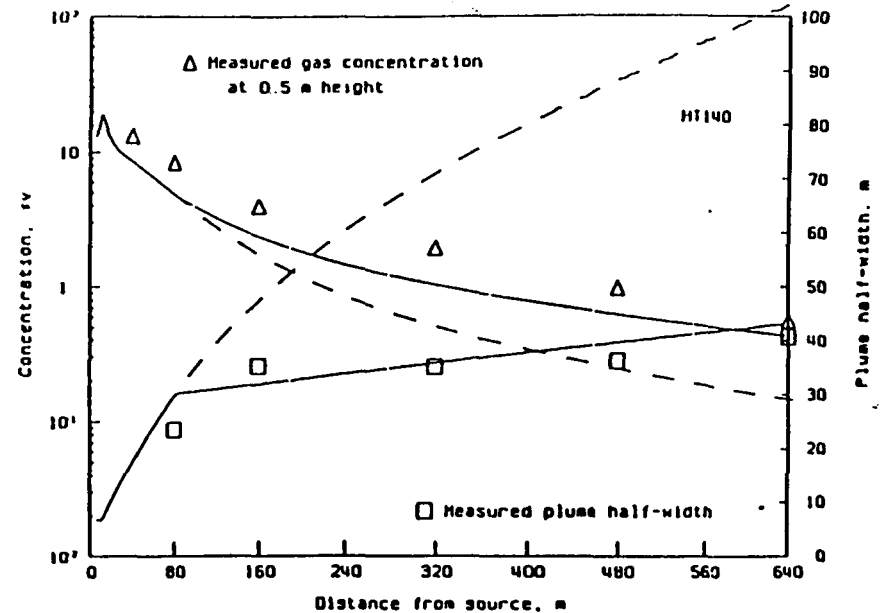
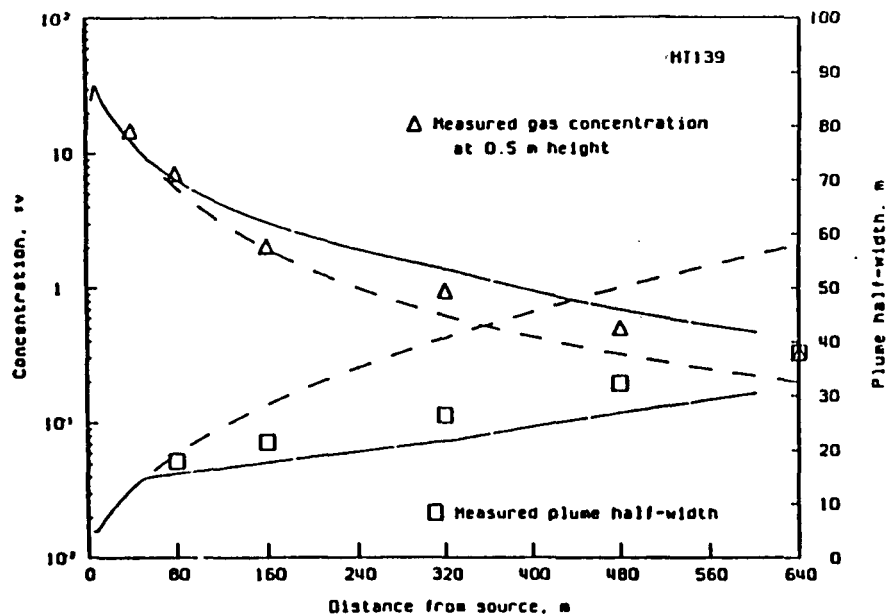


Figure 10. Effect of changing the gravity spreading formulation in HEGADASS to describe the plume spread observed in the course of the HTAG dispersion experiments. The dashed lines show the plume widths and centerline concentrations predicted by the original HEGADAS model. The HTAG data (squares) show a sharp reduction in the plume spread at about 80 m. The solid lines show the revised HEGADAS model predictions that take this into account.

Above left density ratio 1.4 and above right density ratio 3.9.
Results are for the R3 roughness distribution.

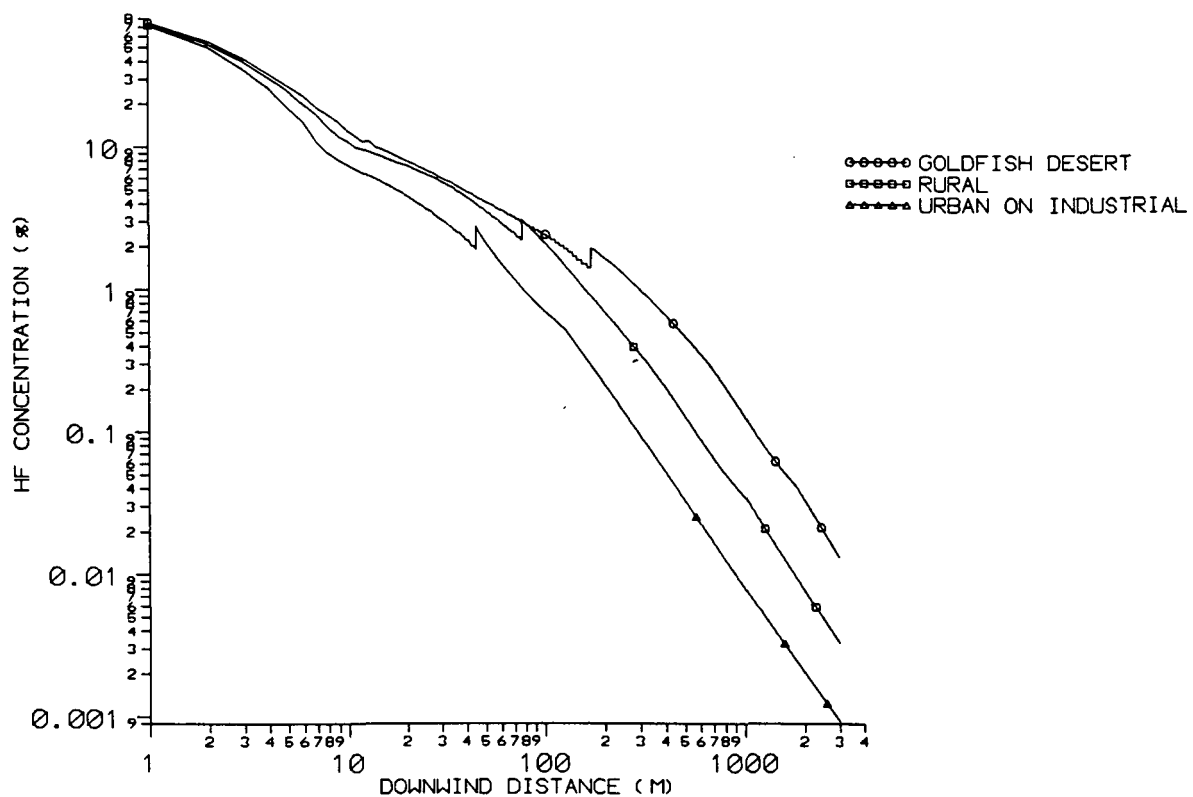


FIGURE 11. EFFECT OF SURFACE ROUGHNESS ON HFPLUME/HEGADAS-5 CONCENTRATION PREDICTIONS.

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Glossary

1. INTRODUCTION

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1. INTRODUCTION

1.1 Background

This report describes the results of work carried out on the development of models to predict atmospheric dispersion of gas releases taking into account the specific properties of hydrogen fluoride (HF). This work was performed under contract to the Ambient Impact Subcommittee of an ad-hoc Industrial Cooperative HF Mitigation and Assessment Group.

The dispersion of hydrogen fluoride is unlike that of simpler gases because of the possibility of marked changes in cloud density due to the chemical's complex thermodynamic properties. HF forms polymers when mixed with air at high concentrations. Depolymerisation occurs as the gas dilutes. This reduces the mean molecular weight and cools the gas. Water vapour in the atmosphere reacts with the gas, and this reaction is strongly exothermic. Both effects change the temperature of an HF-air mixture. Since the dispersion of a gas cloud is strongly dependent on its density, it is necessary that dispersion calculations are performed using models which take specific account of these thermodynamic effects.

The major objective of the study is to develop and validate computer-based models that may be used to calculate the release behaviour and jet and plume dispersion of accidental releases of HF. The dispersion models are required to have the following capabilities:-

- 1) to account for both HF/H₂O/air thermodynamics and aerosol effects on cloud density;
- 2) to simulate both pressurised (jet release, both vertical and horizontal) and non-pressurised (boiling pool) releases;
- 3) to predict concentrations accurately over a wide range of surface roughness conditions (possibly multiple surface roughness

conditions);

- 4) to predict concentrations for user-specified concentration averaging times consistent with release duration at user-specified (ground-based) locations;
- 5) to consider both steady continuous and time-varying release rates;
- 6) to compute crosswind and vertical concentration profiles;
- 7) to treat both dense-gas and passive (ground-based and elevated) phases of dispersion;
- 8) to compute release rates from storage vessels.

In preparing research proposals for the development of the above models, we considered that the key area was the modelling of the ground-level dispersion of a dense HF/moist-air cloud, and that the existing Shell HEGADAS model provided an excellent starting point for the development of a model with HF-specific attributes.

The Shell model for steady and transient releases of dense gases, HEGADAS, was first developed in 1979 and details were published by Colenbrander (1980). Subsequent papers have described the validation of the model using a variety of data (Puttock et al., 1983, 1984, Colenbrander and Puttock, 1984, Puttock, 1987b). Developments in the model have been described by Colenbrander and Puttock (1983, 1989). HEGADAS has been released in the public domain through the U.S. National Technical Information Service (NTIS). A description of the public release version of HEGADAS (Colenbrander and Puttock, 1989) is included as Appendix 3 of this report. This version of HEGADAS is denoted by HEGADAS-4 in this report.

We considered that HEGADAS would be a particularly appropriate model for use with HF, since much of its validation had been performed against data from field releases of liquefied natural gas (LNG) (Maplin Sands, Puttock et al, 1982). For LNG, as for HF, the thermodynamics are very

important; major issues are the effect of humidity and the effects of density changes on dispersion of a gas cloud which may become slightly buoyant. Although the vapour from LNG releases is dense because of its low temperature, heat transfer from the surface and heat released by the condensation of water vapour can make an LNG cloud slightly buoyant for a time if the ambient humidity is high enough. This positive buoyancy has a marked effect in reducing dispersion distances (Puttock, 1987a). Much of the analysis of the Maplin Sands experiments has related to quantification of these effects. With allowance for water vapour effects, HEGADAS has been very successful in reproducing the observed field data. (It should be noted that the field data have only been used for validation, not to tune parameters in the model. This is further discussed in section 9.1 of Chapter 9).

To illustrate the influence such thermodynamic effects can have on dispersion predictions, Table 1.1 shows the results of calculations for Maplin Sands continuous LNG releases. The first column of predictions shows the results of early model runs before the effects of surface heat transfer and surface water-vapour transfer were included and before allowance was made for a humidity gradient in the atmosphere. Note that the important thermodynamic effect of water-vapour condensation was already included in these calculations. The second column of predictions shows the results of final runs of the model HEGADAS-4, which included the above effects. The model predictions all then fall within the range of the observations except for one experiment where we are fairly sure that a steady-state was not reached. If the comparison were made in terms of concentration, rather than distance, then the effect would be approximately a factor of two difference between the two sets of calculations. Thus, for such materials, thermodynamic effects on dispersion can be very significant.

A mathematical model for the simulation of flashing liquid jets of hydrocarbons, WETJET, had also been developed prior to the start of this work (McFarlane, 1988, reproduced as Appendix 1). The WETJET model successfully represented the mixing and evaporation of propane in the two-phase region immediately downstream of the release point. The model provides a good basis for the formulation of a model to describe the

high-momentum behaviour of a pressure-driven release of HF, and its early dispersion as an elevated plume. This would be followed by touchdown at the ground and subsequent transition to modelling by HEGADAS, or by further dispersion as a passive elevated plume.

We can thus make the following observations about the required attributes of the models listed above. Items 3 to 6 were already capabilities of the HEGADAS model. Further study and validation of surface roughness effects, and development of the longitudinal diffusion approach, are included in this programme of work. Aerosol effects on cloud density (item 1) were already covered by the standard thermodynamic subroutine in HEGADAS; the properties of HF are incorporated by the addition of a special thermodynamic subroutine for HF. Pressurised jet releases and dispersion as an elevated plume (item 2) are catered for by the development of an elevated plume model based on WETJET. Models have also been developed for calculation of release rates, pool evaporation and far-field elevated passive plume dispersion.

1.2 Outline of the Technical Reference Manual

Chapter 2 of this report describes the thermodynamic properties of mixtures of HF and moist air. Depolymerisation of HF, as the gas concentration dilutes, reduces the mean molecular weight and cools the gas. Water vapour in the atmosphere associates with the gas, and this reaction is strongly exothermic. Both effects change the temperature and density of an HF-air mixture and strongly influence dispersion behaviour. The thermodynamics model used in this work is based on the model published (1987), and later revised in some details, by Schotte. The model determines equilibrium concentrations of an ideal gas mixture containing air, water vapour, HF monomer, dimer $(\text{HF})_2$, hexamer $(\text{HF})_6$, octamer $(\text{HF})_8$, and the complex $\text{HF}-\text{H}_2\text{O}$, as well as the possible existence of a liquid HF/water aerosol. Implementation of the thermodynamics model in HEGADAS and HFPLUME is outlined; Appendix 5 contains details of the incorporation into HEGADAS. The implementations of the thermodynamic models have been checked and are in agreement with calculations and measurements reported by Schotte.

Chapters 3 and 4 are concerned with source modelling. In an accident, a spill of HF may either form a liquid pool on the ground, or be released under pressure as a liquid or two-phase jet. The program HFSPILL predicts the release rate and release conditions at the spill point for a variety of possible spill scenarios involving release from pressurised containment. The program EVAP describes evaporation from a pool of liquid on the ground. The pool may be spreading out over the ground, in which case the output is a time-dependent evaporation rate suitable for input to the time-dependent HEGADAS model.

Chapter 5 describes the formulation and testing of a new jet/plume model that may be used to predict the behaviour of an elevated pressurised release of HF from the source, both as a high-momentum jet and as an elevated plume. The model HFPLUME calculates the behaviour of flashing liquid HF, or a gas release, as a jet directed horizontally downwind, vertically, or at any angle between. The subsequent plume behaviour is also modelled, whether the plume stays aloft or drops to the ground. The influence of gravity and the ambient wind, atmospheric turbulence (Appendix 2) and gradients in the atmosphere are taken into account. If the plume impinges on the ground, the transition to a ground-based dense plume is modelled. Detailed calculation of the thermodynamic behaviour of HF is incorporated in the HFPLUME model.

A version of the jet/plume model, PLUME, that may be used for any ideal gas release has also been implemented. The PLUME model differs from HFPLUME only in the thermodynamics model used. (See Appendix 2 of the User's Manual).

HFJET is a much simplified version of the model valid only for the prediction of high-momentum conditions in a horizontal HF jet close to the release point; it has the advantage of running significantly faster than HFPLUME for computations under these restricted conditions. The model is described in Appendix 4.

Chapter 6 contains a description of the transition from the elevated plume modelled by HFPLUME or PLUME to the Gaussian plume model PGPLUME for passive dispersion in the far-field. PGPLUME reproduces the standard Pasquill-Gifford dispersion curves.

Chapter 7 summarises the developments which have been made in preparing the new version of HEGADAS, called HEGADAS-5. These include the implementation of the HF thermodynamics model described in Chapter 2. The representation of crosswind dispersion is generalised to allow the use of Briggs' formulae for the lateral dispersion coefficient σ_y . The transition from lateral gravity spreading to diffusional spreading of a dense cloud is analysed in some detail in Chapter 8, and the proposed revision to HEGADAS is summarised in this chapter. An improved representation of downwind dispersion has been developed and incorporated in the transient model HEGADAS-T. Other features include post-processors and additional "breakpoint" facilities, including the ability to deal with changes in surface roughness during the dispersion or to start calculations with given conditions at some point downwind of the source. The interfaces with HFPLUME and a simpler flash calculation HFFLASH are also described.

Chapter 8 examines the effects on dense-gas dispersion of changes in surface roughness. The principal data available for such a study are derived from wind-tunnel experiments. Predictions of HEGADAS are compared with measurements from an extensive set of wind-tunnel experiments covering a variety of surface roughnesses, gas densities, and release types. This study has also prompted a re-evaluation of the treatment of lateral gravity spreading in dense gas dispersion models, and a new criterion is developed to define the point of sudden breakdown of gravity spreading that is apparent in the wind tunnel experiments.

Chapter 9 contains details of the comparison of predictions given by HFPLUME and HEGADAS-5 with the experimental results of the large scale field releases of HF at Frenchman Flat, the Goldfish series of experiments. The comparisons are used to provide an independent validation of these models, whose formulation has been not been based on the Goldfish test results. Simulations are reported of the three tests in which water sprays were not used.

Chapter 10 presents the results of sensitivity calculations carried out using the HFPLUME and HEGADAS-5 models. Two base cases are defined, and the effects of changes in both the input data variables, particularly ambient conditions, and model parameters are examined.

1.3 The HGSYSTEM Computer Programs

The primary products of this project are the HGSYSTEM computer programs, whose formulation, testing and validation are described in this Technical Reference Manual. Full details on implementing and running the HGSYSTEM programs, and detailed user guides to the programs, are contained in the HGSYSTEM Program User's Manual (Witlox, McFarlane, Rees and Puttock, 1990), which forms the second volume of the documentation for the project. These will be referred to subsequently in this report simply as the "User Guides". These programs are supplied in a form suitable for running on IBM personal computers. (They have also been successfully ported to UNIX and IBM VM/CMS operating systems.)

The models in HGSYSTEM are stand-alone computer programs which may either be run individually, or alternatively may be linked together to simulate successive aspects of the behaviour of an accidental release of material into the atmosphere. Where models can be linked, the first model calculates parameters which are required as input by the following model. For instance, the pool-evaporation program EVAP calculates the evaporation data needed for further dispersion calculations by the heavy-gas-dispersion program HEGADAS.

Four types of release scenarios can be analysed by linkage of models in HGSYSTEM, i.e. the unpressurised or pressurised release of HF, and the unpressurised or pressurised release of a non-reactive gas. Figures 1.1, 1.2, 1.3, 1.4 illustrate the consecutive phases (spillage, evaporation or flashing, jet-flow, near-field dispersion, far-field dispersion) for these four scenarios, indicating which models are used to model these phases. Table 1.2 includes a short summary description of each model and a description of the type of release for which the model might be applied (pressurised or unpressurised release; release of HF-gas or a non-reactive, 'ideal' gas; steady-state, finite-duration or transient release).

To provide an easy way to run one model, or to perform a linked series of model runs, the HGSYSTEM interactive program has been prepared. This interface leads the user through the editing of input data and automates the running of the programs. Use of the interactive program provides a simple introduction to the models, and a straightforward means of running the programs (see Chapter 10 of the User's Manual).

The needs of the more experienced user of such programs, who wishes to do multiple production runs easily and efficiently, can often conflict with the requirement for ease of use initially. These needs have been catered for by the development of a system for batch running of the programs, and automatically produced linking files between programs which need to be run successively.

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TABLE 1.1

Observed and Predicted Distances to Lower Flammable Limit
for Maplin Sands Continuous LNG Spills (surface release)

<u>Trial Number</u>	<u>Spill Rate M³/s</u>	<u>Wind Speed m/s</u>	<u>Distance to LFL</u>		
			<u>Observed</u>	<u>Predicted¹</u>	<u>Predicted²</u>
27	3.2	5.5	200 ± 25	260	210
29	4.1	7.4	165 ± 20	250	180
34	3.0	8.6	170 ± 25	195	145
35	3.8	9.8	180 ± 30	205	160
39	4.7	4.1	130 ± 20 ³	355	220
56	2.5	5.1	115 ± 30	210	125

- Notes:
- 1) Initial model runs without surface heat or water vapour transfer and taking relative humidity observed at 10m level.
 - 2) Model runs with surface heat and water vapour transfer. Also measured humidity of air at 1m elevation used.
 - 3) The full steady plume may not have developed in the short time available for dispersion in trial 39, with a resulting low observed LFL distance.

(From Puttock, 1987)

Table 1.2 Programs available in HGSYSTEM

Program	Description of model	gas ¹	release ²		doc. ³
HFSPILL	spillage from a pressurised vessel	HF	pr	tr	Ch.4
EVAP	spreading/evaporation of a liquid pool	both	unpr	st, tr	Ch.5
HFFLASH ⁴	flashing of HF	HF	pr	st ⁴	Ch.7
HFJET ⁵	jet flow	HF	pr	st	App.1
HFPLUME	jet flow and near-field dispersion	HF	pr	st ⁶	Ch.6
PLUME	jet flow and near-field dispersion	ideal	pr	st ⁶	App.2
HEGADAS-S	ground-level heavy-gas dispersion	both	both	st, FD ⁷	Ch.8
HEGADAS-T	ground-level heavy-gas dispersion	both	both	tr	Ch.8
PGPLUME	elevated passive dispersion	both	pr	st, FD	Ch.9

¹ Type of released gas: HF-gas or non-reactive, 'ideal' gas

² Type of release: pressurised (pr) or unpressurised (unpr); steady-state (st), finite-duration (FD) or transient (tr)

³ Each model is documented by a User's Guide included as a Chapter (Ch.) or Appendix (App.) in the HGSYSTEM User's Manual

⁴ If HFPLUME is not run, HFFLASH is used to set HF post-flash data required as input to HEGADAS. Although HFFLASH is a steady-state program, it can be interfaced with both HEGADAS-S and HEGADAS-T.

⁵ HFJET is a simplified version of HFPLUME and should not normally be used.

⁶ Although HFPLUME and PLUME are steady-state programs, they do accept a finite-duration input parameter (e.g. from HFSPILL in case of HFPLUME). This parameter is not used in HFPLUME/PLUME, but passed through to PGPLUME or HEGADAS-T.

⁷ HEGADAS-S is a steady-state program. Although a finite-duration error-function correction can be applied in its post-processor HSPOST, the use of the (more CPU-expensive) transient program HEGADAS-T is advocated for modelling finite-duration releases.

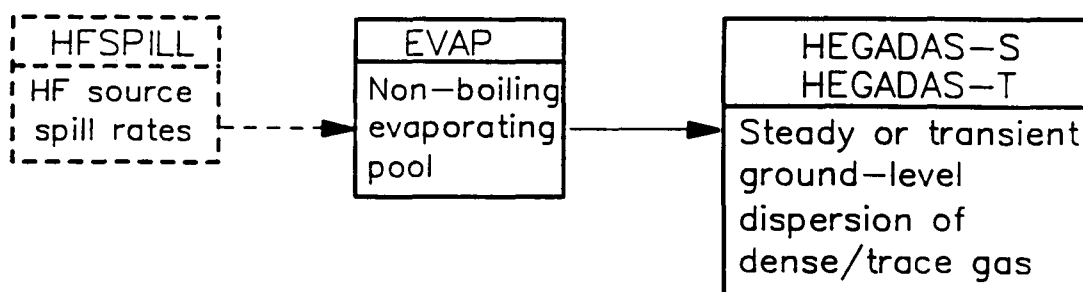
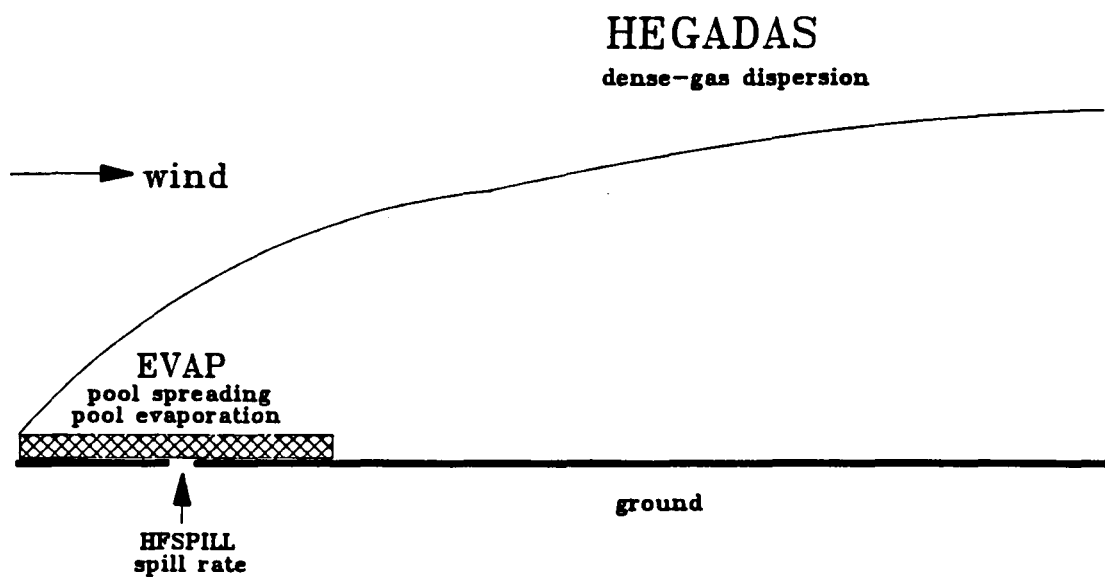


Fig. 1.1. Sequence of HGSYSTEM models for unpressurised release of HF

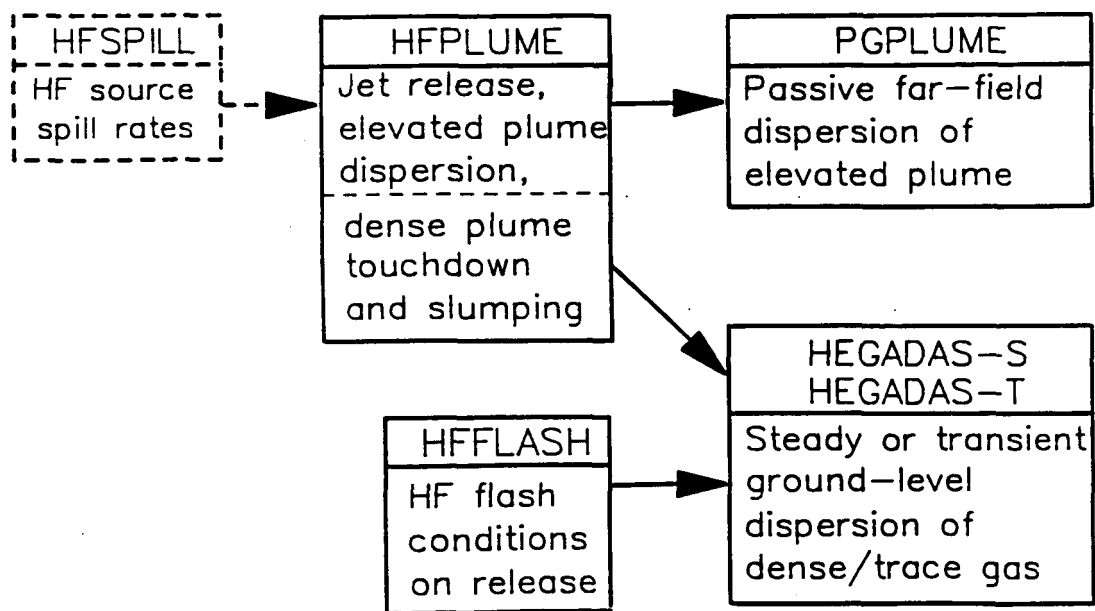
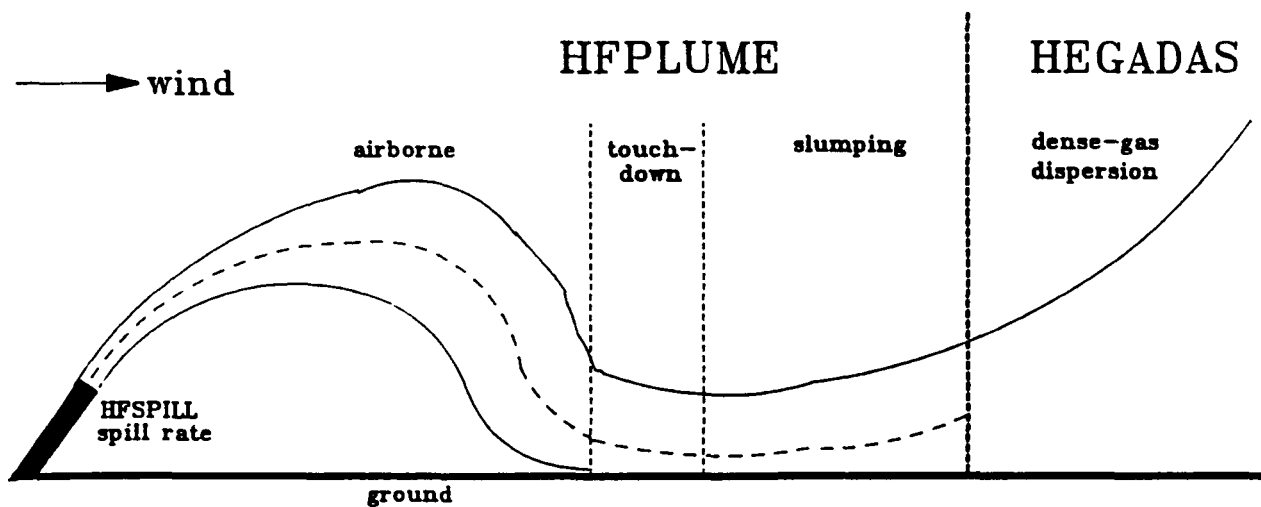
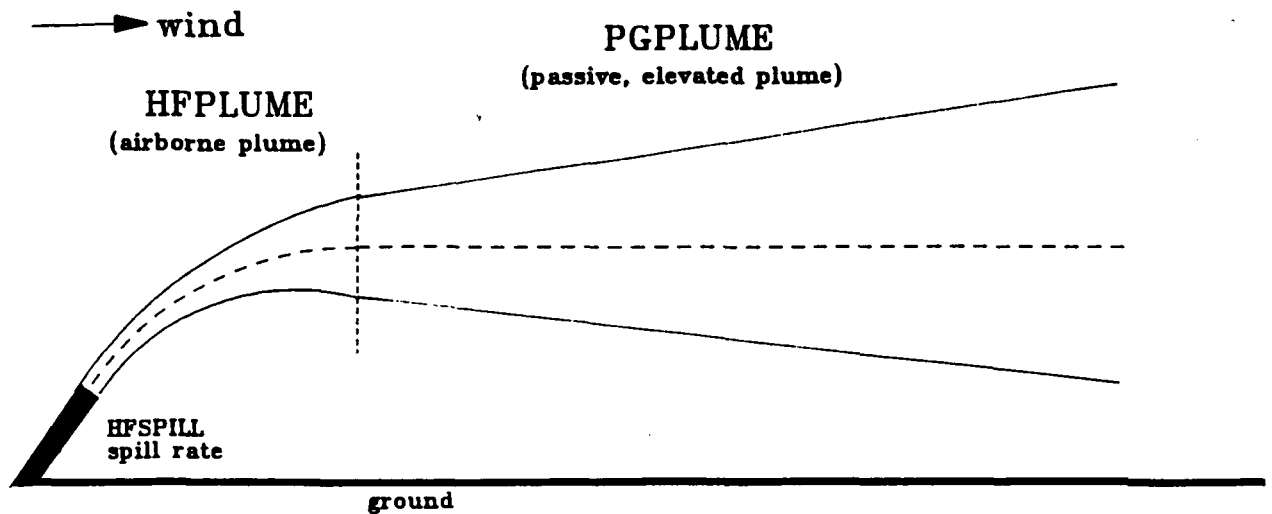


Fig. 1.2. Sequence of HGSYSTEM models for pressurised release of HF. A transition is made from HFPLUME to either PGPLUME (elevated dispersion) or HEGADAS (ground-level dispersion). If HFPLUME is not run, HFFLASH is used to set the flash data needed by HEGADAS.

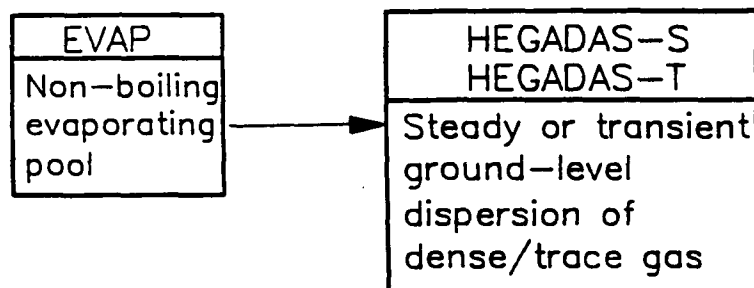
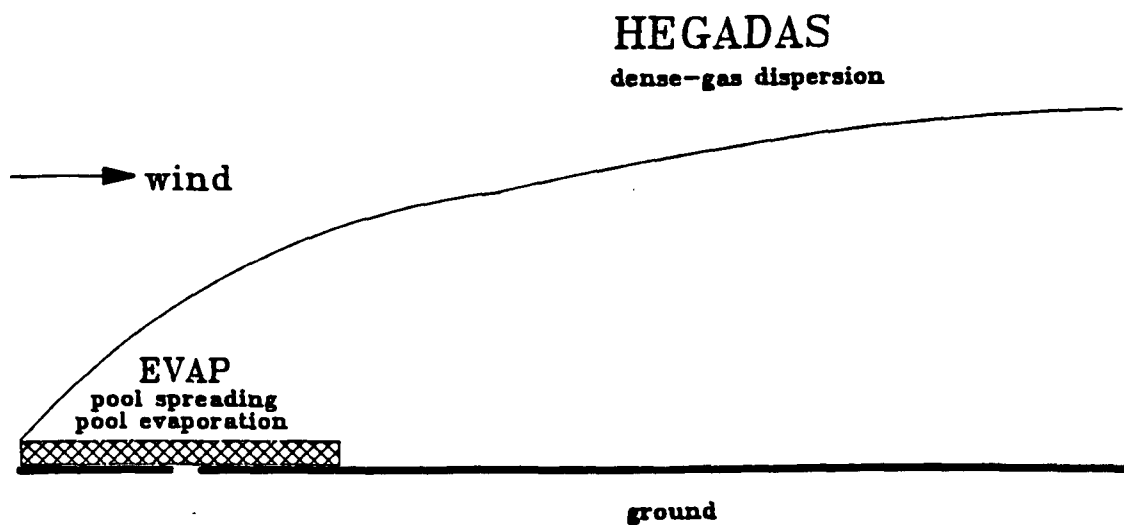


Fig. 1.3. Sequence of HGSYSTEM models for unpressurised release of non-reactive gas.

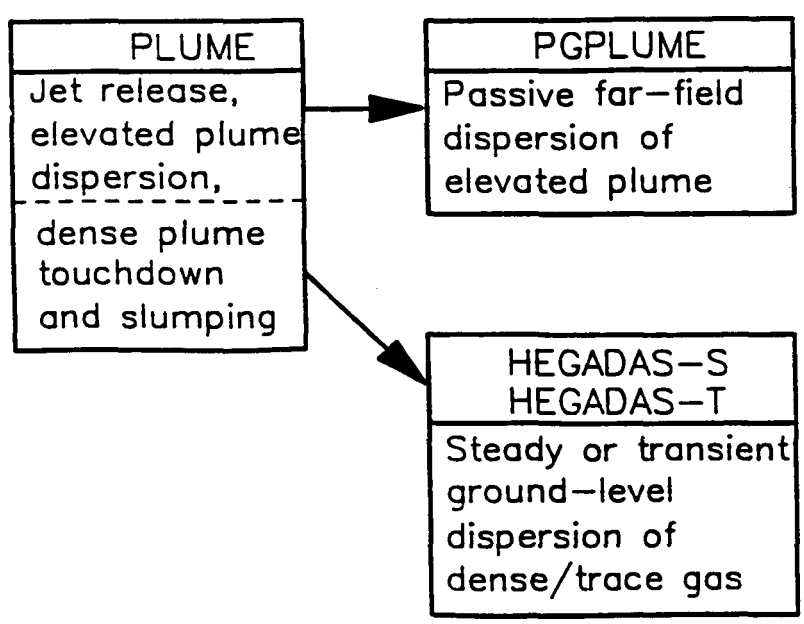
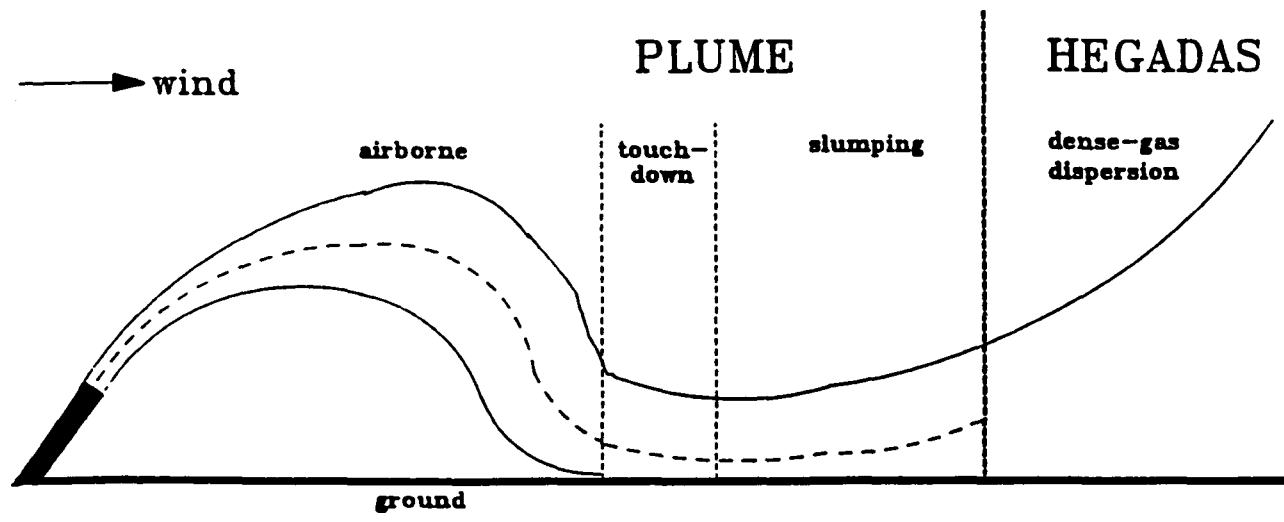
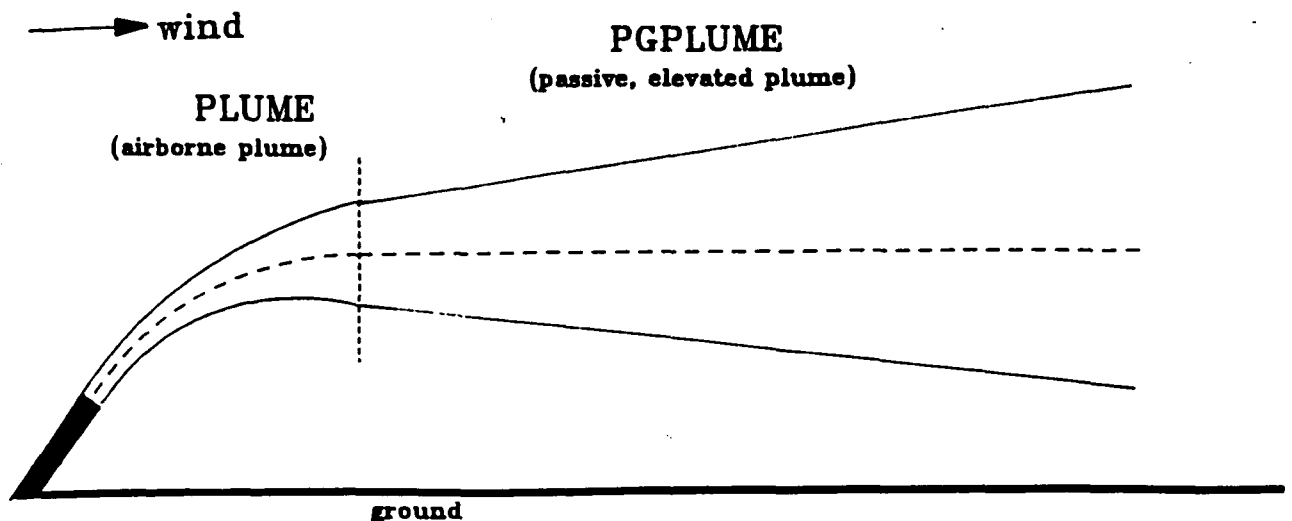


Fig. 1.4. Sequence of HGSYSTEM models for pressurised release of non-reactive gas. A transition is made from PLUME to either PGPLUME (elevated dispersion) or HEGADAS (ground-level dispersion).

2. The Thermodynamics of Hydrogen-Fluoride/Air Mixtures

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§2.1: Introduction.

Hydrogen fluoride undergoes in the presence of moist air a complex series of polymerization and hydration reactions which may result in the formation of acid fog at a temperature widely different from that of (pressurized) storage or of the ambient atmosphere. Progressive dilution may result in initially dense, subsequently buoyant, plumes whose density variation significantly affects local air entrainment and the whole nature of plume dispersion.

Figures 2.1 and 2.2 illustrate the striking variation in plume density and temperature that accompanies the (isobaric) mixing of anhydrous HF and moist air. These results have particular importance for the interpretation of large scale experimental data on the release of anhydrous HF carried out under conditions of extremely low humidity and high ambient temperature at Frenchman Flat in the Nevada desert (Blewitt, Yohn, Koopman and Brown 1987; Blewitt, Yohn, and Ermak 1987; Blewitt 1988). Dispersion under such desert conditions results (Figure 2.2) in a permanently dense, grounded cloud, entrainment within which is inhibited by the density difference between cloud and air. By contrast, plumes released to a high humidity ambient are initially dense but subsequently buoyant. Dispersion, initially similar to that under desert conditions, is later considerably enhanced by mixing associated with the unstable interface between (underlying) buoyant cloud and ambient atmosphere. Dispersion distances obtained for desert conditions may prove significantly misleading (overly conservative) when extrapolated to conditions of high humidity. Accurate account must be taken of the reaction chemistry of anhydrous HF and moist air in simulating a release to atmosphere of anhydrous HF.

The following thermodynamic model is essentially identical to that first proposed and later revised by Schotte (1987, 1988). An exposition is given of

the chemistry of HF/moist air, and (in view of the model complexity) of the methodology underpinning numerical solution.

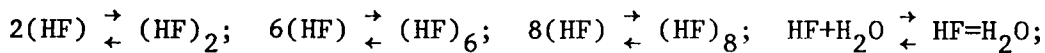
§2.2: The Vapour Phase.

Consider first the vapour-phase polymerization reactions resulting from the strongly polar structure of the HF-monomer. These reactions have been studied *inter alia* (Vierweg 1963; Strohmeier and Briegleb 1953; Clough, Grist and Wheatley 1987) by Schotte (1987, 1988) who identified the oligomer species $(\text{HF})_2$, $(\text{HF})_6$, and $(\text{HF})_8$ as of the greatest importance. In addition, in the presence of water-vapour, there is a significant association of the polar molecules H_2O and HF to form the complex $\text{H}_2\text{O}=\text{HF}$. For the (essentially ambient) pressures within the developing jet or plume the several reacting species may be regarded as ideal gases of constant (isobaric) specific heats (Zemansky 1968). Reaction equilibrium is described by constant heats (enthalpies) and entropies of reaction. Thermal equilibrium is assumed throughout. The state functions for the species HF, H_2O , N_2 , and O_2 are referred to a reference (zero entropy) vapour/gaseous state at a reference temperature of 25C and the standard pressure of 101kPa. The vapour-phase model is determined when the mixture equilibrium temperature, absolute pressure, and molar fraction HF-monomer, respectively the variables $(T, P_\infty, y_{\text{HF}})$, are prescribed.

For a moist-air HF system the vapour-phase is modelled as follows.

Species Present:

HF, $(\text{HF})_2$, $(\text{HF})_6$, $(\text{HF})_8$, H_2O , $\text{HF}=\text{H}_2\text{O}$, N_2 , O_2 ;

Reactions Present:

[Notation: " $\rightleftharpoons$ " denotes the presence of a reversible chemical reaction.]

Reaction Dynamics:

$$y_{\text{HF}_2} = (y_{\text{HF}})^2 K_{(\text{HF})_2}^{\text{HF}}(P_\infty, T); \quad y_{\text{HF}_6} = (y_{\text{HF}})^6 K_{(\text{HF})_6}^{\text{HF}}(P_\infty, T);$$

$$y_{\text{HF}_8} = (y_{\text{HF}})^8 K_{(\text{HF})_8}^{\text{HF}}(P_\infty, T); \quad y_{\text{H}_2\text{O}}^{\text{HF}} = (y_{\text{HF}})(y_{\text{H}_2\text{O}}) K_{\text{H}_2\text{O}}^{\text{HF}}(P_\infty, T).$$

[Notation: y molar fraction, K reaction rate coefficient; P absolute pressure, T absolute temperature; the affices HF , $(\text{HF})_2$, $(\text{HF})_6$, and $(\text{HF})_8$ refer to the several oligomer species of anhydrous hydrogen fluoride, the affix H_2O to water-vapour; the affix " ∞ " to conditions within the ambient atmosphere.]

Reaction Rate Coefficients:

$$K_{(\text{HF})_2}^{\text{HF}} = \text{Rate}(\Delta h_{(\text{HF})_2}^{\text{HF}}, \Delta S_{(\text{HF})_2}^{\text{HF}}, \mu_{(\text{HF})_2})(P/P_{\text{rtp}});$$

$$K_{(\text{HF})_6}^{\text{HF}} = \text{Rate}(\Delta h_{(\text{HF})_6}^{\text{HF}}, \Delta S_{(\text{HF})_6}^{\text{HF}}, \mu_{(\text{HF})_6})(P/P_{\text{rtp}})^5;$$

$$K_{(\text{HF})_8}^{\text{HF}} = \text{Rate}(\Delta h_{(\text{HF})_8}^{\text{HF}}, \Delta S_{(\text{HF})_8}^{\text{HF}}, \mu_{(\text{HF})_8})(P/P_{\text{rtp}})^7;$$

$$K_{\text{H}_2\text{O}}^{\text{HF}} = \text{Rate}(\Delta h_{\text{H}_2\text{O}}^{\text{HF}}, \Delta S_{\text{H}_2\text{O}}^{\text{HF}}, \mu_{\text{H}_2\text{O}}^{\text{HF}})(P/P_{\text{rtp}});$$

$$\text{Rate}(\Delta h, \Delta S, \mu) = \exp[-\mu/R(\Delta h - \Delta S/T)].$$

[Notation: Δh , ΔS heat and entropy of reaction at a temperature of 25C and standard (absolute) pressure (101kPa), K reaction rate coefficients, μ species molecular weight; P system (absolute) pressure, T (absolute) temperature, R universal gas constant; the affices HF , $(\text{HF})_2$, $(\text{HF})_6$, and $(\text{HF})_8$ denote the

several oligomer species of anhydrous hydrogen fluoride; the affix H_2O identifies water-vapour; "rtp" reference temperature (25C) and pressure (101kPa).]

Mixture Properties:

$$\begin{aligned}
 c_g &= c_{HF}^g + c_{(HF)_2}^g + c_{(HF)_6}^g + c_{(HF)_8}^g + c_{g,H_2O}^{HF}; \\
 p_g &= p_{HF}^g + p_{(HF)_2}^g + p_{(HF)_6}^g + p_{(HF)_8}^g + p_{g,H_2O}^{HF} + p_{H_2O}^g + p_{N_2O_2}^g; \\
 h_g &= x_{HF} h_{HF}^g + x_{(HF)_2} h_{(HF)_2}^g + x_{(HF)_6} h_{(HF)_6}^g + x_{(HF)_8} h_{(HF)_8}^g \\
 &\quad + x_{H_2O}^{HF} h_{g,H_2O}^{HF} + x_{H_2O} h_{H_2O}^g + x_{N_2O_2} h_{N_2O_2}^g.
 \end{aligned}$$

[Notation: c species or mixture mass-concentration, p species partial or mixture total vapour-density, h species partial or mixture total specific-enthalpy, x species mass-fraction; the affices HF , $(HF)_2$, $(HF)_6$, and $(HF)_8$ denote the several oligomer species of anhydrous hydrogen fluoride, the affices H_2O and N_2O_2 denotes water and dry air respectively; the affix "g" identifies the vapour phase.]

For a **stable** vapour phase thermodynamic consistency requires the single equation,

$$1 = y_{HF} + y_{(HF)_2} + y_{(HF)_6} + y_{(HF)_8} + y_{H_2O}^{HF} + y_{H_2O} + y_{N_2O_2},$$

which states simply that the molar fractions of all vapour-phase constituents must sum to unity.

§2.3: Two-Phase Equilibrium.

Turning next to the associated problem of two-phase equilibrium mixtures, we follow Schotte (1988) in adopting his (revised) correlations for the **saturation** partial pressures of hydrogen fluoride, in whatever state of aggregation, and of water-vapour. These correlations have the dimensioned form,

HF Partial Pressure:

$$P_{\text{sat}}^{\text{HF}} = 101\text{kPa} \exp[A_{\text{HF}}(y_{\ell}^{\text{HF}}) + B_{\text{HF}}(y_{\ell}^{\text{HF}})/T];$$

$$A_{\text{HF}}(y_{\ell}^{\text{HF}}) = 16.92 + 21.8(y_{\ell}^{\text{HF}}) - 52.39(y_{\ell}^{\text{HF}})^2 + 82.43(y_{\ell}^{\text{HF}})^3 - 106.2(y_{\ell}^{\text{HF}})^4 + 54.43(y_{\ell}^{\text{HF}})^5;$$

$$B_{\text{HF}}(y_{\ell}^{\text{HF}}) = -5903 - 586.9(y_{\ell}^{\text{HF}}) + 1341(y_{\ell}^{\text{HF}})^2 + 6822(y_{\ell}^{\text{HF}})^3 + 2114(y_{\ell}^{\text{HF}})^4 - 6819(y_{\ell}^{\text{HF}})^5.$$

H₂O Partial Pressure:

$$P_{\text{sat}}^{\text{H}_2\text{O}} = 101\text{kPa} |1 - y_{\ell}^{\text{HF}}| \exp[A_{\text{H}_2\text{O}}(y_{\ell}^{\text{HF}}) + B_{\text{H}_2\text{O}}(y_{\ell}^{\text{HF}})/T];$$

$$A_{\text{H}_2\text{O}}(y_{\ell}^{\text{HF}}) = \begin{cases} 21.36 + 47.29(y_{\ell}^{\text{HF}} - 0.4738) + 4.269(y_{\ell}^{\text{HF}} - 0.4738)^2, & y_{\ell}^{\text{HF}} \geq 0.4738, \\ 21.36 + 4.263(y_{\ell}^{\text{HF}} - 0.4738) + 7.907(y_{\ell}^{\text{HF}} - 0.4738)^2, & y_{\ell}^{\text{HF}} < 0.4738, \end{cases}$$

$$\begin{cases} 21.36 + 4.263(y_{\ell}^{\text{HF}} - 0.4738) + 7.907(y_{\ell}^{\text{HF}} - 0.4738)^2, & y_{\ell}^{\text{HF}} < 0.4738, \end{cases}$$

$$B_{\text{H}_2\text{O}}(y_{\ell}^{\text{HF}}) = \begin{cases} -5765 - 17670(y_{\ell}^{\text{HF}} - 0.4738) + 192.2(y_{\ell}^{\text{HF}} - 0.4738)^2, & y_{\ell}^{\text{HF}} \geq 0.4738, \\ -5765 - 3082(y_{\ell}^{\text{HF}} - 0.4738) - 4.269(y_{\ell}^{\text{HF}} - 0.4778)^2, & y_{\ell}^{\text{HF}} < 0.4738. \end{cases}$$

$$\begin{cases} -5765 - 3082(y_{\ell}^{\text{HF}} - 0.4738) - 4.269(y_{\ell}^{\text{HF}} - 0.4778)^2, & y_{\ell}^{\text{HF}} < 0.4738. \end{cases}$$

The notation is that y_{ℓ}^{HF} denotes the molar fraction of the liquid phase that is hydrogen fluoride (in whatever state of combination), and that T denotes the absolute temperature.

We interpret these partial pressures in the context of an assumed (reacting) ideal gas vapour for which the partial pressure attributed to HF is the sum of the partial pressures of each oligomer species, together with a proportion of the partial pressure attributed to the complex $\text{HF}=\text{H}_2\text{O}$. The corresponding H_2O partial pressure comprises two terms, the partial pressure due to free water-vapour, and the remaining proportion of that attributed to the complex $\text{HF}=\text{H}_2\text{O}$. For such an ideal vapour these partial pressures are a proportion of the total pressure equal to the species molar-fraction. This formulation, that

$$\begin{aligned} p_{\text{sat}}^{\text{HF}}/p_{\infty} &= y_{\text{HF}} + y_{(\text{HF})_2} + y_{(\text{HF})_6} + y_{(\text{HF})_8} + \mu_{\text{HF}}/(\mu_{\text{HF}} + \mu_{\text{H}_2\text{O}}) y_{\text{H}_2\text{O}}^{\text{HF}}, \\ p_{\text{sat}}^{\text{H}_2\text{O}}/p_{\infty} &= y_{\text{H}_2\text{O}} + \mu_{\text{H}_2\text{O}}/(\mu_{\text{HF}} + \mu_{\text{H}_2\text{O}}) y_{\text{H}_2\text{O}}^{\text{HF}}, \end{aligned}$$

is essentially that adopted by Schotte (1988).

In addition to this characterisation of saturated equilibrium information is needed regarding the enthalpy and density of the liquid phase. The density of (dilute) hydrofluoric acid is a complex function of temperature and concentration (Du Pont 1988). Nevertheless this complexity has little impact upon enthalpy distribution between liquid and vapour phases of a HF/moist-air mixture. We agree with Schotte that accurate representation of the liquid density is not needed in the (accurate) simulation of plume conditions, at least at the level of a homogeneous equilibrium model. We take the mass-averaged form

$$\rho_{\ell} = 1/[x_{\ell}^{\text{HF}}/\rho_{\ell}^{\text{HF}} + (1-x_{\ell}^{\text{HF}})/\rho_{\ell}^{\text{H}_2\text{O}}].$$

$0 \leq x_{\ell}^{\text{HF}} \leq 1$ is the HF mass-fraction; ρ_{ℓ}^{HF} and $\rho_{\ell}^{\text{H}_2\text{O}}$ are representative **constant** densities for anhydrous hydrogen fluoride and for water.

The enthalpy of dilute hydrofluoric acid is constructed by an enthalpy of condensation from the pure monomer, an enthalpy of dilution or mixing at constant temperature and pressure, and an empirical mixture specific heat at constant pressure. Condensation and mixing occur at reference temperature (25°C) and (standard) pressure. Consider first the condensation of (thermodynamically unstable) pure monomer vapour at reference temperature and pressure. Schotte quotes Vanderzee and Rodenburg (1970) and the latent heat $h_{lg,rtp}^{HF} = 1.51 \text{ MJ/kg}_{HF}$. The heat of condensation of water-vapour is similarly $h_{lg,rtp}^{H2O} = 2.45 \text{ MJ/kg}_{H2O}$.

The heat of mixing at reference temperature and pressure of pure anhydrous HF and liquid water in the molar-proportions y_{ℓ}^{HF} HF to $1-y_{\ell}^{HF}$ water is (Johnson, Smith and Hubbard 1973),

$$\Delta h_{mix}^{rtp} = 941 \text{ kJ/kg}_{HF} [1 - (y_{\ell}^{HF})^2],$$

a result expressed per unit mass HF. The enthalpy of dilute acid of given molar/mass fraction HF at reference temperature and pressure is, therefore,

$$h_{\ell}(T_{rtp}, P_{rtp}; x_{\ell}^{HF}) = -x_{\ell}^{HF} h_{lg,rtp}^{HF} - (1-x_{\ell}^{HF}) h_{lg,rtp}^{H2O} - x_{\ell}^{HF} \Delta h_{mix}^{rtp},$$

$0 \leq x_{\ell}^{HF} \leq 1$ being the mass-fraction HF.

It remains to deduce, given a mean mixture specific heat, the liquid-phase enthalpy at general temperature T and absolute pressure P . For temperatures in the range $0^{\circ}\text{C} < T < 50^{\circ}\text{C}$, Schotte (1987) proposed that the mean isobaric specific heat at or near standard pressure be represented by the dimensioned form

$$c_{p, HF}^{H2O} = [18.05 + 0.000397(T - T_{1s}^{H2O})] \\ - y_l^{HF} [13.97 - 0.0152(T - T_{1s}^{H2O})] \\ + (y_l^{HF})^2 [8.528 + 0.00187(T - T_{1s}^{H2O})],$$

in which T_{1s}^{H2O} is the temperature of melting ice at standard pressure, and $c_{p, HF}^{H2O}$ the mean specific heat expressed in Cal/mol/C. The liquid enthalpy per unit mass is therefore

$$h_l(T, P; x_l^{HF}) = c_{p, HF}^{H2O}(T - T_{rtp}) + (P - P_{rtp}) / \rho_l(T, P; x_l^{HF}) + h_l(T_{rtp}, P_{rtp}; x_l^{HF}).$$

The pressure correction is deduced from the (incompressible) mixture density adopted above.

The system of thermodynamic equations comprises, for two-phase equilibrium, a set of explicit formulae for such mixture parameters as void-fraction, vapour mass-fraction, mixture specific enthalpy, density, and total mass-concentration HF, together with **two** consistency relations which govern the relationships amongst the principal thermodynamic coordinates $(x_1^{HF}, y_{HF}, T, P_\infty)$. The consistency relations may take several equivalent forms from which we choose the following pair:

$$1 = y_{HF} + y_{(HF)_2} + y_{(HF)_6} + y_{(HF)_8} + y_{H_2O}^{HF} + y_{H_2O} + y_{N_2O_2},$$

$$\beta x_{N_2O_2} \rho_g(T, P_\infty; y_{HF}) = \rho(1 - c/\rho) x_{N_2O_2}^\infty.$$

[Notation: β mixture void fraction, c HF mass-concentration, ρ mixture density, $x_{N_2O_2}$ mixture mass-fraction **dry** air, $x_{N_2O_2}^\infty$ atmosphere mass-fraction **dry** air, y_{HF} molar fraction HF monomer, ... , $y_{N_2O_2}$ molar fraction dry air; (T, P_∞) (absolute) temperature and pressure. By "void fraction" we intend the vapour

volume-fraction; by "dry" air we intend air the relative and absolute humidity of which are zero.]

These conditions express the physical requirements that the sum of molar fractions over all species within the vapour phase must equal unity, and second that the total dry-air mass per unit volume mixture must equal that calculated from the entrainment of moist-air in the proportion $1-c/\rho$ moist air to c/ρ released HF, and from the known mass-fraction of water-vapour within the ambient air.

§2.4: Phase Stability.

The above sections **assume** a given phase composition, whether single vapour or two-phase, and calculate the associated thermodynamic state. The two-phase solution has a physical range of applicability limited by the vapour mass-fraction parameter x . A saturated equilibrium system is thermodynamically stable if and only if the parameter x lies in the physical range $[0,1]$. Complete droplet evaporation corresponds exactly to the transition criterion $x=1$. It is possible in certain atmosphere conditions for droplet formation to recur following earlier and complete evaporation. Such transitions might be associated with the repeated intersection of plume and cloud-layers. The stability of an assumed vapour phase system must, therefore, be examined. We follow Clough, Grist and Wheatley (1987), and consider (Figure 2.3) the phase envelope defined by the parametric equations,

$$0 \leq x_{\ell}^{\text{HF}} \leq 1,$$

$$X(x_{\ell}^{\text{HF}}) = p_{\text{sat}}^{\text{HF}}(P, T; x_{\ell}^{\text{HF}});$$

$$Y(x_{\ell}^{\text{HF}}) = p_{\text{sat}}^{\text{H}_2\text{O}}(P, T; x_{\ell}^{\text{HF}}).$$

It is always possible to determine a solution to the thermodynamic equations for given P , and T , and assumed vapour-phase equilibrium. From the solution may be deduced a set of partial pressures P_g^{HF} , and P_g^{H2O} such that

$$\begin{aligned} P_g^{HF}/P_\infty &= y_{HF} + y_{(HF)_2} + y_{(HF)_6} + y_{(HF)_8} + \mu_{HF}/(\mu_{HF} + \mu_{H_2O}) y_{H_2O}^{HF}, \\ P_g^{H2O}/P_\infty &= y_{H_2O} + \mu_{H_2O}/(\mu_{HF} + \mu_{H_2O}) y_{H_2O}^{HF}. \end{aligned}$$

These define (Figure 2.3) a point (X_g, Y_g) in the envelope space. The phase is stable if and only if the point (X_g, Y_g) lies within the phase envelope defined parametrically in terms of the liquid-phase mass-fraction x_ℓ^{HF} . There exists a (unique) x_ℓ^{HF} marking the intersection of the phase envelope and the line linking (X_g, Y_g) to the origin. The point (X_g, Y_g) is then internal to the phase envelope (the vapour phase is stable) if and only if the line segment linking intersection to the origin is greater in length than that linking the points (X_g, Y_g) and $(0,0)$. The criterion for vapour-phase stability is therefore,

$$\begin{aligned} 1 - y_{N_2O_2} &< P_{sat}^{HF}(T, P; x_\ell^{HF}) / (P + P_{sat}^{H2O}(T, P; x_\ell^{HF})) / P \\ \eta P_{sat}^{HF}(P, T; x_\ell^{HF}) &= (1 - \eta) P_{sat}^{H2O}(P, T; x_\ell^{HF}); \\ \eta &= (1 - y_{N_2O_2})^{-1} [y_{H_2O} + \mu_{H_2O} / (\mu_{H_2O} + \mu_{HF}) y_{H_2O}^{HF}]. \end{aligned}$$

§2.5: Solution Methodology:

The solution of a differential plume or jet model requires the repeated calculation of states of thermodynamic equilibrium amongst HF and moist air. Each such calculation requires the solution of a set of three strongly non-linear equations. Efficiency of calculation is therefore an absolute priority if fast executing code is to be produced. Attention must therefore be given to the most

efficient or computationally advantageous means of solution of the coupled differential plume model and algebraic thermodynamic system.

Such systems of coupled differential/algebraic equations have been much studied by numerical analysts: their solution optimally requires a general purpose differential/algebraic solver, developed by numerical analysis specialists, and incorporating automatic "step" determination subject to prescribed local tolerances on all variables (Petzold 1982, Petzold and Lotstedt 1986). More efficient solutions **may** be possible (for example in the limit of great dilution) in circumstances for which inexpensive yet accurate approximations to the (algebraic) solution may be found.

It has been suggested that solution of the thermodynamic model might be carried out prior to the dispersion calculation and the results summarized for later interpolation. However, the thermodynamic calculations are dependent on the temperature of the entrained air, and this is not constant in a non-neutral boundary layer. It is dependent on the elevation of the plume in HFPLUME and the height of the plume in HEGADAS and so is **determined** by the dispersion calculations. Surface heat transfer in HEGADAS is also dispersion dependent. Furthermore, in HFPLUME, even if it were possible to perform the thermodynamic calculations in advance, it would take more time. The differential/algebraic solver integrates the thermodynamic equations together with the dispersion equations to the degree of convergence needed to achieve the desired accuracy in the solution variables. If solving in advance, one would have to calculate to greater accuracy and at more points just in case these were needed. Thus the alternative approach is neither feasible, given the generality of the model formulations, nor potentially more efficient.

§2.6: Incorporation in HFJET and HFPLUME:

Both HFPLUME and HFJET incorporate the differential/algebraic package SPRINT (Berzins, Dew and Furzeland 1983; Berzins and Furzeland 1985), complemented by the robust non-linear solver NAESOL (Scales 1989a,b). The savings are in code clarity, in efficiency, and in particular in execution speed, with increased execution rates perhaps 50 times larger than the fully nested iterative solution method proposed for thermodynamic flash calculations by Exxon (Gray 1987).

The advantage of a differential/algebraic description is that the thermodynamic model is defined as a set of explicit formulae, together with a set of physically evident consistency equations. The structure of the system thermodynamics may be coded exactly as set-out in the theoretical description above.

For two-phase equilibrium we regard the quantities $(x_l^{HF}, y_{HF}, T, P_{\infty})$ as independent variables subject to a (different) pair of constraints. Phase stability is assured in this case provided that the liquid phase mass-fraction lies in the range (0,1). Similarly the vapour phase is described by the independent variables (T, P_{∞}, y_{HF}) . Phase stability may be examined by augmenting the variable set to include the "saturation" mass-fraction x_l^{HF} , and by adding an auxiliary (stability linked) constraint. This is efficient, preserves program structure, and places upon an equal footing the computational complexity of both two- and single-phase thermodynamic systems.

§2.7: Incorporation in HEGADAS:

The HEGADAS program has been structured so that the thermodynamic model is contained within a separate FORTRAN 77 subroutine THERMO. Details of the incorporation of HF/moist-air thermodynamics into the HEGADAS program are given in Appendix 5.

Inasmuch as the computational structure of HEGADAS was already in place, it is not practicable to implement a full differential/algebraic algorithm within HEGADAS as with HFJET and HFPLUME. The numerical separation of heavy-gas advection from mixture thermodynamics is less efficient than a full differential/algebraic solution. Equally HEGADAS gains over HFJET and HFPLUME in ease of generality: different thermodynamics may simply be "plugged in" to the HEGADAS driver. Notwithstanding, computational efficiency in the solution of HF thermodynamics within HEGADAS remains a key issue. Attention has therefore been given to the solution method within the "stand-alone" thermodynamic routine THERMO.

The underlying physics, and numerical predictions, of the formulations implemented in HFJET, HFPLUME and HEGADAS are identical. Nevertheless the formulation and coding of HF thermodynamics within HEGADAS differs substantially from that of HFPLUME and from the exposition of mixture thermodynamics given above. The routine THERMO follows closely a formulation introduced, and later revised, by Schotte (1987, 1988), in which (imagined) flows of pure HF and of moist-air are mixed and equilibrated. Discussion is phrased in terms of mole-flows, enthalpy deficits, and of fugacities. The model is formulated in terms of a set of either two or three non-linear algebraic equations for a single vapour phase, or a two-phase system respectively. No check is made for phase stability following transition to a vapour-phase plume. The equations are solved simultaneously by means of a robust "state of the art" non-linear equation solver NAESOL (Scales 1989a, b). Initial estimates correspond to converged values from the last numerical "step" from the (stiff) ordinary differential equation solver STINT (Prothero and Robinson 1975) incorporated within the HEGADAS driver.

§2.8: Model Validation:

The thermodynamic models encoded in HFJET, HFPLUME, and HEGADAS have been compared with predictions of Schotte (1987, 1988), of Clough, Grist and Wheatley (1987), and have been validated directly against experiment (Schotte 1987, 1988).

Consider first the thermodynamic model for the HF/moist air system set out in §2.2 through §2.4 above. This is closely similar but not identical to that proposed (Schotte 1987), and later revised by Schotte (1988). These models differ in several particulars from that of Clough, Grist and Wheatley (1987). The composition of the vapour phase, the oligomer species present, and their heats of reaction, significantly differ, as do the representation of phase equilibrium, partial pressure correlations, and the isothermal heat of mixing of anhydrous HF and water. The sensitivity of concentration/temperature behaviour to such model uncertainties should clearly be examined.

Reference to Figures 2.5 through 2.16 (Schotte 1987, 1988) confirms that no significant differences in the concentration/temperature behaviour result from uncertainties in thermodynamic structure or coding. The models are, moreover, successful in predicting the temperature/ humidity/ concentration behaviour as observed by Schotte (1987), and Vierweg (1963). The degree of accord amongst these differing descriptions is at once remarkable and reassuring. Uncertainties attributed to this source are insignificant compared with those arising from the dynamics of air entrainment.

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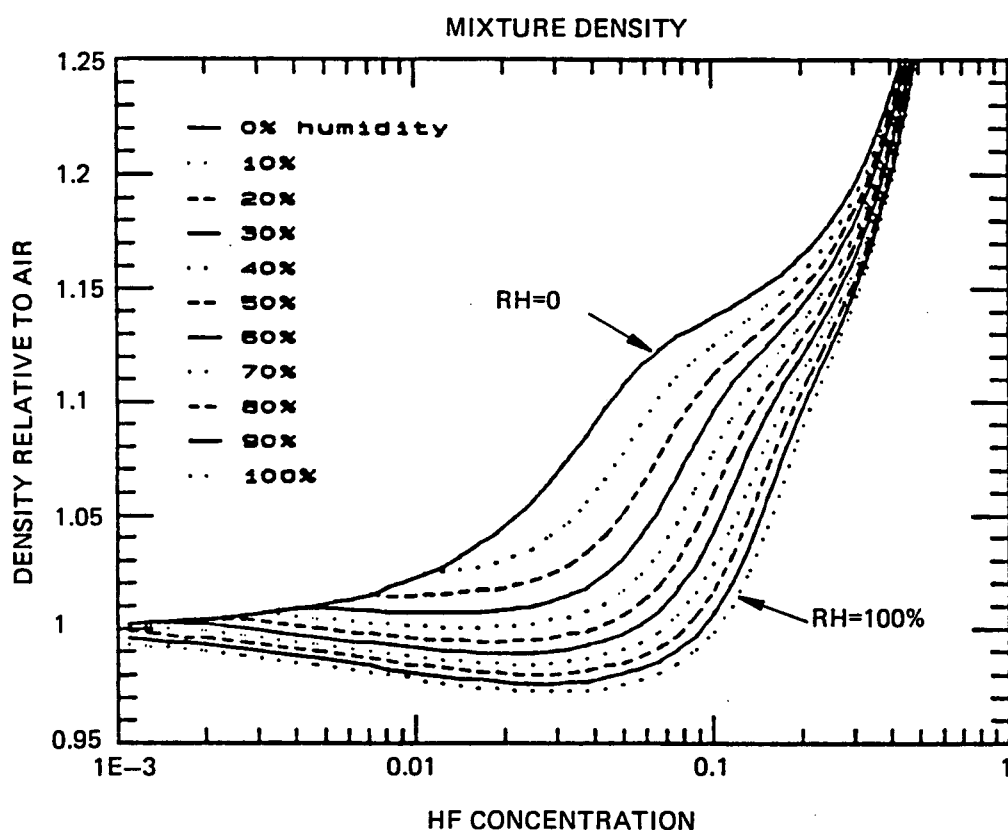
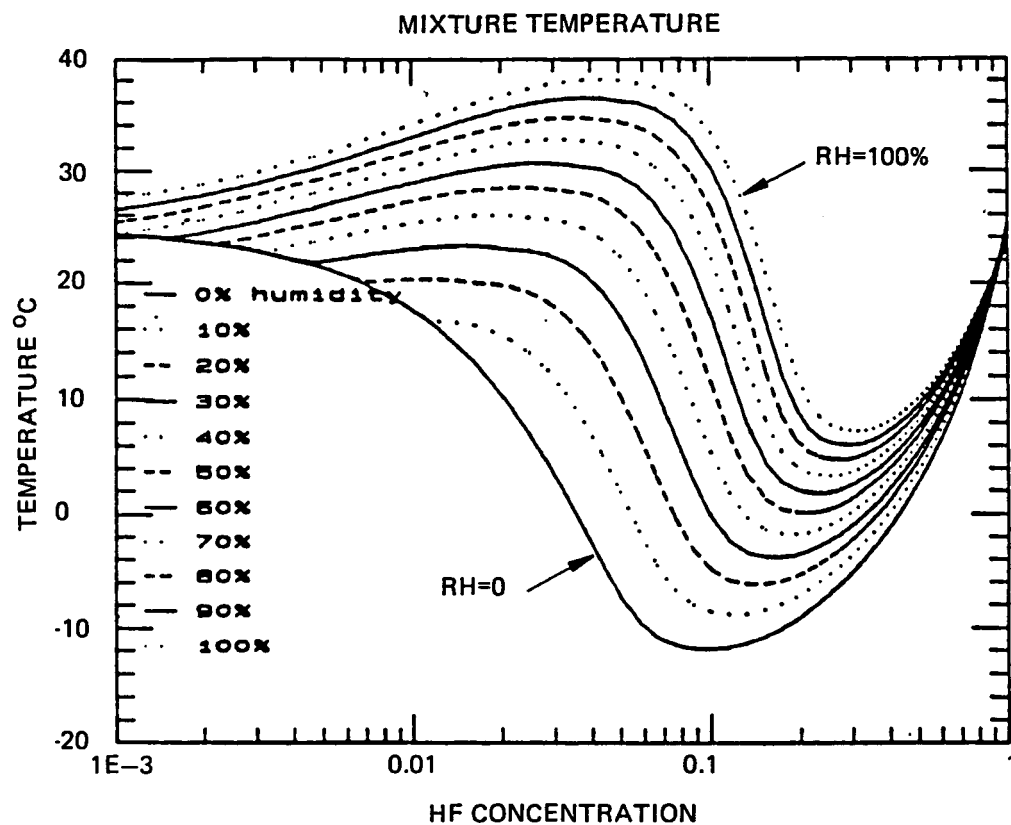


FIG. 2.1 - Cloud temperature and density variations with HF concentration and humidity when HF vapour at 25°C is mixed with moist air at 25°C.

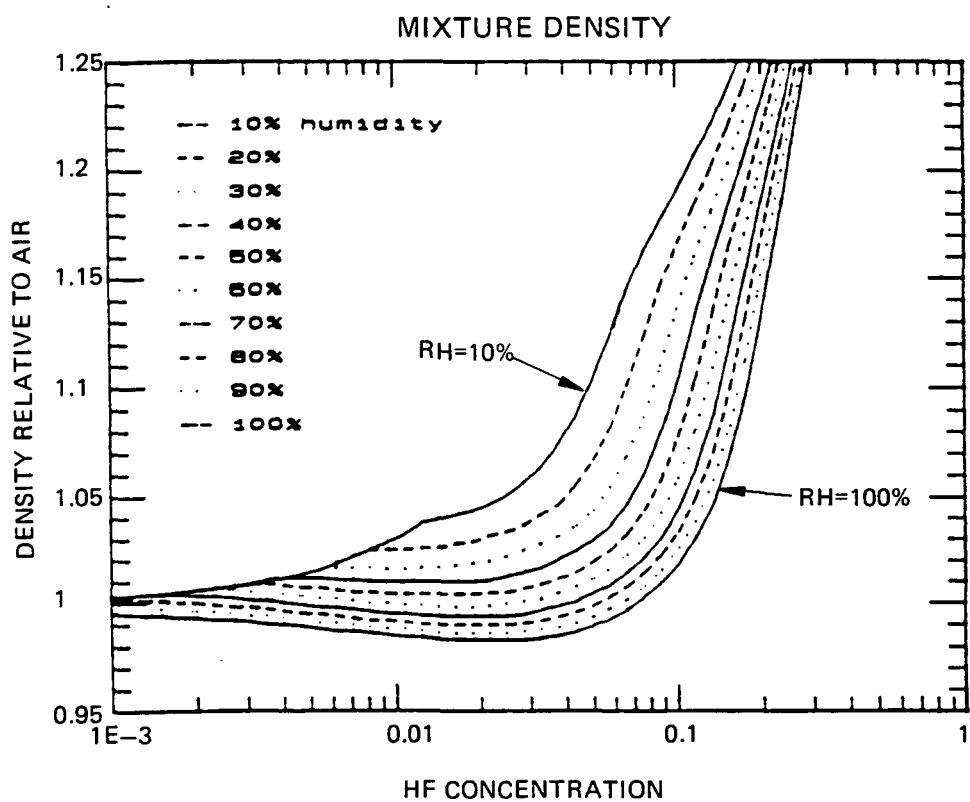
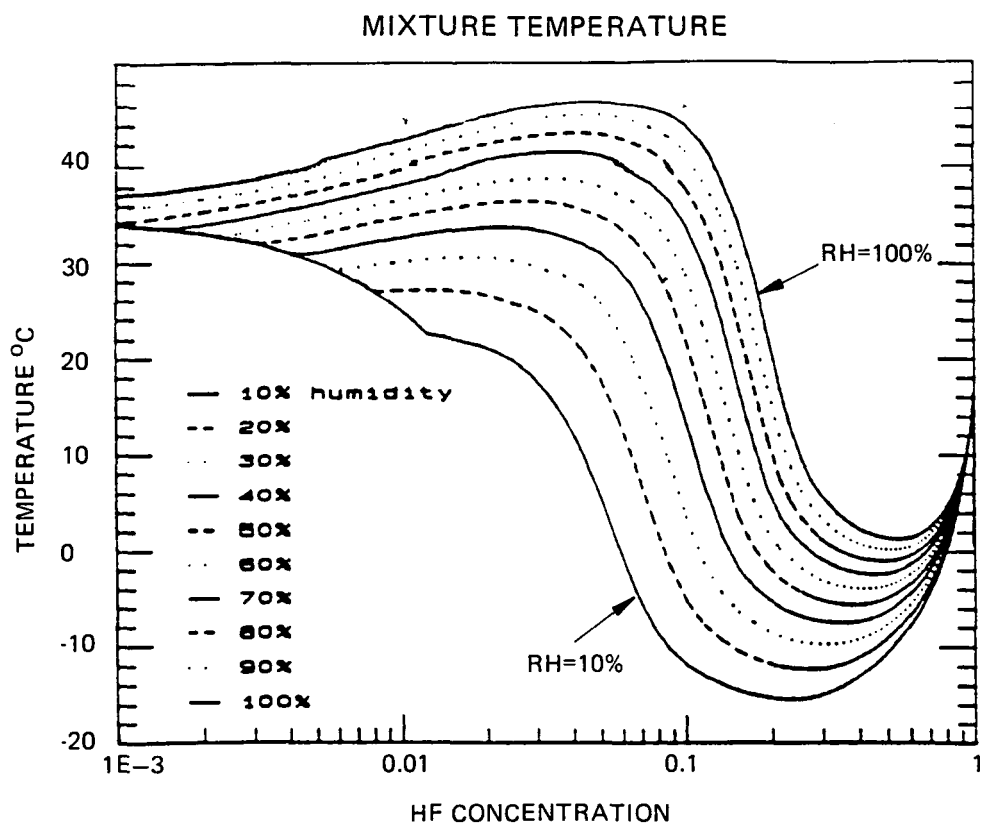


FIG. 2.2 – Cloud temperature and density variations with HF concentration and humidity when liquid HF at 37.8°C is mixed with moist air at 35°C.

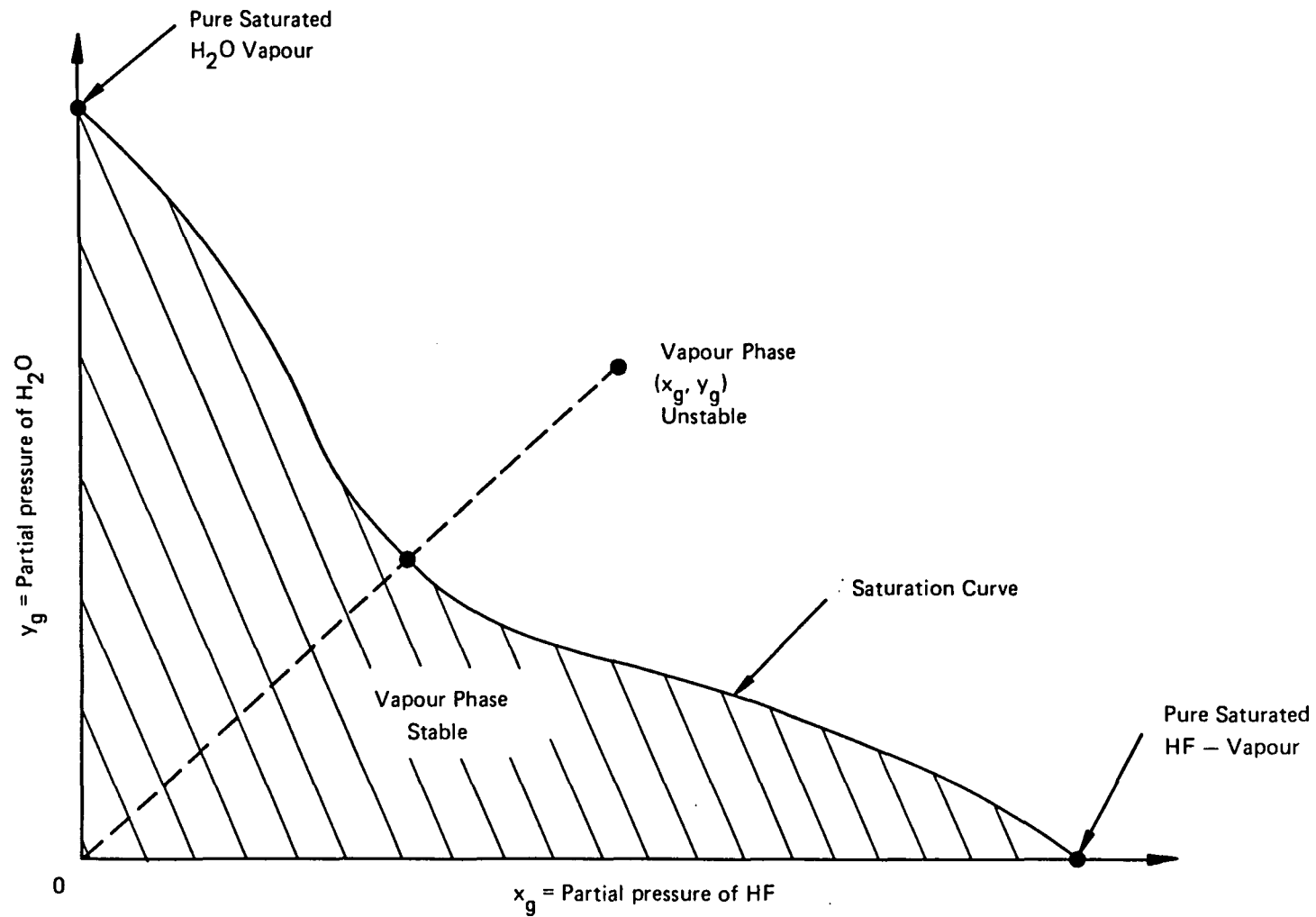


FIG. 2.3 – Stable vapour phase region (shaded) for a mixture of HF/H₂O in dry air, for given total pressure and temperature.

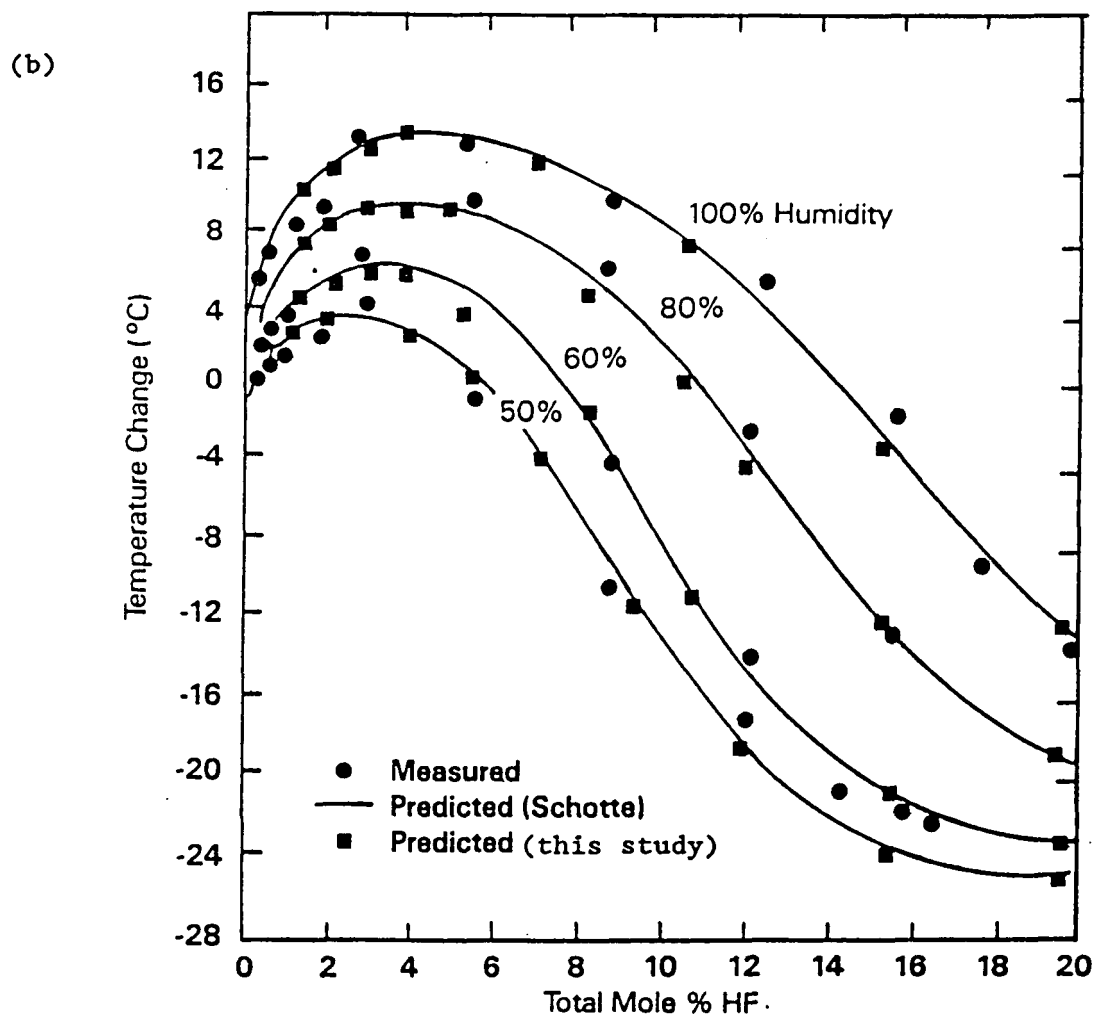
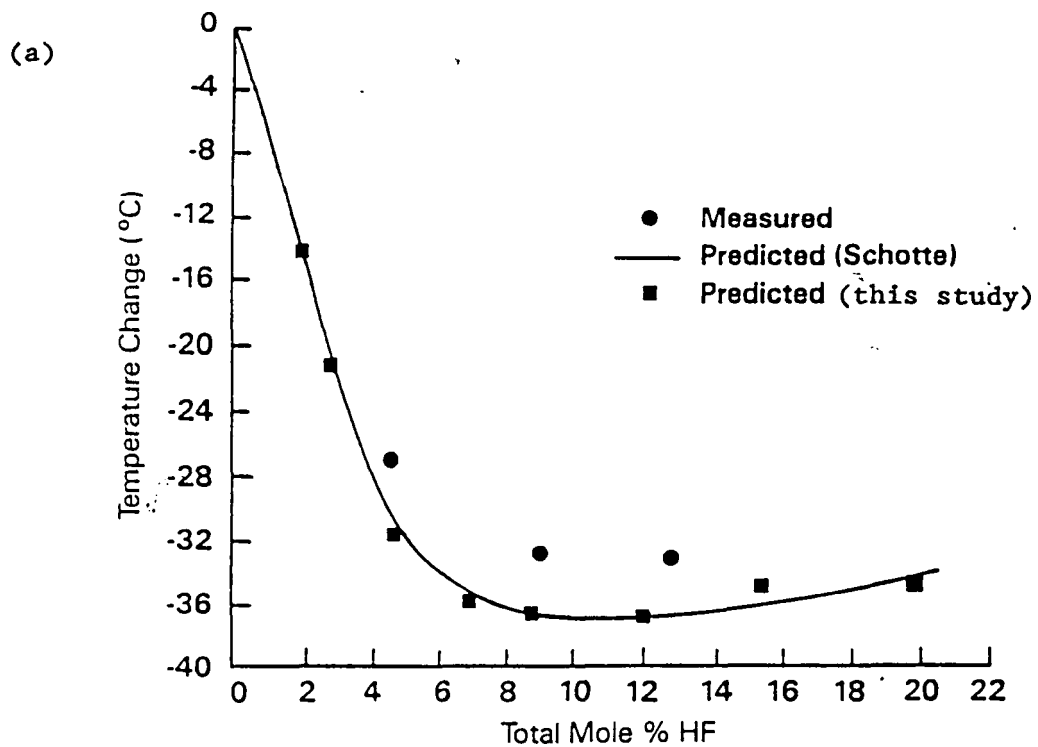


Figure 2.4 Temperature variation with humidity and HF concentration when liquid HF at 25°C is mixed with (a) dry air at 25°C , and (b) moist air at $25\text{--}26^{\circ}\text{C}$. Comparison of model predictions with experimental data from Schotte (1987)

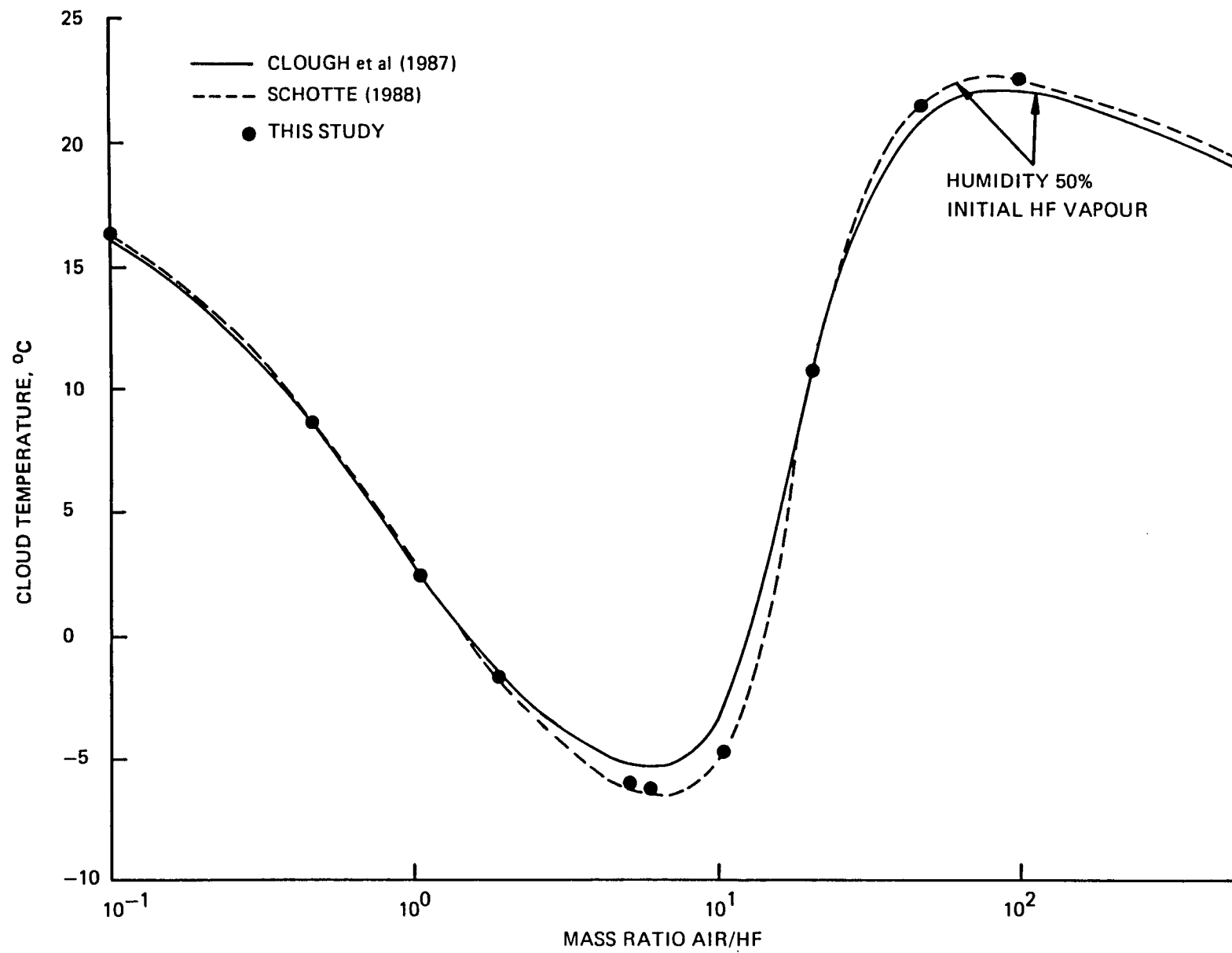


FIG. 2.5 – Predicted cloud temperature variations with mixing ratio of air at 20°C and HF at 19.54°C.

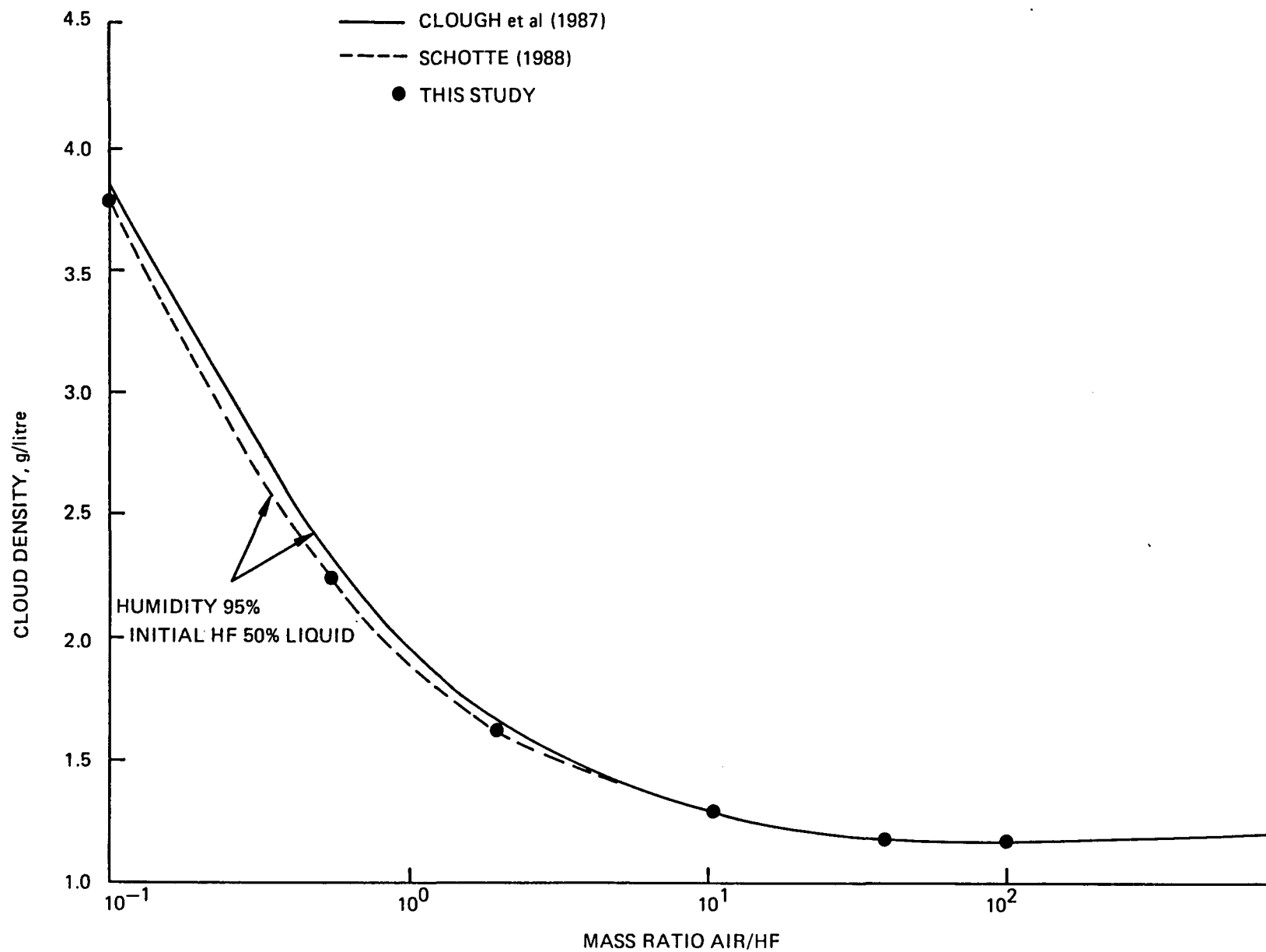


FIG. 2.6 — Predicted cloud density variations with mixing ratio of air at 20°C and HF at 19.54°C.

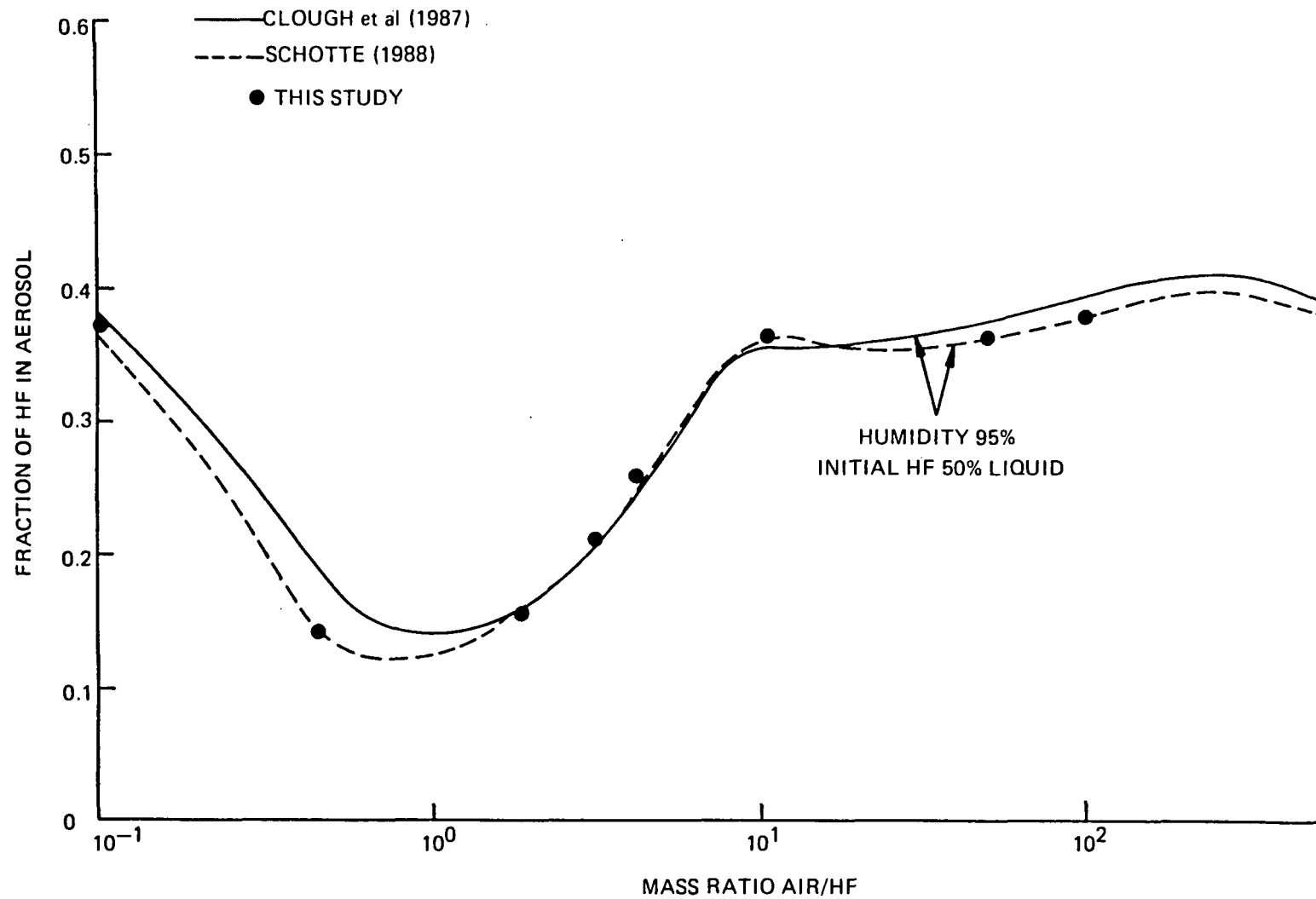


FIG. 2.7 — Predicted variations in the fraction of HF in aerosol with mixing ratio of air at 20°C and HF at 19.54°C.

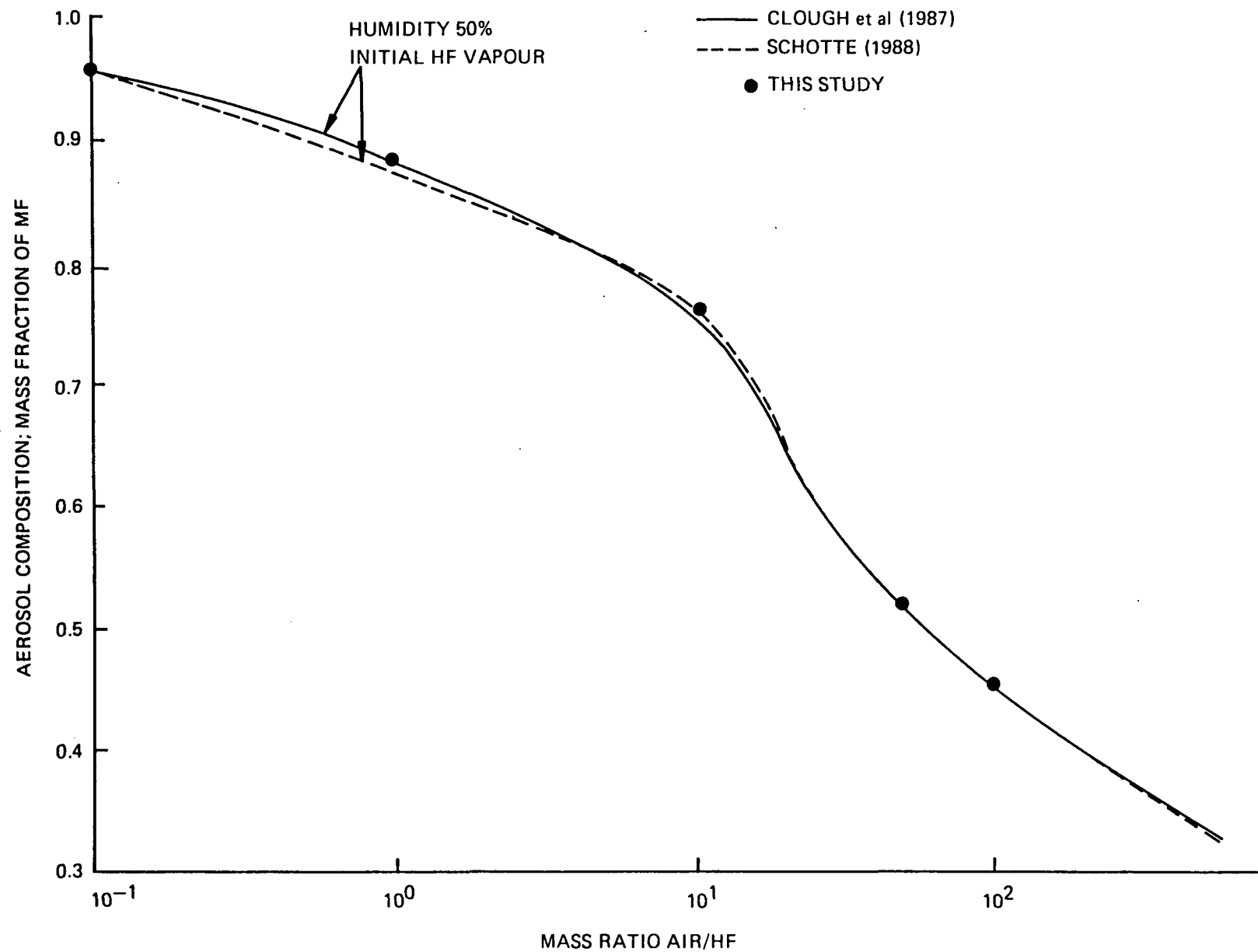


FIG. 2.8 — Predicted variations in aerosol composition with mixing ratio of air at 20°C and HF at 19.54°C.

3. PREDICTION OF RELEASE RATES FROM PRESSURISED CONTAINMENT

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§3.1: Introduction.

This Chapter develops a model (HFSPILL) for the venting-rate and orifice pressure of a pressurized vessel containing hydrofluoric acid. The pressurizing gas is nitrogen; the effects of gravity are assumed negligible. The storage vessel is assumed to be in thermodynamic equilibrium; the efflux of mass is governed by well established correlations (Boucher and Alves 1963, Wallis 1969, Collier 1972, Fox 1974, Fauske and Epstein 1988).

Conditions at the release orifice, in terms of mass-flux and pressure histories, are required input to the near-field jet/plume dispersion models, HFPLUME (Chapter 5) and HFJET (Appendix 1). HFSPILL has been developed for this purpose; HFSPILL is comparable in accuracy and complexity to source models adopted in a similar context by Raj and Morris (1987).

§3.2: The reservoir model.

The reservoir is assumed to be in thermal equilibrium with liquid, when present, confined to the lower vessel. Depressurization and fluid loss is then governed by the (slow) efflux of fluid-mass via a reservoir or pipe break, by the influx of heat from the (atmospheric) environment, and (possibly) by an imposed variation in reservoir volume. The mass discharge-rate (dm/dt), the rate of heat influx (dQ/dt), and the assumed volumetric variation (dV/dt), are each expressed as known functions (correlations) of ambient and reservoir state and (possibly) of the elapsed time. Currently HFSPILL discharge from an adiabatic vessel of fixed (fluid) volume.

The reservoir fluid is assumed to be either pure vapour or else a separated mixture of liquid and vapour; discharge is of pure liquid of reservoir equilibrium composition, or else of pure vapour. The fluid is assumed pressurized by means of an inert (ideal) gas insoluble in the liquid phase; gravity is assumed negligible. Thermodynamic equilibrium is defined by the ideal-gas liquid-phase model proposed (1986) and later revised (1988) by Schotte.

The reservoir is described by the (extensive) variables (U,m,V) of (total) internal energy, fluid mass, and reservoir volume; and by the (intensive) variables (T,P, y_{HF} , x_{ℓ}^{HF} , x_{HF} , $x_{\text{H}_2\text{O}}$) denoting reservoir (absolute) temperature, (absolute) pressure, mole-fraction HF-monomer in the vapour-phase, mass-fraction anhydrous HF in liquid-phase, average mass-fractions of anhydrous HF and of water in the reservoir fluid.

Mathematically the model comprises a differential/algebraic system of four algebraic and five differential equations in the nine state variables (U,m,V,T,P, y_{HF} , x_{ℓ}^{HF} , x_{HF} , $x_{\text{H}_2\text{O}}$). Solution is carried out by the differential/algebraic solver SPRINT (Berzins and Furzeland 1985), supplemented as necessary by the robust non-linear solver NAESOL (Scales 1988). The full equation system is as follows (refer Chapter 2):

Vapour phase equilibrium:

$$\begin{aligned}
 1 &= y_{\text{HF}} + y_{\text{HF}_2} + y_{\text{HF}_6} + y_{\text{HF}_8} + y_{\text{H}_2\text{O}}^{\text{HF}} + y_{\text{H}_2\text{O}} + y_{\text{N}_2}; \\
 1 &= x_{\text{HF}} + x_{\text{H}_2\text{O}} + x_{\text{N}_2}; \quad U/m = h - P/\rho; \\
 \phi P_{\text{HF}}^{\text{lg}}/P &= (1-\phi) P_{\text{H}_2\text{O}}^{\text{lg}}/P; \quad \phi = [y_{\text{H}_2\text{O}} + u_{\text{HF}} / (u_{\text{HF}} + u_{\text{H}_2\text{O}}) y_{\text{H}_2\text{O}}^{\text{HF}}] / (1 - y_{\text{N}_2}); \\
 dm/dt &= -dm/dt|_{\text{exit}}; \quad dU/dt = h_g dm/dt + dQ/dt|_{\text{wall}}; \\
 dV/dt &= dV/dt|_{\text{res}}; \quad dx_{\text{HF}}/dt = 0; \quad dx_{\text{H}_2\text{O}}/dt = 0.
 \end{aligned}$$

[Notation: $t > 0$: elapsed time since pipe/vessel failure; U : reservoir total internal energy; m : total stored fluid-mass; P : reservoir (absolute) pressure; (ρ, ρ_g) : mean (reservoir-fluid, reservoir-vapour) density; (h, h_g) : mean (reservoir-fluid, reservoir-vapour) specific-enthalpy; $(y_{HF}, y_{HF_2}, y_{HF_6}, y_{HF_8})$ mole-fraction HF (monomer, dimer, tetramer, octomer) in the reservoir vapour-phase; $y_{H_2O}^{HF}$: mole-fraction $HF=H_2O$ complex in vapour-phase; (y_{H_2O}, y_{N_2}) mole-fractions (water-vapour, nitrogen) in vapour; $(x_{HF}, x_{H_2O}, x_{N_2})$ reservoir mass-fractions (anhydrous HF, water, nitrogen); $\bar{x}_{N_2}^g$: mass-fraction of vapour-phase that is nitrogen; The affices "wall", "res", and "exit" refer to heat-influx through the vessel wall, to imposed volume change of the reservoir, and to the release orifice or fluid exit; $dQ/dt|_{wall}$, $dV/dt|_{res}$, and $dm/dt|_{exit}$ are prescribed functions of the reservoir and ambient conditions and of the elapsed time.]

Two-phase equilibrium:

$$\begin{aligned}
 1 &= y_{HF} + y_{HF_2} + y_{HF_6} + y_{HF_8} + y_{H_2O}^{HF} + y_{H_2O} + y_{N_2}; \\
 1 &= x_{HF} + x_{H_2O} + x_{N_2}; \quad U/m = h - P/\rho; \quad \beta x_{N_2}^g \rho_g = x_{N_2} \rho; \\
 dm/dt &= -dm/dt|_{exit}; \quad dV/dt = dV/dt|_{res}; \quad dx_{HF}/dt = (x_{\ell}^{HF} - x_{HF})(1/m)(dm/dt); \\
 dU/dt &= h_{\ell} dm/dt + dQ/dt|_{wall}; \quad dx_{H_2O}/dt = (1 - x_{\ell}^{HF} - x_{H_2O})(1/m)(dm/dt).
 \end{aligned}$$

[Notation: $t > 0$: elapsed time since pipe/vessel failure; U : reservoir total internal energy; m : total stored fluid-mass; P : reservoir (absolute) pressure; β : reservoir void-fraction; ρ : mean (reservoir-fluid) density; (h, h_{ℓ}) : mean (reservoir-fluid, reservoir-liquid) specific-enthalpy; $(P_{HF}^{lg}, P_{H_2O}^{lg})$: saturation partial pressure of water and anhydrous HF; $(y_{HF}, y_{HF_2}, y_{HF_6}, y_{HF_8})$ mole-fraction HF (monomer, dimer, tetramer, octomer) in the reservoir vapour-phase; $y_{H_2O}^{HF}$: mole-fraction $HF=H_2O$ complex in vapour-phase; (y_{H_2O}, y_{N_2}) mole-fractions

(water-vapour, nitrogen) in vapour; $(x_{\text{HF}}, x_{\text{H}_2\text{O}}, x_{\text{N}_2})$ reservoir mass-fractions (anhydrous HF, water, nitrogen); $x_{\text{N}_2}^g$: mass-fraction of vapour-phase that is nitrogen; x_l^{HF} : mass-fraction liquid that is anhydrous HF. The affices "wall", "res", and "exit" refer to heat-influx through the vessel wall, to imposed volume change of the reservoir, and to the release orifice or fluid exit; $dQ/dt|_{\text{wall}}$, $dV/dt|_{\text{res}}$, and $dm/dt|_{\text{exit}}$ are prescribed functions of the reservoir and ambient conditions and of the elapsed time.]

It might appear that vapour-phase equilibrium is over-specified by the above differential/algebraic system. Certainly the vapour-phase has one less degree of freedom than has two-phase equilibrium, being characterized by the condition $\beta=1$. We have, however, retained the auxiliary variable $0 \leq x_l^{\text{HF}} \leq 1$ necessary for the monitoring of phase stability. This permits the onset of condensation within the vapour phase to be recognized and phase transition made (Chapter 2).

Discussion and limitations:

The assumption of thermal equilibrium throughout the reservoir is valid for slowly varying reservoir conditions for which thermodynamic equilibrium can be re-established by material transport between and within phases, and for which bulk boiling is absent. Features of highly transient depressurization such as bulk "flashing", significant liquid "boil-up", and the prospect of near homogeneous two-phase conditions within the reservoir are discounted. The neglect of such highly transient phenomena is consistent with the requirements of the subsequent (near-field) dispersion models HFJET (Appendix 1) and HFPLUME (Chapter 5); these models assume that "quasi steady-state" conditions are established near to the point of release.

The range of validity of the models HFPLUME (and HFJET) is limited to that downwind range for which the flow development time is short compared to the time required for significant variation in the reservoir discharge. Highly transient releases imply valid quasi-static ranges short compared to the development length for heavy-gas advection. In such circumstances no link to such far-field models as HEGADAS-S (Chapter 7) for heavy-gas advection, or PGPLUME (Chapter 6) for passive (Pasquill/Gifford) advection, is possible.

The assumption of (separated phase) equilibrium within the HF reservoir is, therefore, (contextually) reasonable, offers major savings in model complexity, and eliminates the need for (uncertain) assumptions regarding the extent and distribution of disequilibrium within the vessel and discharge flow.

The final simplifying assumption is the neglect of gravity. We anticipate that for typical HF storage conditions pressurization will be to of order 10bar gauge, so that for much of the discharge gravity-head will be negligible. A significant increase in the level of description of the storage vessel and discharge line is needed if gravity is to be represented. For example calculation of a gravity-head requires details of vessel shape and orientation, not merely its volume.

§3.3 Mass-discharge correlations.

The reservoir model is completed by means of an appropriate choice of empirical correlations for the efflux of mass and heat from the vessel into the atmospheric environment. These correlations replace (at least in part) a detailed pipe/orifice discharge model in which such effects as inter-phase slip, thermal

disequilibrium, and the influence of wall-friction and heat-transfer may all be significant.

Reference to Fauske and Epstein (1988) produced a correlation valid for the discharge of liquid subcooled at storage, but superheated at ambient, pressure. In addition HFSPILL incorporates standard correlations for the discharge of subcooled liquid (Fox 1974), and for the discharge of ideal-gases (Raj and Morris 1987).

No attempt has been made to take account of pipe-wall friction, of disequilibrium in "stub" (short) pipes, or to model efflux rates associated with two-phase flows whichever (vapour or liquid) phase is continuous. Equilibrium amongst the several vapour-phase species is assumed "frozen" during transit of the discharge path between reservoir and atmosphere. Other assumptions are possible, but of (much) greater computational complexity. The chosen correlations are as follows:

Vapour discharge:

$$\begin{aligned} dm/dt|_{\text{exit}} &= C_D^g A_{\text{exit}} y [2(P - P_{\text{exit}}) \rho_g]^{1/2}; \\ y &= [F^{2/\gamma} / (1 - 1/\gamma)]^{1/2} [(1 - F^{1-1/\gamma}) / (1 - F)]^{1/2}; \\ F &= P_{\text{exit}}/P = \max\{P_{\text{atm}}/P, [2/(1+\gamma)]^{1/(1-1/\gamma)}\}. \end{aligned}$$

[Notation: $C_D^g (\approx 1.0)$: coefficient of discharge (vapour); $\gamma = c_p^g/c_v^g$: ratio of (ideal) vapour specific heats at constant pressure and volume ($\gamma > 1$); ρ_g : reservoir vapour-phase density P : reservoir (absolute) pressure; P_{atm} : atmosphere ambient pressure A_{exit} : orifice (pipe-break) cross-sectional area; y : orifice contraction factor (Boucher and Alves 1963); $F > 1$: ratio of ambient (or choke) pressure to the

reservoir pressure. Note that the formulae assume "frozen" equilibrium during the formation of an external choke as well as in the preceeding pipe-flow.]

Liquid discharge:

$$\begin{aligned} dm/dt|_{\text{exit}} &= C_D^l A_{\text{exit}} [2\rho_l (P - P_{\text{atm}})]^{1/2}; \quad P_{\text{HF}}^{lg} + P_{\text{H}_2\text{O}}^{lg} \leq P_{\text{atm}}; \\ dm/dt|_{\text{exit}} &= C_D A_{\text{exit}} [2\rho_l (P - P_{\text{HF}}^{lg} - P_{\text{H}_2\text{O}}^{lg} + P_{\text{sat}}^{\text{eff}})]^{1/2}; \\ (P_{\text{sat}}^{\text{eff}}/\rho_l)/h_{lg} &= (1/2)[h_{lg}/(c_p^l T)]/(\rho_l/\rho_g - 1)^2; \quad P_{\text{HF}}^{lg} + P_{\text{H}_2\text{O}}^{lg} > P_{\text{atm}}. \end{aligned}$$

[Notation: $C_D^l (\approx 0.6)$: coefficient of discharge (Fox 1974); A_{exit} : orifice (pipe-break) cross-sectional area; P : reservoir (absolute) pressure; P_{atm} : atmosphere ambient pressure; ρ_l : reservoir liquid-phase density; c_p^l : reservoir liquid (isobaric) specific heat; h_{lg} : latent heat of evaporation reservoir liquid; P_{HF}^{lg} : saturation (partial) vapour-pressure reservoir water; $P_{\text{H}_2\text{O}}^{lg}$: saturation (partial) vapour-pressure anhydrous HF. $P_{\text{sat}}^{\text{eff}}$: effective pressure-drop associated with the (choked flow) discharge of reservoir saturated liquid. The affix "atm" refers to the external atmosphere, "sat" to saturated (two-phase) equilibrium.]

Discussion and limitations:

The possibility of droplet flow resulting from condensation within the vapour phase is discounted. First such flows are likely to be complex, but might be well represented by a homogeneous equilibrium model; second the issue of vapour phase stability is "clouded" by limitations of Schotte's thermodynamic model of the HF/water system. Specifically the failure of Schotte's (1987, 1988) correlations for saturation partial pressures to satisfy the Gibbs-Duhem equation (Guggenheim

1957) appears to induce repeated "switching" back and forth between two-phase and vapour phase equilibrium at or near complete exhaustion of liquid from the reservoir. This prevents the consistent introduction of a mass-efflux correlation for droplet flows until this matter is resolved. Such (notional) "instability" within the newly formed vapour-phase is first "flagged", and thereafter tolerated. Note that Guggenheim (1957) outlines a methodology for the introduction of successive **thermodynamically consistent** approximations to a thermodynamic system. This methodology underpins the formulation of the HF/water system adopted and tested by Clough, Grist, and Wheatley (1987).

HFSPILL takes no account of (pipewall) friction in estimating mass discharge rates and choke pressures at the point of release to atmosphere. Such frictional forces are typically of minor interest in the context of pressurized releases, though they assume importance for mass flow-rates for exceptionally long or narrow pipes ($l_{\text{pipe}}/D \gg 1$). Such pipes present the possibility of choke formation in vapour flow at the pipe exit, rather than externally. Additionally the longer the pipe the greater the relaxation of (presumed "frozen") reservoir equilibrium towards equilibrium at the choke pressure and temperature. Both these effects cause departures of (quasi-steady) mass-flow from that calculated for a free orifice and "frozen" equilibrium by (inter alia) Raj and Morris (1987).

The greater the role of friction, the greater its influence upon choke formation for (ambient superheated) liquids and the greater the importance of pipe related factors upon the mass discharge-rate. Correlations are given by Fauske and Epstein (1988) which attempt to correct for frictional losses as a function of the length to diameter ratio (l_{pipe}/D) of the discharge pipe, at any rate for reservoir-saturated flows. However, in view of radically different pressure gradients associated with two-phase equilibrium and subcooled liquid flows within

long pipes, we anticipate that the frictional dependence of the mass flow-rate will depend substantially upon the thermodynamic substance, and in particular upon the degree of reservoir subcooling appropriate to reservoir- subcooled / ambient-superheated liquid discharge. The prediction of orifice pressure requires in the presence of friction the use of a homogeneous equilibrium pipe-flow model. It was to avoid such complexity that mass-flux correlations were first introduced.

§3.4: Entry, Pipe, and Orifice Flow.

An (albeit brief) search of the literature failed to discover correlations for the orifice pressure, that is the pressure just within the discharge pipe, appropriate to the release of reservoir subcooled, ambient superheated, liquid. This parameter is needed for input to subsequent jet or plume release models HFJET (Appendix 1) and HFPLUME (Chapter 5). We therefore introduce a homogeneous equilibrium model of entry, pipe, and orifice flow in order to estimate the pipe exit-pressure. The flow will be presumed steady, inviscid, adiabatic, and (other than entry-flow) quasi one-dimensional (Wallis 1969, Collier 1972, Fox 1974).

Entry flow:

$$(1/2)u^2_{\text{entry}} = \int_{P_{\text{entry}}}^{P_{\text{res}}} \rho(P;S)|_{S=S_{\text{res}}} dP;$$

$$[h + (1/2)u^2]|_{\text{entry}} = h_{\text{res}}; \quad dm/dt|_{\text{exit}} = (A\rho u)|_{\text{entry}};$$

[Notation: u : flow-speed; h : specific enthalpy; ρ : (mean) fluid density; P : (absolute) fluid pressure; dm/dt : mass flow-rate. The affix "res" denotes "reservoir" conditions, "entry" conditions at the entrance to the discharge system or pipe, "exit" to conditions at the release orifice.]

Pipe-flow:

$$d/ds(\rho u) = 0; \rho u (du/ds) + dp/ds + (2f/D)\rho u^2;$$

$$(\rho u)d/ds[h + (1/2)u^2] = 0; T(ds/ds) = (2/D)fu^2;$$

$$d/ds[(1/2)u^2] = (2fu^2/D)(u^2/c^2)/(1-u^2/c^2);$$

$$dp/ds = -(2f/D)\rho u^2/(1-u^2/c^2); dA/ds = 0;$$

$$c^2 = (\partial P/\partial \rho)|_{h+(1/2)u^2}; dm/dt|_{\text{exit}} = A\rho u; A = \pi D^2/4.$$

[Notation: $0 < s \leq \ell_{\text{pipe}}$: displacement from pipe entry $f \rightarrow 0$: pipe-wall (Fanning) friction-factor; A : pipe cross-sectional area; D : pipe (effective) diameter; ℓ_{pipe} : pipe length ρ : mean fluid density; P : fluid (absolute) pressure; T : fluid(absolute) temperature; u : fluid flow-speed; c : homogeneous equilibrium sound-speed; h : specific enthalpy; S : specific entropy.]

Orifice flow:

$$d/ds[h + (1/2)u^2] = 0; d/ds(A\rho u) = 0; c^2 = (\partial P/\partial \rho)|_{S_{\text{exit}}};$$

$$dp/ds = -(1/A)(dA/ds)(\rho u^2)/(1-u^2/c^2);$$

$$d/ds[(1/2)u^2] = (1/A)(dA/ds)u^2/(1-u^2/c^2); A = \pi D^2/4.$$

[Notation: $\ell_{\text{pipe}} < s$: displacement from pipe exit ℓ_{pipe} : pipe length A : flow cross-sectional area; D : flow effective diameter; ρ : mean fluid density; P : fluid (absolute) pressure; T : fluid (absolute) temperature; u : fluid flow-speed; c : homogeneous equilibrium (isentropic) sound-speed; h : specific enthalpy; S : specific entropy.]

Discussion and limitations:

Reference to the Navier-Stokes and continuity equations for entry flow reveals the flow acceleration from reservoir fluid at rest to flow (just) within the discharge pipe is governed (we neglect gravity) by the Bernoulli equation for compressible flow (Batchelor 1970). This assumes that entry losses typically associated with flow expansion following discontinuities in pipe diameter are negligible (Fox 1974). In the absence of significant friction within the discharge line the equations of motion for homogeneous equilibrium flow imply no change in fluid velocity or thermodynamic state between entry flow and the pipe exit. Thereafter flow evolution occurs within flow immediately downstream of the orifice, so that for incompressible liquid and (ideal) gas flow we obtain equations for vapour phase ("frozen") equilibrium;

$$u^2 = (2P/\rho)|_{\text{res}} [1 - F^{1-1/\gamma}] / (1 - 1/\gamma); \quad F = P/P_{\text{res}};$$

$$A/A_{\text{exit}} = [F^{1/\gamma} (1 - F^{1-1/\gamma})^{1/2}] / [F^{1/\gamma} (1 - F^{1-1/\gamma})^{1/2}]|_{\text{exit}};$$

and for liquid-phase flow;

$$u^2 = 2(P_{\text{res}} - P)/\rho_l; \quad A/A_{\text{exit}} = [(P_{\text{res}} - P)/(P_{\text{res}} - P_{\text{exit}})]^{1/2}.$$

Explicit solution is not possible for two-phase equilibrium flow in the orifice flow. The mass-flux is then governed by conditions at choke formation, or else upon attainment of ambient pressure in accordance with the equation,

$$dm/dt|_{\text{exit}} = (A\rho u)|_{\text{vena contracta}}.$$

We then relate the area of the "vena contracta" to that of the orifice by means of the coefficient of discharge C_D . Details of the flow contraction cannot be derived from a one-dimensional equilibrium flow, but follow either as the solution of a free boundary problem in axisymmetric flow (Batchelor 1970), or else (more credibly) as the result of experiment (Boucher and Alves 1963). Rather than pursue complex formulae for C_D expressed as a function of the flow Reynolds' number and of the orifice shape we are content to make the simple assumptions (Fox 1974, Boucher and Alves 1963) $C_D^l = 0.6$; $C_D^g = 1.0$. There result the following conditions at the exit plane ($A = A_{\text{exit}}$, $C_D^g = 1$):

Vapour-phase Discharge:

$$P_{\text{exit}}/P_{\text{res}} = F = \max\{P_{\text{atm}}/P_{\text{res}}, [2/(1+\gamma)]^{1/(1-1/\gamma)}\};$$

$$(1/2)u^2|_{\text{exit}} = (P_{\text{res}}/\rho)|_{\text{res}}[1-F^{1-1/\gamma}]/(1-1/\gamma);$$

Liquid-phase Discharge:

$$P_{\text{exit}} = [1-(C_D^l)^2]P_{\text{res}} + (C_D^l)^2P_{\text{atm}}; u_{\text{exit}} = [2(P_{\text{res}} - P_{\text{exit}})/\rho_l]^{1/2}.$$

Two-phase exit conditions:

Finally consider the (presumed choked) discharge of ambient saturated or superheated liquid from pressurized storage. The mass flow-rate is that suggested by Fauske and Epstein (1988). In the absence of losses at entry and within the discharge line flow acceleration and flashing necessarily occur within the (external) orifice flow. Such orifice flow may be expected to be of metastable liquid rather than of a two-phase equilibrium mixture. This suggests that the

influence of friction whilst small is not entirely negligible, and that frictional losses are sufficient to permit two-phase equilibrium flow within the discharge line. The flow is then choked at the pipe exit (van den Akker and Bond 1984), corresponding to negligible flow contraction in the external (orifice) flow, and a coefficient of discharge C_D^{lg} of essentially unity. The presence of choking within the pipe implies an aphysical increase in pressure downstream of the choke-front.

The use of the choked flow equation $u = c$ at the orifice (van den Akker and Bond 1984) is uncertain owing to difficulties arising from the interpretation of the "sound-speed" for two-phase flow. Inter-phase heat transfer is especially uncertain in the context of (infinitesimal) wave-speeds (Wallis 1969). We view the calculation of the pipe-exit conditions for such two-phase flow as particularly uncertain, but suggest that the pressure (whether or not thermodynamic equilibrium is established) satisfies the approximate identity,

$$(P + \rho u^2)|_{\text{exit}} = (P + \rho u^2)|_{\text{entry}};$$

for sufficiently small pipe-wall friction ($f \rightarrow 0$). If the entry flow is assumed to be of meta-stable liquid and to be loss-free, then the entry conditions are related to the reservoir conditions by the equation

$$P_{\text{res}} = (P + \rho_l u^2/2)|_{\text{entry}}.$$

This is analogous to the expected orifice flow for "stub" pipes (Fauske and Epstein 1988), and for storage vessel wall failure.

The exit-plane state for assumed homogeneous equilibrium flow is therefore determined by mass, momentum, and energy conservation, together with the equations of two-phase equilibrium:

Two-phase equilibrium flow:

$$\begin{aligned}(P+\rho u^2)|_{\text{exit}} &= P_{\text{res}} + [(dm/dt)/A]|_{\text{exit}}^2 / (2\rho_l); \\ [h + (1/2)u^2]|_{\text{exit}} &= h_{\text{res}}; 1 = y_{\text{HF}} + y_{\text{HF}_2} + y_{\text{HF}_6} + y_{\text{HF}_8} + y_{\text{H}_2\text{O}}^{\text{HF}} + y_{\text{H}_2\text{O}} + y_{\text{N}_2}; \\ 1 &= x_{\text{HF}} + x_{\text{H}_2\text{O}} + x_{\text{N}_2}; \beta x_{\text{N}_2}^g \rho_g = x_{\text{N}_2} \rho.\end{aligned}$$

This equation system is problematical: multiple solutions exist corresponding to saturated liquid as well as two-phase flow at the exit-plane. Further, the existence of a two-phase solution for a (correlation given) mass-flux is not guaranteed, so that difficulties can (and do) arise in the numerical solution for the exit conditions using the non-linear solver NAESOL (Scales 1988). These problems are not solved, but circumvented, by the observation that flow "immediately post flash" is (essentially) independent of stable two-phase or metastable liquid assumptions at the pipe-break (orifice plane).

External flashing and exit conditions:

Immediately beyond the exit-plane discharging fluid undergoes rapid depressurization to (near) ambient pressure accompanied by the flashing of superheated liquid and the re-establishment of homogeneous equilibrium flow. Air entrainment (against an adverse pressure gradient) is assumed negligible. A control volume analysis yields the conservation laws linking fluid states immediately before and after external flashing.

$$\begin{aligned}
 u_{\text{flash}} &= u_{\text{exit}} + (P_{\text{exit}} - P_{\text{atm}}) / (\rho u) |_{\text{exit}}; \\
 [h + (1/2)u^2] |_{\text{flash}} &= [h + (1/2)u^2] |_{\text{exit}} = h_{\text{res}}; \\
 d/dt |_{\text{exit}} &= (A\rho u) |_{\text{exit}} = (A\rho u) |_{\text{flash}}; \quad P_{\text{flash}} = P_{\text{atm}}.
 \end{aligned}$$

For assumed homogeneous equilibrium at the exit-plane we deduce, in the absence of entry losses or pipe-wall friction, the following expression for the jet velocity "immediately post flash";

$$u_{\text{flash}} = A_{\text{exit}} (P_{\text{res}} - P_{\text{atm}}) / (dm/dt) |_{\text{exit}} + (dm/dt) |_{\text{exit}} / (2A_{\text{exit}} \rho_{\ell}),$$

in which ρ_{ℓ} is the (incompressible) liquid density of (possibly dilute) hydrofluoric acid. Remarkably if metastable liquid is presumed to exist at the exit-plane **precisely the same** formula is derived.

This suggests that the behaviour "immediately post flash" is (for "loss-free" discharges) substantially independent of conditions at the release orifice or exit-plane, provided, that is, that a mass-flux can be assigned from an appropriate correlation. That this is indeed the case may be seen by a modified control volume analysis in which the control volume links conditions "immediately post flash" to conditions at pipe entry. For low-loss flow there is by assumption no significant drag acting over the inner pipe-wall surface; no forces act over that section of the control-volume. We deduce directly the following equations marking conservation of mass and momentum,

$$\begin{aligned}
 dm/dt |_{\text{exit}} &= (A\rho u) |_{\text{entry}} = (A\rho u) |_{\text{flash}}; \\
 [AP + u(dm/dt)] |_{\text{entry}} &= [AP + u(dm/dt)] |_{\text{flash}}.
 \end{aligned}$$

These equations are valid **whether or not** thermal and mechanical equilibrium exists anywhere within the discharge pipe, provided only that equilibrium exists at entry and immediately post flash. The velocity "immediately post flash" follows directly, as do the auxiliary conditions expressing prescribed mass-flux, and the invariance of the total energy $h+(1/2)u^2$.

Given that HFSPILL is intended only as a pre-processor to the atmospheric jet and plume entrainment models HFJET (Appendix 1) and HFPLUME (Chapter 5), we choose to avoid problems associated with two-phase equilibrium at the exit-plane by assuming instead that the release is of metastable liquid. The exit-plane pressure is then simply,

$$P_{\text{exit}} = P_{\text{res}} - (dm/dt|_{\text{exit}})^2 / (2A_{\text{exit}}^2 \rho_{\ell}).$$

§3.5 Summary and Conclusions.

A simple model assuming thermodynamic equilibrium within the storage vessel and correlation given mass-flux has been developed. Discharge is from an initially closed, pressurized vessel. The pressurizing gas is nitrogen; gravity is assumed negligible. Heat-influx and mass-efflux are given by literature standard correlations. Exit-plane pressures for liquid and "frozen" equilibrium vapour are obtained from an analysis of homogeneous equilibrium pipe-flow in the limit of negligible pipe-friction and entry losses.

Problems arise with the existence and uniqueness of saturated two-phase exit conditions when coupled to correlations (Fauske and Epstein 1988) for the mass-flux. In view of the typically weak influence of exit conditions upon equilibrium flow "immediately post flash", we take the exit conditions for entry

to the jet/plume models HFJET and HFPLUME as corresponding to the existence at the exit-plane of (possibly) metastable liquid. This (conventional) assumption results in considerable computational savings and in identical predictions with two-phase equilibrium choking "immediately post flash".

A FORTRAN 77 (Monro 1982) computer program HFSPILL has been written incorporating the reservoir model and mass-flux correlations outlined above. The basic model presumes a fixed orifice area and an adiabatic reservoir (storage vessel). If variable orifice area or atmosphere/reservoir heat exchange are important or need be modelled, the code structure requires only the substitution of the required correlation or valve closure assumptions within the FORTRAN 77 subroutine RELIEF. HFSPILL returns a depressurization history of the storage vessel together with conditions at the release (exit-) orifice. HFSPILL is a "pre-processor" to HFPLUME (HFJET) to be used when information regarding orifice conditions and discharge mass-flux is not available.

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4. The program EVAP for prediction of spreading and
mass-transfer-limited evaporation of
a liquid pool on land or water

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4. THE PROGRAM EVAP FOR PREDICTION OF SPREADING AND MASS-TRANSFER LIMITED EVAPORATION OF A LIQUID POOL ON LAND OR WATER

4.1. Introduction

This section describes the program EVAP, which predicts the steady-state or time-dependent spreading and mass-transfer limited evaporation of a liquid pool on land or water. EVAP is an extension of the time-dependent pool evaporation program EVAPW (Colenbrander, 1977), and includes capabilities of the steady-state spills program SPILLS (Fleischer, 1980).

The Shell program EVAPW calculates the time-dependent spreading and evaporation of a liquid pool on water. It assumes that the liquid is a cryogenic liquid having a boiling point much below ambient. Thus the vapour emission rate is entirely dependent on the heat transfer from the water to the pool. Because of negligible cooling of the water, conditions do not change and the evaporation flux may be taken constant. In EVAPW this constant flux must be specified by the user. Note that EVAPW is not applicable for the case of a liquid pool on land, because cooling of the land gives a heat flux decreasing with time and hence an evaporation flux decreasing with time.

The pool evaporation program EVAP may be used for both steady and non-steady pools. EVAP includes the EVAPW treatment of a boiling liquid pool on water (with liquid density smaller than water density), as well as a non-boiling liquid pool on land (for a general type of liquid, or HF). The controlling process is not heat transfer from the ground (as for a boiling liquid pool on land), but mass transfer above the pool. This mass transfer is assumed to occur predominantly by forced convection caused by the flow of air above the pool. To describe this mass transfer, a relationship between the pool evaporation rate and the pool radius is adopted, which has been used previously by M.T. Fleischer (1980) in the Shell program SPILLS. Thus for the option in EVAP of a non-boiling liquid pool on land, the evaporation flux needs not to be specified by the user, but is calculated by the program.

The EVAP model is applicable for releases of fluids (e.g. HF) which will form a liquid pool. While at the present time there is no exact criterion to determine when pool formation will occur, it can be assumed that pool formation is likely to occur for releases where the fluid is stored at reduced temperature and pressure.

In Section 4.2 the mathematical model for EVAP is formulated. The reader is referred to the EVAP user's guide contained in the User's Manual for details on the use of EVAP. The user's guide also describes how the (steady-state or time-dependent) pool data calculated by EVAP can be input to (the steady-state or transient version of) the heavy-gas-dispersion program HEGADAS; see Chapter 7 in this document for details on HEGADAS.

4.2. Mathematical model

This section describes the mathematical model adopted for EVAP. Sections 4.2.1 and 4.2.2 present a discussion of the time-dependent and steady-state model, respectively.

4.2.1. Time-dependent model: equations for pool volume and pool radius

The shape of the liquid pool is assumed to be cylindrical, with a radius $R(t)$, a volume $V(t)$, height $H(t) = V/(\pi R^2)$, and mass $M(t) = \rho_L V(t)$. The density ρ_L is taken to be uniform and constant. For HF, ρ_L (kg/m³) is related to the temperature T_L (Celsius) of the liquid by $\rho_L = 1015. - 2.2 \cdot T_L$ (see Figure 7 in Du Pont (1982)).

The spillage of liquid is given by the spill rate $S(t)$ (m³/s). The spill rate can be entered by the user in two difference ways:

- by means of the analytical formula,

$$S(t) = A_1 + A_2 t^{A_3}, \quad (0 < t < t_s) \quad (4.1a)$$

$$= 0, \quad (t < 0, t > t_s) \quad (4.1b)$$

in which the parameters A_1 , A_2 , A_3 , and the spill duration t_s are user-specified

- at incremental steps, i.e. specification of $S(t)$ at the times $t = 0, t_1, t_2, \dots, t_n$ ($n \geq 1$); in between these times $S(t)$ is linearly interpolated, and $S(t)=0$ for $t < 0$ and $t > t_n$. Thus the spill duration equals $t_s = t_n$. In the case of an HF-pool on land, the incremental values for $S(t)$ might be derived from the program HFSPILL. HFSPILL automatically generates a link file to EVAP, that includes incremental values for $S(t)$; see the User's Manual for further details

Note from the above that spillage starts at time $t = 0$ and stops at $t = t_s$, and that at time $t = 0$,

$$V(t) = 0, \quad R(t) = 0, \quad (t=0) \quad (4.2)$$

For $t>0$, the volume of the pool increases due to spillage of liquid, and decreases due to evaporation. Conservation of mass implies

$$dV/dt = (1-r_f) S - E(R) / \rho_L \quad (4.3)$$

Here the flash/spill ratio r_f is the proportion of spilled liquid converted into gas immediately after the flash, and $E(R)$ is the evaporation rate (kg/s). For liquid on water, the evaporation rate is taken to be $E(R) = \pi R^2 Q$, with the flux Q (kg/m²/s) constant and user-specified. For liquid on land, the evaporation rate is calculated as a function of R ; see Section 4.2.3 for details.

Gravitational spreading of the liquid pool is taken into account by the simple spreading law

$$dR/dt = C_L \{g' \max(0, H-H_{\min})\}^{1/2} \quad (4.4)$$

with C_L a spreading constant, g' the reduced gravity, and $H_{\min}$ a minimum, user-specified height. Here the spreading constant is taken to be $C_L = 2^{1/2} \approx 1.41$, and the reduced gravity equals

$$g' = g(1-\rho_L/\rho_w), \quad (\text{liquid on water; } \rho_L < \rho_w) \quad (4.5a)$$

$$g' = g, \quad (\text{liquid on land}) \quad (4.5b)$$

Here ρ_w ($= 1000 \text{ kg/m}^3$) is the density of the water. The correction factor $(1-\rho_L/\rho_w)$ in eq. (4.5a) represents the effect of subsidence of the liquid into the water, and vanishes for $\rho_L \ll \rho_w$. The spreading law for the liquid pool is derived from the simplified Bernoulli equation $0.5 (dR/dt)^2 = gH$. The latter equation leads to $C_L = 2^{1/2}$, but a smaller value may be used in order to account for obstacles on the ground. The spreading law for water is derived from a type of "dam burst" equation for the leading edge velocity of a liquid pool; see eq. (21) in Enger (1972). Validation of these spreading laws against experimental data has not been carried out in this study.

Starting from the initial values in eq. (4.2), the pool volume $V(t)$ and the pool radius $R(t)$ are found as a function of time by integrating the differential equations (4.3) and (4.4) with respect to time. Equations (4.3) and (4.4) are assumed to be valid up to the time t_1 , at which the pool height reduces to the minimum value $H(t_1) = H_{min}$.

The minimum pool height H_{min} is related to physical properties of the liquid such as surface tension and viscosity. See Appendix 4.A for a discussion of the appropriate choice for H_{min} .

Let $t_2 = \max(t_1, t_s)$, i.e. the maximum of t_1 and the time t_s at which the spillage stops. The following subsequent phases in time can now be distinguished in the process of spreading and evaporation of the liquid pool.

1. Time $0 < t < t_1$ [$S(t) > 0$, $H > H_{min}$].

The pool volume $V(t)$ and the pool radius $R(t)$ are found from equations (4.3) and (4.4). The pool height equals $H(t) = V(t)/(\pi R^2) > H_{min} = H(t_1)$.

2. Time $t_1 < t < t_2$ [$S(t) > 0$, $H = H_{min}$].

The pool height equals the minimum pool thickness, $H(t) = H_{min}$. The differential equation (4.4) is replaced by $R = \{V/(\pi H_{min})\}^{1/2}$, and the differential equation (4.3) is solved for $V(t)$ by integration with respect to time.

3. Time $t > t_2$ [$S(t) = 0$, $H = H_{min}$].

The height equals the minimum pool thickness, $H(t) = H_{min}$. Spreading is assumed to stop, i.e. the pool radius equals $R(t) = R(t_2)$. The liquid now breaks up into separate blobs (of height H_{min}). Here the evaporation rate is assumed to be proportional to the reducing pool area $A(t) = V(t)/H_{min}$. Thus $E(t) = a \rho_L V(t)$, with a a constant. By inserting this equation into equation (4.3) (with $S(t) = 0$), it is found that $E(t)$ decays exponentially in time, i.e. $E(t) = E(t_2) \exp[-a(t-t_2)]$. By imposing conservation of mass,

$$M(t_2) = \rho_L V(t_2) = \rho_L \pi R^2(t_2) H_{min} = \int_{t_2}^{\infty} E(t) dt \quad (4.6)$$

it is found that $a = E(t_2)/M(t_2)$.

4.2.2. Steady-state model: equation for pool radius

The time-dependent model formulated in the previous section can also be used for the calculation of data for steady pools, i.e. pools with a constant and indefinite spill rate S . To this purpose the spill rate $S(t)=S$ in the transient model must be applied in the transient model for a sufficiently large time t_s , such that at $t = t_s$ steady-state is closely achieved.

This model can be derived from the time-dependent model by adopting in the latter model a constant spill rate $S(t)=S$. This steady-state model is described in the present section. This model has the advantage of being more economical to use (in terms of computer usage) than the time-dependent model.

The shape of the steady liquid pool is assumed to be cylindrical, with a radius R and a uniform density ρ_L . For HF, ρ_L (kg/m³) is related to the temperature T_L (Celsius) of the liquid by $\rho_L = 1015 - 2.2 \cdot T_L$ (see Figure 7 in Du Pont (1982))

The spillage of liquid is given by the spill rate S (m³/s). Conservation of pool mass implies (cf. eq. (4.3))

$$E(R) = \rho_L (1-r_f) S \quad (4.3^*)$$

Here the flash/spill ratio r_f is the proportion of spilled liquid converted into gas immediately after the flash. For liquid on water, the evaporation rate (kg/s) is taken to be $E(R) = \pi R^2 Q$, with the flux Q (kg/m²/s) constant and user-specified. For liquid on land, the evaporation rate is calculated as a function of R ; see Section 4.2.3 for details.

The conservation equation (4.3*) can be solved for the pool radius R. For liquid on water, R equals

$$R = \{ \rho_L (1-r_f) S / (\pi Q) \}^{1/2}$$

For liquid on land, equation (4.3*) is solved iteratively for the pool radius R by means of the Newton-Raphson method.

The EVAP steady-state model has been compared against the EVAP transient model by adopting in the latter model the steady-state spill rate S for a sufficiently large time; see e.g. Fig. 4.2 for the case of HF on land. The development in time of the pool radius R(t) and the evaporation E(t) in Fig. 4.2 can be explained from the phases 1,2 of the spreading/evaporation process described in Section 4.2.1:

- Initially (start of phase 1) the radius R(t) and the evaporation rate E(t) are lower than their steady-state values, the rate of spillage of mass is larger than the rate of evaporation, and the pool mass increases. While the pool is spreading R(t), E(t) overshoot the steady-state values. Subsequently the rate of spillage is less than the rate of evaporation; the pool mass decreases and the pool height H(t) reduces to the minimum pool height H_{min} (end of phase 1).
- Finally (phase 2) $H(t) = H_{min}$, $R(t) = (V / \pi H_{min})^{1/2}$ and the evaporation rate E(t) reduces to the rate of spillage; the pool radius reduces to its steady-state value.

4.2.3. Relationship between pool evaporation rate and pool radius

In order to describe the evaporation rate of a liquid pool on land, a relationship between the pool evaporation rate and the pool radius is necessary. This relationship has been used previously by M.T. Fleischer (1980) in the Shell program SPILLS for steady pools. In this section the relationship will be given, and the basic steps and assumptions in the derivation of this relationship will be summarised. See Fleischer (1980) for full details. Note that the SPILLS program was tested for non-reactive

fluids only, and the validity of the method for reactive fluids such as HF has yet to be validated. In particular, the expression for the binary diffusivity may not be applicable for HF.

MASS TRANSFER RELATION

The mass transfer is assumed to occur predominantly by forced convection caused by the flow of air over the surface of the chemical pool. The rate of evaporation E (kg/s) is given by the mass transfer equation

$$E = k_c A \rho_g = Sh_L (v_c/L) L^2 \rho_g \quad (4.7)$$

with k_c the convective mass transfer coefficient (m/s), $L = \pi^{1/2} R$ the length of an equivalent square pool, $A = \pi R^2 = L^2$ the pool area, v_c the binary diffusivity of the gas-air mixture (m^2/s), $Sh_L = k_c L/v_c$ the dimensionless Sherwood number, and ρ_g the saturated vapour density.

ANALOGY BETWEEN MASS AND HEAT TRANSFER

The dimensionless Sherwood number Sh_L and Schmidt number Sc for mass transfer are assumed to be correlated via an analogy with the dimensionless Nusselt number Nu_L and Prandtl number Pr for heat transfer. An expression for Nu_L can be found from the Pohlhausen solution of the problem of heat transfer by forced convection due to wind blowing over a flat plate of length L in the downwind direction. Here the boundary layer is taken to be laminar for Reynolds number $Re < 3.2 \times 10^5$, and turbulent for $Re > 3.2 \times 10^5$. Thus, via the analogy, it is found that the Sherwood number is given by

$$Sh_L = 0.664 Sc^{1/3} Re_L^{0.5}, \quad (Re_L < 3.2 \times 10^5) \quad (4.8a)$$

$$Sh_L = 0.037 Sc^{1/3} (Re_L^{0.8} - 15200), \quad (Re_L > 3.2 \times 10^5) \quad (4.8b)$$

Here the Schmidt number and Reynolds number are given by

$$Sc = v_m/v_c, \quad Re = V L / v_m \quad (4.9)$$

with ν_m being the kinematic viscosity of air (m^2/s) and V the wind speed (m/s).

The wind speed V should be typical for the mass-transfer processes, and might be chosen equal to e.g. the ambient friction velocity u_* . In the EVAP program V is taken to be the wind speed at 10 m height, because the program SPILLS has been validated against experimental data for this choice of V ; see pp. 36-43 in Fleischer (1980). The SPILLS program has also been validated against experimental data assuming mass transfer taking place at atmospheric conditions. Therefore in EVAP the air and gas properties are presently evaluated at ambient pressure and ambient temperature. It might be more realistic to assume that mass transfer takes place at film conditions, i.e. to evaluate the air and gas properties at the film temperature (mean of air temperature and liquid temperature).

EVALUATION OF AIR AND GAS PROPERTIES

The air property ν_m , and the gas properties ν_c , ρ_g occurring in the equations (4.7) and (4.9) are all evaluated at ambient temperature and pressure (= 1 atmosphere). Thus it is assumed that the mass transfer takes place at ambient conditions. The properties are calculated as follows (see Appendix IV in Fleischer (1980) for further details).

- The kinematic air viscosity ν_m is derived as a function of temperature from NBS Circular 564.
- The binary diffusivity ν_c of the gas-air mixture is given by a kinetic theory expression as a function of the temperature and the pressure. The function contains as parameters three gas properties, i.e. the molecular weight M_g (kg/kmole), the normal boiling point T_g^{NBP} , and the liquid volume V_g^{NBP} (m³/kmole) at T_g^{NBP} .
- The saturated vapour density ρ_g (kg/m³) of the gas is the ratio of the molecular weight of the gas M_g and the saturated vapour volume V_g (m³/kmole). By the model of Edwards and Thodos, V_g is expressed as a function of the vapour pressure and temperature. The function contains as parameters the critical temperature, the critical pressure, and the critical volume of the gas.

For a general type of gas, the reduced vapour pressure (= vapour pressure / critical pressure) is calculated as a function of the reduced temperature (= temperature / critical temperature) by solving the Frost-Kalkwarf equation. This equation contains as parameters the gas constants B_r and C_r , which can be found by fitting.

For HF, the reduced vapour pressure is taken as a function of the temperature from Figure 6 in Du Pont (1982); see Figure 4.1.

See Table 4.1 for a list of the above properties for a large number of liquids.

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Appendix 4.A. Minimum height of a spreading vaporising pool

The minimum height $H_{\min}$ of a vaporising pool spreading on a surface will depend on properties of both the liquid and the surface. This appendix contains some discussion for the appropriate choice of $H_{\min}$.

In most pool-spreading models $H_{\min}$ is taken to be of the same order as the capillary depth $h_c = (\sigma_L / g \rho_L)^{1/2}$, with σ_L being the surface tension (N/m), $g = 9.8 \text{ m/s}^2$ the gravitational acceleration and ρ_L the liquid density (kg/m^3). On theoretical grounds $H_{\min}$ should never be lower than h_c . Batchelor (1967) quotes that an empirical rule is that the surface tension σ_L is proportional to the temperature difference between the liquid temperature T_L (or should we use the film temperature?) and the critical temperature T_c .

Simulations of experiments of steady spreading of LNG on a concrete surface were carried out by two different models developed by Moorhouse and Carpenter (1986) and Webber and Jones (1987) respectively. For both models the model predictions were found to lead to a best fit of the experimental data with a value of $H_{\min} = 10 \text{ mm}$, which is considerably larger than the capillary depth for LNG ($h_c = 1.8 \text{ mm}$).

For a steady, axisymmetric vaporising pool Webber (1990,1991) formulated a pool-spreading model based on shallow-layer equations for mass and momentum conservation. The mass equation assumes a constant uniform evaporation flux, and the momentum equation includes a resistance term proportional to the liquid viscosity ν_L . An approximate solution to these equations leads to the estimate $H_{\min} = (6\nu_L S / \pi g)^{1/4}$, in which S is the steady spill rate (m^3/s). Application of this formula to the above experiments leads to $H_{\min} = 7.8 \text{ mm}$, which is reasonably close to the value of 10 mm required to fit the data.

It is recalled that EVAP includes the EVAPW treatment of a boiling liquid pool on water (with liquid density smaller than water density). EVAPW was used by Colenbrander and Puttock (1984) to simulate the spreading of a boiling pool of LNG on water (Maplin Sands experiments). They found

that a value $H_{\min} = 6$ mm was needed in EVAPW to agree with observations of maximum pool diameter and evaporation time. They suggested that $H_{\min}$ was larger than h_c because of ice formation at the edges of the pool.

In conclusion it follows from the above that the precise choice for $H_{\min}$ is somewhat insecure. The capillary depth h_c is in any case a lower bound for $H_{\min}$. However this value may be too low, and thus lead to pools with a too short spill duration and extending to a too large distance. This will result in too high predictions for the (initial) concentrations and dispersion distances and to a too low prediction of the hazard duration. Following the steady-state model of Webber, one could suggest for slowly-varying release rates to take $H_{\min}$ variable as a function of the time t , i.e. to take $H_{\min} = H_{\min}(t) = \max[h_c, (6v_L S(t)/\pi g)^{1/4}]$, where $S(t)$ is the spill rate at the present time t . However it is doubtful (because of lack of experimental data) that there is sufficient evidence to justify this formula.

Let us apply the results of the above discussion to HF. According to Du Pont (1982), the critical temperature T_c equals 188.5 C, the surface tension at the boiling point $T_L = 19.55$ C equals $\sigma_L = 8.6 \times 10^{-3}$ N/m, and the liquid density ρ_L is related to T_L by $\rho_L = 1015 - 2.2 \cdot T_L$. By assuming σ_L being proportional to $(T_c - T_L)$, it is now found that

$$\sigma_L = \sigma_L(T_L) = 5.1 \times 10^{-5} (188.5 - T_L),$$

$$h_c = (\sigma_L / g \rho_L)^{1/3} = 2.3 \times 10^{-3} * [(188.5 - T_L) / (1015 - 2.2 T_L)]^{1/3}$$

The above formula results in $h_c = 0.96$ mm for $T_L = 19.55$ C (boiling point of HF at 1 atm.), $h_c = 0.975$ mm for $T_L = 10$ C and $h_c = 0.99$ mm for $T_L = 0$ C. Thus an approximate value of the capillary depth for a wide range of HF-liquid temperatures equals $h_c = 1$ mm.

The dynamic viscosity μ_L of liquid HF equals 2.6×10^{-4} kg/m/s at $T_L = 0$ C and 2.3×10^{-4} kg/m/s at $T_L = 10$ C (Du Pont, 1982). Using $\nu_L = \mu_L / \rho_L$ and $\rho_L = 1015 - 2.2 \cdot T_L$, it is thus derived that for temperatures in or close to the range of $0 \leq T_L \leq 10$ C the above suggested formula becomes ($H_{\min}$ in m; $S(t)$ in m^3/s)

$$H_{\min}(t) = \max[h_c, (6\nu_L S(t)/\pi g)^{1/4}] \approx \max[0.001, 0.015 S(t)^{1/4}]$$

Table 4.1. List of liquid/gas properties to be input to EVAP in the case of a liquid non-boiling pool spreading on land: molecular weight M_g (kg/kmole), critical temperature T_c (Celsius), critical pressure p_c (N/m²), critical volume V_c (m³/kmole), normal boiling point T_g^{NBP} (Celsius), liquid volume V_g^{NBP} (m³/kmole) at T_g^{NBP} , and the constants B_r , C_r needed in the vapour pressure equation. The values listed below correspond to those used in the Shell program SPILLS; see Fleischer (1980).

Type of liquid/gas	M_g	T_c	p_c	V_c	T_g^{NBP}	V_g^{NBP}	B_r	C_r
acetaldehyde	44.05	188.00	5.54E+07	0.152	20.40	0.056	9.78	4.40
acetone	58.08	236.40	4.74E+07	0.213	56.19	0.077	10.41	5.15
acrolein	56.06	237.00	5.22E+07	0.189	52.69	0.069	10.03	4.76
allyl alcohol	58.08	272.00	5.71E+07	0.203	97.08	0.074	15.46	9.50
allyl chloride	76.52	240.35	4.71E+07	0.234	45.10	0.084	9.99	5.62
benzene	78.11	288.94	4.89E+07	0.259	80.10	0.096	10.12	5.40
butadiene	54.09	151.84	4.33E+07	0.220	-4.41	0.083	9.49	4.72
butane	58.12	152.01	3.80E+07	0.254	-0.50	0.096	9.57	4.79
n-butyl alcohol	74.12	289.83	4.41E+07	0.274	117.73	0.102	18.83	13.48
t-butyl alcohol	74.12	233.00	3.97E+07	0.274	82.42	0.103	19.74	14.41
butylene	56.10	146.39	4.02E+07	0.239	-6.30	0.089	9.54	4.81
chlorine	70.90	144.00	7.70E+07	0.124	-34.05	0.045	8.21	3.93
diallyl amine	97.16	284.00	3.32E+07	0.367	111.00	0.139	11.85	6.03
epichlorohydrin	92.25	320.15	5.60E+07	0.235	116.11	0.087	11.00	5.12
ethanol	46.07	243.10	6.38E+07	0.167	78.30	0.062	14.62	8.11
ethyl chloride	64.51	187.15	5.26E+07	0.199	12.27	0.071	9.55	4.81
ethylene dichloride	98.96	287.85	5.36E+07	0.220	83.47	0.085	10.27	5.12
ethylene glycol	62.06	372.26	6.51E+07	0.185	197.40	0.064	11.72	1.45
ethylene oxide	44.05	195.66	7.15E+07	0.140	10.62	0.049	9.45	4.61
2-ethyl hexanol	130.23	347.95	2.73E+07	0.493	184.60	0.188	18.23	11.81
isoamylene	70.13	197.39	3.44E+07	0.318	38.57	0.109	10.20	5.01
isobutane	58.12	134.98	3.64E+07	0.263	-11.73	0.097	9.37	4.64
isoprene	68.12	210.17	3.73E+07	0.268	34.07	0.102	10.20	5.81
isopropanol	60.09	235.16	4.76E+07	0.220	82.26	0.082	17.21	11.06
isopropyl ether	102.17	226.90	2.87E+07	0.386	68.30	0.152	11.47	6.21
mesityl oxide	98.14	321.50	3.26E+07	0.359	129.50	0.131	12.35	7.21
methyl ethyl ketone	72.10	262.40	4.15E+07	0.267	79.60	0.097	10.40	4.97
meth. isobutyl ket.	100.16	298.30	3.27E+07	0.371	116.00	0.141	12.15	6.79
phenol	94.11	421.10	6.12E+07	0.229	181.80	0.101	13.62	8.20
propane	44.09	96.78	4.25E+07	0.200	-42.07	0.075	8.87	4.23
propylene	42.08	91.73	4.61E+07	0.181	-47.70	0.069	8.87	4.29
styrene	104.15	363.69	3.67E+07	0.349	145.20	0.133	11.52	6.71
toluene	92.14	318.56	4.10E+07	0.315	110.62	0.117	10.54	5.56
vinyl chloride	62.49	156.50	5.60E+07	0.178	-13.37	0.064	8.49	3.86
xylene	106.16	343.90	3.54E+07	0.376	139.11	0.140	11.20	5.97

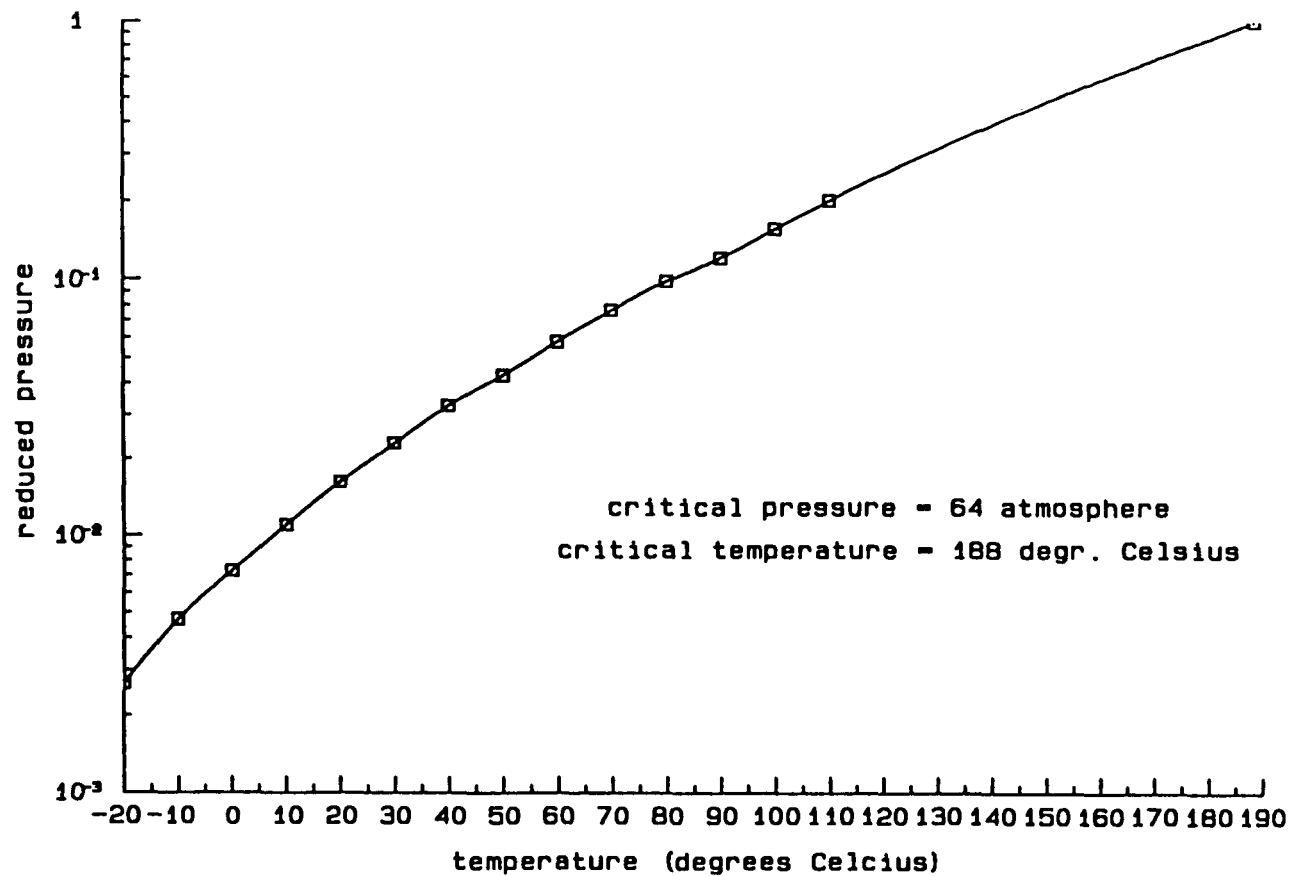


Fig. 4.1. Reduced vapour pressure of HF (= vapour pressure / critical pressure) as a function of the temperature of the gas (from Fig. 6 in Du Pont (1982))

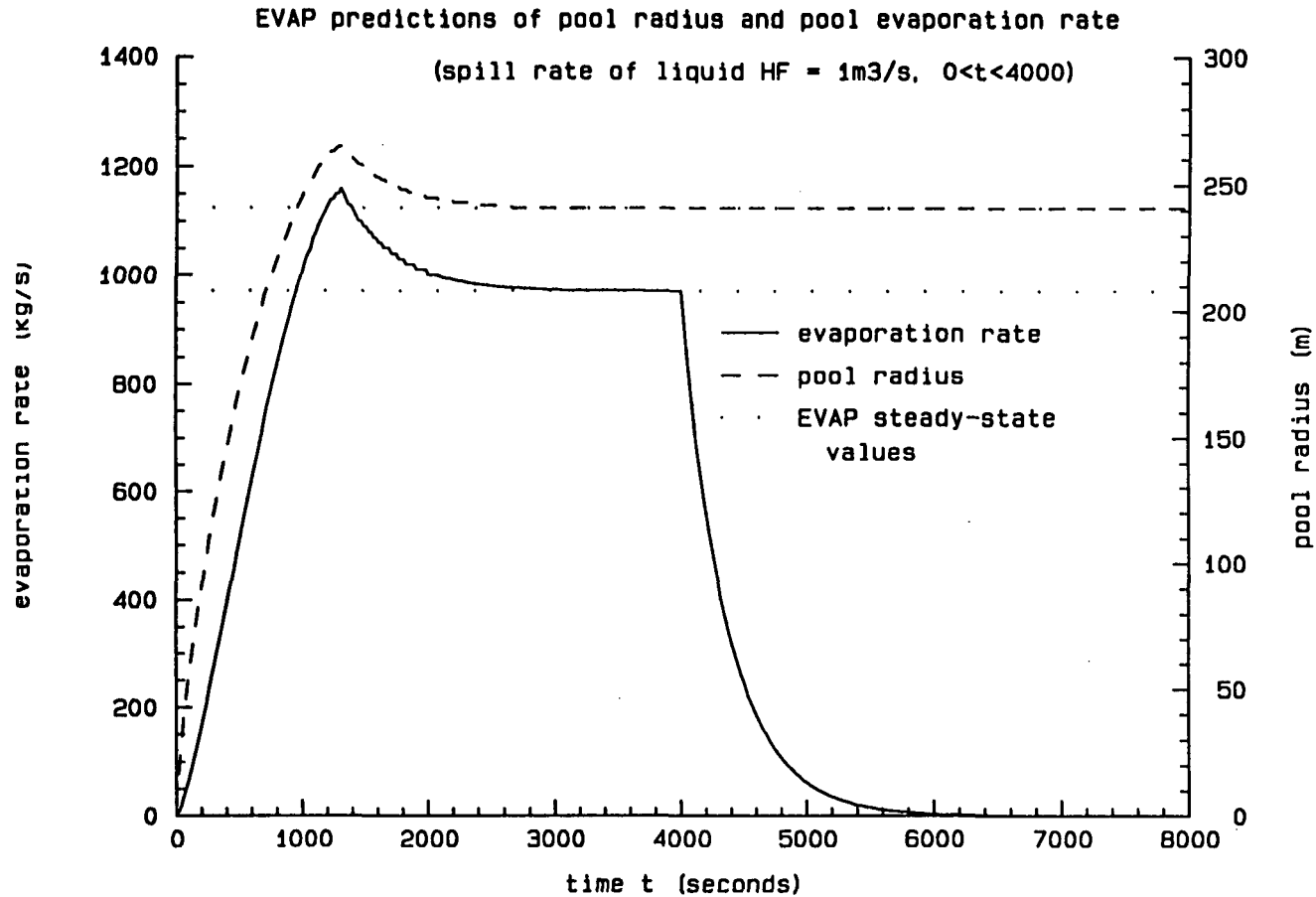


Fig. 4.2. Comparison of steady-state model against time-dependent model for the case of HF on land; in the steady-state model the input data are $S = 1\text{ m}^3/\text{s}$, $r_f = 0$, $T_a = T_s = 20^\circ\text{C}$, $V = 5\text{ m/s}$, and the calculated pool data are $R = 241\text{ m}$, $E = 971\text{ kg}$; observe that in the transient model steady-state is closely achieved after about 2800 seconds

5. Development of Plume and Jet Release Models

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§5.1: Introduction.

This chapter sets out the formulation and structure of the jet/plume model HFPLUME. The model describes initial jet flow, elevated plume, plume touchdown, and gravity-slumping following a pressurized release of anhydrous hydrogen fluoride. HFPLUME is a comprehensive model of dispersion in the near-field. Prediction of far-field dispersion requires that HFPLUME be "matched" (linked) either to a heavy-gas advection model, such as HEGADAS-S (Appendix 3, Appendix 5, Colenbrander and Puttock 1988), or else, for neutral or buoyant releases, to a passive dispersion model PGPLUME (Chapter 6, Hanna 1982).

Previous work (Ooms 1972; Wheatley 1987a, 1987b); Forney and Droescher 1985; Birch and Brown 1988; McFarlane 1988; Raj and Morris 1987) on dense and buoyant plumes, two-phase and pressurized gas jets, reactive and ground-affected jets, supported the view that predictions accurate in context could be obtained by means of an essentially simple, one-dimensional, integral-averaged model.

The models HFPLUME, and the simplified variant HFJET (Appendix 4), have been validated against thermodynamic data for HF/moist-air systems (Schotte 1987, 1988); their entrainment formulations have been checked against observed dispersion of buoyant (Petersen 1987) and dense (Hoot, Meroney and Peterka 1973) (ideal) gases, and against (atmospheric) releases of liquid propane gas (Cowley and Tam 1988, McFarlane 1988).

In addition the model combination HFPLUME/HEGADAS-S has been used (Chapter 9) to simulate recent large-scale experimental releases of anhydrous hydrogen fluoride (Blewitt, Yohn, Koopman and Brown 1987; Blewitt, Yohn and Ermak 1987; Blewitt 1988).

The indications are that HFPLUME, and within circumscribed limits HFJET, are satisfactory predictors of the early dispersion (plume rise, fall, touchdown, and early slumping) of a dense (neutral), or buoyant release of anhydrous hydrogen fluoride.

§5.2: The Stages of Plume Development: Physical Description, Literature, and Areas of Uncertainty:

Prior to the development of HFPLUME, we conducted a literature review in order to determine whether any existing model could be adapted to simulate a jet of anhydrous hydrogen fluoride (HF). The following sub-sections describe the results of that review for a number of models. The discussion is presented for the various zones of importance: external flashing, flow establishment, airborne plume, touchdown plume, slumped plume, and the far field.

From point of release to the far-field a dense plume passes through a series of (phenomenological) stages. These stages form the basis of the computer based model HFPLUME: the identification, sequence, and characteristics of these stages is therefore of considerable importance. This section should make clear the need for a careful selection of literature available models, and for their extension to cover regions not previously considered.

External Flashing:

Consider a pressurized release of evaporating liquid HF. Such a release forms at the orifice a narrow zone in which take place pressure relaxation and violent "flashing". "Flashing" is the sudden and disruptive evaporation of superheated liquid in response to a sharp fall in fluid pressure. This results in prompt

atomisation of any residual liquid and in the development of a two-phase flow. This stage of plume development is extremely complex. Fortunately details of "flashing" flow are not needed: it is sufficient to "bridge" this zone by means of integral conservation laws and by assuming that air entrainment during flashing is negligible (Wheatley 1987a, Raj and Morris 1987). The flashing zone ends when approximate thermal equilibrium, ambient pressure, and negligible inter-phase slip between vapour and liquid (droplet) phases are established. The velocity profile is roughly uniform; the cross-section may be assumed circular; deflection due to ambient pressure in cross-flow is typically negligible (Figure 5.1).

Flow Establishment:

Immediately beyond the flashing zone there exists a second zone "of flow establishment": air entrainment as the result of shear-induced turbulence results in the progressive dilution of the evaporating liquid jet, and in the radial diffusion of air towards the plume centre-line. The flow is described by an unperturbed "core" region, which diffusion of air has not reached, and by an axi-symmetric "outer" region, in which turbulent diffusion has resulted in a near Gaussian distribution of entrained air. This zone ends with the complete "erosion" of the core region and with the establishment of approximately self-similar conditions within the flow. The cross-section may be assumed circular (Figure 5.2). Generally this region is either neglected (Raj and Morris 1987; Hoot, Meroney and Peterka 1973; Forney and Droescher 1985), or else considered in conjunction with such effects as stack "downwash" (Hanna 1982; Ooms 1972; Havens 1987) and represented by an empirically derived correlation (Keffer and Baines 1963, Kanotani and Greber 1972). The discussion follows an analysis of Albertson Dai, Jensen and Hunter Rouse (1948), and of Abramovich (1963).

Airborne Plume:

Following flow establishment, plume development is described by the interaction of plume, ambient wind, and buoyancy effects: the influence of the ground, except as a generator of ambient turbulence and of wind-shear is negligible. This is the simplest of all the stages of plume development: nonetheless it is not without controversy. Arguments exist over the level of description necessary: whether Gaussian (Ooms 1972; Ooms and Duijm 1983; Petersen 1986; Schatzmann 1979) or "top-hat" (Hoot, Meroney and Peterka 1973; Forney and Droescher 1985; Davidson 1986) models are preferable; whether the effects of gradients within the atmosphere need be considered (Schatzmann and Policastro 1984); and whether or not significant "drag" forces act upon a plume in cross-wind (Briggs 1984; Ooms 1972; Schatzmann 1979; Hoult, Fay and Forney 1969; Coelho and Hunt 1989). Several different formulations for the crosswind entrainment have been proposed and checked against experimental data (Petersen 1978, 1987; Schatzmann 1978, Spillane 1983). Even the basic formulation of the equations of motion has resulted in discussion (Schatzmann 1978, 1979; McFarlane 1988), and in the use of special devices, such as plume "truncation" and dilute gas thermodynamics (Ooms 1972, Petersen 1978). The cross-section is generally assumed to be circular; the flow axisymmetric. However the presence of trailing vortices in cross-flow, and the cumulative effect of differences in vertical and horizontal diffusivity in the undisturbed atmosphere, will result in asymmetry and ultimately in an elliptic cross-section (Bloom 1980; Li, Leijdens and Ooms 1986). The role of dilute plume asymptotics in allowing estimation of certain entrainment coefficients from plume-rise and other data should be emphasised. Such early work as that of Briggs (1975) in the development of semi-empirical plume-rise correlations based on such analyses should not be neglected. (Figure 5.3).

Touchdown Plume:

Dense plumes must ultimately drift to ground or at any rate expand as the result of entrainment so as to intersect the ground surface. The ground interacts with a descending plume in several ways. First it acts as a geometrical constraint resulting in the redistribution of plume material. Second the ground allows the development of pressure forces as the result of pre-existing vertical momentum within the plume. These are impact forces resulting in the conversion of vertical to horizontal momentum. Third the ground permits the development of internal pressure within the plume as the result of gravity-slumping, in which the transverse motion of a gravity current is driven by an internally generated pressure acting at the ground surface. Finally drag forces must act at the ground as the result of differences in horizontal speed between plume and ambient wind.

In this region a transition must be made between a circular cross-section appropriate to an airborne plume, and a semi-elliptical (say) cross-section appropriate to an advected heavy-gas plume resting upon the ground (Figure 5.4). The touchdown region is described by a cross-section in the form of a circular segment. The region ends when a semi-circular cross-section first develops.

This transition region is neglected by Havens (1987,1988a) following Ooms (1972) and Ooms and Duijm (1984), as well as (inter alia) by Bloom (1980), by Schatzmann (1979) and by Raj and Morris (1987). No previous model exists which attempts to make a **smooth** transition from airborne dense to advected slumped plume. Limited experimental evidence does exist in the form of an unpublished study of dense salt water plumes (Karman 1986). In addition photographic evidence collected but not published by Hoot, Meroney and Peterka (1973) may form a useful dataset for model validation.

Slumped Plume:

Following touchdown the plume cross-section may be assumed semi-elliptic. Changes in plume eccentricity (aspect ratio) accommodate gravity slumping and the influence of residual ground-drag and impact pressure-forces. Vertical motions will be small compared to horizontal (Figure 5.5). An asymptotic approach, based on assumed horizontal flow, prescribed air entrainment, and a representation of gravity-spreading, is therefore possible.

Such a model is that proposed by Raj and Morris (1988) for dense plumes released horizontally at or near ground-level. The model incorporates jet entrainment, ground drag, and a formula for dense-gas gravity spreading. This model is (however) **not** valid for buoyant slumped plumes; neither is an interface for initially vertical releases provided.

Havens (1988) does not attempt to deal rigorously with the transition zone, for which horizontal momentum may be significant, but rather makes a simple transition from first plume/ground contact to heavy-gas advection. It may be questioned whether such a transition is physically appropriate.

The Far-Field:

Ultimately differences in velocity between (heavy-gas) plume and ambient atmosphere must become negligible, so that the representation of HFPLUME or that of Raj and Morris (1988) must merge into a heavy-gas advection model such as HEGADAS (Appendix 3, Colenbrander and Puttock 1988) or DEGADIS (Havens 1988). This is accomplished (Chapter 7, §7.8) by means of asymptotic matching. Alternatively for asymptotically buoyant plumes a transition may be made directly to a passive

advection (Gaussian) model such as PGPLUME (Chapter 6, Hanna 1982). It is also possible to incorporate the observed horizontal and vertical diffusion for a passive plume into the near-field formalism (Bloom 1980, Disselhorst 1984). This procedure is computationally costly; its advantage over simple matching unclear.

Curiously for horizontal slumped releases Raj and Morris (1988) are content to use their grounded jet model throughout the heavy-gas advection region, matching ultimately with a passive advection model (Figures 5.6, 5.7). This procedure fails to make use of well-validated models for heavy-gas dispersion.

To summarise: A review of the literature revealed clear gaps in existing models of early plume dispersion. These relate particularly to complex thermodynamics, to plume touchdown, and to the dispersion on the ground of possibly buoyant possibly dense clouds, such as arise from the interaction of HF and moist air. There was need of a **consistent** fundamentally-based model capable of describing all of the stages of plume development. No such formalism existed prior to the development of HFPLUME. It is to the development and validation of such a comprehensive model that this Chapter is addressed.

§5.3: Control Volume Analysis: Basic equations of Motion.

Consider a steady plume or jet of anhydrous hydrogen fluoride (HF) issuing from a pipebreak at pressure and at an angle to the horizontal. The atmosphere into which a release takes place is in a state of steady turbulent flow and has a mean wind-speed which is both horizontal and aligned with the horizontal component of the released (HF) jet. This last assumption is inessential, and is introduced to simplify the equations of plume motion.

We shall regard the jet and ambient atmosphere as a single fluid (of variable composition) occupying the upper half-plane above a horizontal ground-surface. The jet and ambient atmosphere merge infinitesimally so that no jet "boundary" exists at finite distance from the jet-axis; entrainment occurs therefore "at infinity". No slip occurs amongst the constituent phases of the developing jet; mean-flow within both ambient atmosphere and jet/plume is everywhere steady.

We begin by introducing a set of control-volumes $\tau(s)$, $s > 0$, an analysis of which results in an integral-averaged description of jet development independent of detailed assumptions regarding induced and ambient turbulence.

The Control-Volume $\tau(s)$: First construct a vertical surface at such distance upwind of the release-point that ambient flow is negligibly perturbed. Second, at arbitrary distance $s > 0$ downwind of the release-point, construct a "cross-section" $A(s)$ through the developing jet. Third link these (semi-infinite) surfaces by skirting the ground and pipe-work surfaces and passing through the jet at the plane of release. Finally construct a fourth bounding surface A_∞ at great (notionally infinite) distance from the jet-axis such as to enclose the (infinite) volume $\tau(s)$. [See Figure 5.1-5.3; Figure 5.8; Appendix 1, Figure A1.1]

By a "cross-section" $A(s)$ we intend a curved surface locally perpendicular to the (turbulent mean) flow-velocity $\mathbf{u}$. We shall assume that these surfaces form a family parameterized by a distance $s > 0$ measured along a (mean flow) stream-line (the plume-axis) originating at the point of release. Such a cross-section is orthogonal to the plume centre-line and asymptotically vertical at great off-axis distance. It reflects the progressive rotation of the mean plume velocity from centre-line to undisturbed atmospheric values. We shall assume that the

characteristic length-scales for plume development parallel and perpendicular to the mean-flow are asymptotically ordered, at any rate in those regions of the flow for which departures between the plume and undisturbed ambient flows are significant. Specifically we shall take the parallel length-scale to be much greater than the perpendicular: it is in this sense that the jet/plume may be described, following Hinze (1959), as "thin". Finally we shall have regard to that part of the ground surface over which there exist significant departures from the undisturbed ambient either in HF concentration, in pressure, or in ground-shear. This area, the intersection of plume and ground, we term the plume "footprint" $F(s)$.

Integration of the basic equations of motion over such a control-volume results, given an assumed "thin" jet, in the integral forms (Hinze 1959):

HF mass-flux:

$$\iint_{A(s)} c u_{\bullet} dA = (c_{\square} / \rho_{\square}) dm/dt|_{\square};$$

Entrained mass-flux:

$$\begin{aligned} \iint_{A(s)} (\rho u - \rho_{\infty} u_{\infty})_{\bullet} dA = \\ A_{\square} (\rho_{\square} u_{\square} - \rho_{\infty} u_{\infty}) - \iint_{A_{\infty}(s)} \rho u_{\bullet} dA; \end{aligned}$$

Horizontal excess-momentum flux:

$$\begin{aligned} \iint_{A(s)} [\rho u (u_x - u_{\infty}) + (p - p_{\infty}) e_x]_{\bullet} dA = (u_x^{\square} - u_{\infty}) dm/dt|_{\square} \\ + A_{\square} \cos \phi_{\square} (p_{\square} - p_{\infty}) - \iiint_{\tau(s)} \rho u_{\bullet} \nabla u_{\infty} d\tau - \iint_{F(s)} (\Sigma_{xz} - \Sigma_{xz}^{\infty}) dA; \end{aligned}$$

Vertical momentum flux:

$$\begin{aligned} \iint_{A(s)} [\rho u u_z + (p - p_{\infty}) e_z]_{\bullet} dA = u_z^{\square} dm/dt|_{\square} \\ + A_{\square} \sin \phi_{\square} (p_{\square} - p_{\infty}) - \iiint_{\tau(s)} (\rho - \rho_{\infty}) g d\tau + \iint_{F(s)} (p - p_{\infty}) dA; \end{aligned}$$

Total energy flux:

$$\iint_{A(s)} [\rho \mathbf{u} (h + (1/2) \mathbf{u}^2 - h_{\infty} - (1/2) \mathbf{u}_{\infty}^2)] \cdot d\mathbf{A} = \iint_{F(s)} (\dot{\Phi} - \dot{\Phi}_{\infty}) dA \\ + (h_{\square} + (1/2) \mathbf{u}_{\square}^2 - h_{\infty}^{\square} - (1/2) \mathbf{u}_{\infty}^{\square 2}) dm/dt|_{\square} - \iint_{\tau(s)} \rho \mathbf{u} \cdot \nabla (h_{\infty} + (1/2) \mathbf{u}_{\infty}^2 + gz) d\tau.$$

[Notation: $dm/dt|_{\square}$, mass flow-rate issuing from the release-point; $(\rho, c, \mathbf{u}, p, h)$, density, pollutant mass-concentration, velocity, absolute pressure, and specific enthalpy of the ensemble-averaged flow. ϕ angle to the horizontal of the plume-axis (coordinate stream-line), $\dot{\Phi}$ the surface to air heat-flux, Σ_{xz} the Reynolds stress as the result (ultimately) of viscous drag at the ground. $\mathbf{e}_x$ and $\mathbf{e}_z$ denote unit vectors in the horizontal (wind aligned) and vertical (upward) directions. The affix " $\square$ " identifies conditions at the release-plane; the suffix " ∞ " conditions within the unperturbed atmosphere.]

These equations express in integral form conservation of hydrogen fluoride mass-flux, air entrainment, conservation of the excess above ambient of momentum (both horizontal and vertical), and conservation of energy.

The HF-continuity equation (**HF mass-flux**) expresses that HF is merely transported and diluted by the atmosphere. Total mass continuity (**Entrained mass-flux**) allows the identification of the entrained air mass-flux with the integrated sum of mass-flows induced "at infinity", that is at great distance from the plume centre-line. The equation is formulated as a difference in mass-flux between the undisturbed atmosphere and the system that exists following a sustained release of hydrogen fluoride. This has advantages over conventional (total mass-flux) formulations (Ooms 1972, Petersen 1987) in that it is not necessary to introduce a "cut-off" point in a Gaussian plume model beyond which conditions revert (discontinuously) to atmosphere values (Schatzmann 1978). This permits **true** Gaussian profiles to be introduced in estimating concentrations and

temperatures within the developing plume or jet, with a consequent improvement in the accuracy of predicted centre-line concentrations (Appendix 1, Davidson 1986, McFarlane 1988).

The horizontal momentum equation (**Horizontal excess-momentum flux**) states that (in the absence of ground drag and significant vertical wind-shear) the excess-flux of horizontal momentum is conserved. Horizontal momentum excess is therefore a natural variable of the jet/plume system (Hinze 1959, McFarlane 1988, Appendix 1). Conventional plume models neglect "ground-effects" (have zero "footprint" area) and consider only the weak effect of vertical wind-shear upon horizontal momentum flux. The present model, in dealing consistently with "jet", buoyant plume, and "slumped" plume, necessarily incorporates a ground-drag force, acting over the plume "footprint", the effect of which is (substantially) to decelerate an "airborne" plume at first ground "impact". Note that the drag force is expressed over the "footprint" area $F(s)$, and in terms of the **difference** between the ground-level stresses Σ_{xz} and Σ_{xz}^{∞} in the presence or absence of released material. Clearly drag forces exist even in the undisturbed atmosphere: these, however, are balanced in steady atmosphere flow by (weak) horizontal gradients in the ambient pressure field, and are therefore absent from the difference formulation adopted here.

The vertical momentum equation (**Vertical momentum-flux**) expresses the variation in the flux of vertical momentum in terms of forces arising from either buoyancy or pressures developed at the ground surface at "touchdown" and beyond. Conventional descriptions model either buoyancy forces alone, or else buoyancy together with "airborne" plume drag, that is the pressure force that arises over the cross-section $A(s)$ as the result of small local differences between undisturbed ambient and plume pressure (Frick 1984). "Airborne" drag is a controversial element (Briggs 1984), being found necessary by some (Ooms 1972,

Petersen 1978, Schatzmann 1979) but not by others (Petersen 1987; Forney and Droescher 1985; Hoot, Meroney and Peterka 1973). The present model necessarily includes pressure forces developed over the plume "footprint" in response to velocity changes implied by air entrainment, buoyancy, ground-drag, and the geometrical constraint of an impermeable (level) ground. Pressure forces at the ground develop in response to the interaction of "top" entrainment and "gravity slumping", and hence are plausibly expressed in terms of the spreading velocity and buoyancy force in a manner consistent with the gravity current spreading (van Ulden 1984, Raj and Morris 1987).

Finally consider the energy equation (**Total energy flux**), which expresses the near constancy of the excess flux above ambient values of the plume total energy (essentially enthalpy). This flux is altered by small vertical gradients in atmospheric enthalpy and wind-speed, and by the potential energy changes associated with vertical motion under terrestrial gravity. The "airborne" plume is assumed to exert negligible influence on the heat transfer from ground to atmosphere. In addition for a touchdown plume whose temperature differs substantially from that of the ground the heat flux at the ground surface may become important. The heat-flux from the ground is mediated via a heat transfer coefficient the magnitude of which is related to the vertical turbulent transport of heat from ground surface into the overlying plume. For the unperturbed atmosphere such fluxes are also present but are balanced by vertical temperature gradients and by (typically small) systematic variation in temperature downwind. This unperturbed heat flux is therefore absent from the difference model here developed, except inasmuch as it determines the Monin-Obukov length, wind-speed and temperature profiles within the undisturbed atmosphere (Plate 1982, Colenbrander 1985). No provision has been made for this enhanced ground/plume heat transfer in the current model formulation. Such provision is however encoded within the heavy-gas advection module HEGADAS (Appendix 3). Inasmuch as HFPLUME

is intended as a "front-end" to a heavy-gas advection model such a HEGADAS, the neglect of heat transfer from the ground at touchdown and beyond was judged (a priori) insignificant.

§5.4: External "flashing": Equilibration of Jet and Ambient Pressure; the Zone of Flow Establishment: Self-similar Flow and Gaussian Profiles.

This section "bridges" the external flash (depressurization) and flow-establishment zones prior to the development within a released plume/jet of (approximately) self-similar conditions. The discussion of flow establishment relates particularly to the prediction of **point-local** from **sectionally averaged** concentrations within the early jet, and to the prediction of the zone length. This analysis is **not** incorporated within the (integral averaged) plume model HFPLUME. Such detailed formulation (as it affects air entrainment) requires careful experimental validation and exerts a modest influence upon predictions in the range of greatest interest, perhaps 10 to 500m downwind of release; it has, however, clear implications for a purely Gaussian plume model.

External Flashing:

Having set up the basic equations of motion in integral form, we specialise in order to "bridge" the external flashing zone, or for a gas-jet the depressurization zone, that occurs immediately beyond the breakpoint in choked flow. In the absence of choked flow this transitional region may still be present. For example, for a purely liquid release, pressure at the orifice may be an appreciable fraction of the storage (reservoir) pressure; this pressure, however,

rapidly relaxes within the vena contracta to an essentially ambient value. During flashing radial and axial velocities within the developing jet are of co-magnitude so that the "thin jet" approximation is invalid. In addition interphase slip and thermal disequilibrium are likely to occur. Nonetheless depressurization occurs so quickly, within a few (perhaps 5) diameters of the release plane, that "thin jet", equilibrated conditions may be presumed to exist everywhere except within a narrow transition zone adjacent to the release point. We shall assume further, in view of the strongly expanding flow of a flashing jet, or the very large density differences between jet and ambient of a liquid jet, that negligible air entrainment occurs within this depressurization zone. The length of the zone will in the context of evaporating liquid jets or plumes ordinarily be negligible and will hereafter be ignored: the models have initial conditions defined "immediately post flash" at (axial) displacement zero.

Neglecting further the influence of gravity and of wind-shear upon the integral conservation laws, we deduce, for the conditions "immediately post flash", the elementary forms (Figure 5.1)

$$u = u_{\square} + A_{\square}(p_{\square} - p_{\infty})/dm/dt|_{HF}; \quad c = \rho; \quad \phi = \phi_{\square}; \quad A_c u = dm/dt|_{HF};$$

$$[h + (1/2)u^2 - h_{\infty}^{\square} - (1/2)u_{\infty}^{\square 2}] = [h_{\square} + (1/2)u_{\square}^2 - h_{\infty}^{\square} - (1/2)u_{\infty}^{\square 2}].$$

[The notation is that ϕ is the angle of inclination to the horizontal, and that $A_{\square}$ is the (true) area of the release orifice. The values of velocity u , density ρ , and area A are averaged values, that is they assume an essentially uniform velocity or density within the jet as it emerges from the depressurization zone.]

This is approximately valid for a liquid jet, (Albertson, Dai, Jensen, and Hunter Rouse 1948) and is at any rate plausible for a gaseous or two-phase jet. Certainly

drag forces at the jet edge and the momentum redistribution associated with the entrainment of air are for consistency necessarily small.

Flow Establishment:

Beyond the zone of depressurization there exists a second transitional zone, a zone of "flow establishment", in which the interaction of jet and ambient result in the progressive turbulent diffusion of air towards, and of jet momentum away from, the jet centre-line. This zone is characterised by a progressive change from a "top-hat" velocity profile to an essentially Gaussian profile (Hinze 1959, Abramovich 1963) in the asymptotic far-field. Within this zone, neither "top-hat" nor Gaussian profiles properly describe the cross-sectional variation in jet velocity and pollutant concentration (Figure 5.2).

What is needed is a transitional profile (Albertson, Dai, Jensen, and Hunter Rouse 1948) in which an inner "core" jet (of uniform velocity and HF concentration of 100%) is "eroded" by a spreading Gaussian profile coupling inner "core" and outer ambient flows. An order of magnitude analysis yield that this zone is of typical length $\ell/D = 1/e_{\text{jet}}$, in which D is a representative diameter "immediately post flash", and in which e_{jet} is a (dimensionless) coefficient whose magnitude measures the effectiveness of jet/ambient shear in causing air entrainment.

For gas jets this magnitude is most probably comparable to that seen following the establishment of self-similar flow (Ricou and Spalding 1961), which for a "top-hat" model yields a value $e_{\text{jet}} = 0.08$. This is certainly reduced for a two-phase system (Appendix 1, McFarlane 1988), and may be much smaller for a liquid jet for which dynamical break-up, rather than flashing "atomization", may dictate the entrainment rate (Wheatley 1987a, Ohnesorge 1936, van de Sande and Smith 1976, McCarthy and Molloy 1973).

We shall assume that all modelled releases result in prompt atomization rather than gradual break-up, as is consistent with the earlier assumptions of negligible interphase slip and thermodynamic equilibrium. This results in a zone of flow establishment whose length is perhaps 20 orifice diameters. This zone is therefore also of a negligible length compared with downwind displacements of order tens or hundreds of metres. More complex models are possible and have been suggested (Jones 1988, Iannello and Rothe 1988): they require further and uncertain details regarding jet and droplet break-up and evaporation.

This zone ends with the diffusion of air to the jet centre-line, the elimination of the undisturbed "core" zone, and the establishment of simple Gaussian profiles for jet velocity and HF-concentration. Given estimates of the fluxes of mass, momentum, and energy, we may locate the zone boundary at least to moderate precision simply by requiring that these principal fluxes be invariable whatever self-similar "profiles" are assumed to describe the cross-sectional variation in velocity and hydrogen fluoride concentration.

The zone boundary is then located at that displacement $s > 0$ for which the centre-line concentration first differs from 100% HF. Let therefore the profiles of jet velocity and HF mass-concentration be described by the Gaussian forms (ground-effects negligible):

$$c/c_* = \phi_c(r/D_*; \gamma^2); (u - u_\infty)/(u_* - u_\infty) = \phi_u(r/D_*);$$

$$\phi_u(r/D_*) = \exp(-4r^2/D_*^2); \phi_c(r/D_*; \gamma^2) = \exp(-4r^2/\gamma^2/D_*^2).$$

The notation is that $r > 0$ is the off-axis displacement, γ^2 is the turbulent Schmidt number (Hinze 1959), $u_*(s)$ the centre-line velocity, and $c_*(s)$ the centre-line concentration. $D_*(s)$ is an effective jet "diameter". Invariance of

the principal fluxes results in a set of (non-linear) integral equations for the parameters u_* , c_* , and D_* , namely (Figure 5.2),

$$\begin{aligned} \iint_{A(s)} c u \, dA &= dm/dt|_{HF}; \\ \iint_{A(s)} (\rho u - \rho_\infty u_\infty) &= dm/dt; \\ \iint_{A(s)} \rho u (u - u_\infty) \, dA &= dP_x/dt - u_\infty dm/dt. \end{aligned}$$

The above non-linear system has a solution space which properly contains the set of physically admissible "self-similar" profiles. Additionally aphysical solutions exist for which $c_* > \rho_*$, that is for which the HF mass-concentration exceeds the total mixture density; for which $u_* > u_{flash}^{post}$, that is for which the centre-line velocity is greater than the velocity immediately post flash; and finally for which $c_* > c_{flash}^{post}$, that is for which the centre-line concentration, consistent with an assumed Gaussian profile, actually exceeds that found at the jet-axis immediately following jet depressurization.

The correct diagnosis from these symptoms is that the set of principal fluxes ($dm/dt|_{HF}$, dm/dt , dP_x/dt) and the atmosphere properties (ρ_∞ , u_∞) correspond not to Gaussian self-similarity, but rather to a cross-section located within the zone of flow development. The zone boundary is therefore defined by the simultaneous solution of the above integral equations, together with the "boundary equation", $c_* = c_{flash}^{post}$.

§5.5: The Airborne Plume: geometry and shear entrainment.

We consider in this section the representation of the "airborne" plume, that is the plume from a point "immediately post flashing" to the point of first plume "touchdown". We have chosen to represent the plume development in terms of a

simple, integral-averaged, or "top-hat" model in which is tracked the plume "centre-line". The plume consists of a set of circular cross-sections, each of defined diameter, mean density, temperature, and mass concentration of HF. Within each cross-section the velocity is assumed uniform; outside conditions are those of the undisturbed atmosphere.

We seek to introduce a (global) coordinate system the level surfaces of which are everywhere orthogonal to the turbulent-mean flow. Such coordinates, however, cannot be found without detailed knowledge of the turbulent flow in the presence of a dense-gas plume. In the circumstances we must be content with an approximate coordinate description valid in the neighbourhood of the plume-axis. We begin by introducing a local ("canonical") coordinate system (s, r, θ) defined in the neighbourhood of the plume centre-line (Figures 5.8, 5.9, Schatzmann 1978):

$$\mathbf{r} = (x, y, z) = \mathbf{r}_\square + \left(\int_0^s \cos \phi ds, 0, \int_0^s \sin \phi ds \right) + r(-\sin \phi \sin \theta, \cos \theta, \cos \phi \sin \theta);$$

$$\mathbf{r}_\square = (x_\square, y_\square, z_\square); (s, r, \theta): 0 \leq s < \infty, 0 \leq r < \infty, -\pi/2 \leq \phi < 3\pi/2, 0 \leq \theta < 2\pi.$$

The coordinate s marks the distance along the plume centre-line from release point to a general plume cross-section $\mathbf{A}(s)$. The coordinate pair (r, θ) defines a set of plane polar coordinates in the cross-section $\mathbf{A}(s)$. The angle $\phi(s)$ is the inclination of the plume centre-line at displacement s from the release point (Figure 5.3).

Such coordinates are not and cannot be globally defined. Neither do the level surfaces $ds=0$ coincide precisely with the surface $\mathbf{A}(s)$ in the sense of the original control-volumes $\tau(s)$ of §5.3. In particular the level surfaces $ds=0$ are not asymptotically vertical as are the original surfaces $\mathbf{A}(s)$. They do nonetheless approximate such cross-sections $\mathbf{A}(s)$ in the vicinity of the plume centre-line, that is in that region of the plume for which the differences between

plume and ambient are most pronounced. This certainly suggests, though it cannot confirm, that it is legitimate to cast the equations of plume motion in terms of a "top-hat" model and its associated, "canonical", coordinate system.

Differentiation of the integral equations of §5.3 then yields, for the canonical coordinates (s, r, θ) , the basic differential equations;

$$\begin{aligned} d/ds(dm/dt) &= \text{Entr}_{\text{Amb}}^{A(s)}; \\ d/ds(dP_x/dt) &= \text{Drag}_{\text{Amb}}^{A(s)} \cdot e_x + \text{Shear}_{\text{Amb}}^{A(s)}; \\ d/ds(dP_z/dt) &= \text{Drag}_{\text{Amb}}^{A(s)} \cdot e_z + \text{Buoy}_{\text{Amb}}^{A(s)}; \\ d/ds(dE/dt) &= \text{Ener}_{\text{Amb}}^{A(s)}; \quad dx/ds = \cos\phi; \quad dz/ds = \sin\phi; \end{aligned}$$

together with the algebraic constraints;

$$\begin{aligned} A &= (\pi/4)D^2; \quad dm/dt = A\rho u; \quad dm/dt|_{\text{HF}} = A c u; \\ dP_z/dt &= dm/dt \, u \sin\phi; \\ dP_x/dt &= dm/dt \, (u \cos\phi - u_\infty); \\ dE/dt &= dm/dt \, (h + (1/2)u^2 - h_\infty - (1/2)u_\infty^2). \end{aligned}$$

[Notation: A cross-section area, D plume diameter (circle), x horizontal axis-displacement, z axis height above level ground, dm/dt released and entrained mass-flux, $(dP_x/dt, dP_z/dt)$ excess (horizontal, vertical) momentum flux, dE/dt excess energy flux, $dm/dt|_{\text{HF}}$ HF mass-flux; u mean flow-speed, ϕ axis inclination, ρ mean plume-density, c mean mass-concentration HF, $h(\rho, c, P_\infty)$ specific enthalpy the suffix " ∞ " denotes ambient conditions at the centroid height $z > 0$.]

The quantities **Drag**, **Shear**, **Entr**, **Buoy**, and **Ener** have the formal definitions,

$$\text{Drag}_{\text{Amb}}^{A(s)} = (d/ds) \iint_{A(s)} (p - p_\infty) dA;$$

$$\text{Shear}_{\text{Amb}}^{A(s)} = \iint_{A(s)} \rho u \sin \phi \left(\frac{du_{\infty}}{dz} \right) |J| dA.$$

$$\text{Entr}_{\text{Amb}}^{A(s)} = \iint_{A_{\infty}} \rho u_{\infty} dA;$$

$$\text{Buoy}_{\text{Amb}}^{A(s)} = \iint_{A(s)} (\rho - \rho_{\infty}) g |J| dA;$$

$$\text{Ener}_{\text{Amb}}^{A(s)} = \iint_{A(s)} \rho u \sin \phi \left(\frac{d}{dz} \right) (h_{\infty} + (1/2) u_{\infty}^2 + gz) |J| dA.$$

[Notation: s displacement along plume centre-line, z height above ground, ϕ plume centre-line inclination, ρ local (turbulent averaged) density, u flow-speed, p (absolute) pressure, h specific enthalpy, $|J| = 1 - r \sin \theta \, d\phi/ds$ Jacobian determinant, g acceleration due to gravity, $dA = r dr d\theta$ (scalar) area element.]

They represent (respectively) the "drag" force $\text{Drag}_{\text{Amb}}^{A(s)}$ acting on the plume in cross-flow as the result of vortex formation in the plume wake (Ooms 1972, Schatzmann 1979), the shear force $\text{Shear}_{\text{Amb}}^{A(s)}$ associated with the vertical gradient of wind-speed, the total entrainment rate $\text{Entr}_{\text{Amb}}^{A(s)}$ per unit axis length, the section-averaged buoyancy force $\text{Buoy}_{\text{Amb}}^{A(s)}$, and the variation in plume total energy $\text{Ener}_{\text{Amb}}^{A(s)}$ resulting from vertical gradients of temperature (enthalpy) and wind-speed. The pressure is that deduced for hydrostatic equilibrium, except insofar as departures result in the (airborne) drag force. These integrals are in actual practice replaced by empirical formulae chosen for compatibility with existing plume models and literature available data. These formulae express, for example, the contribution to air entrainment within the plume of the difference in velocity between mean cross-sectional velocity and the ambient wind-speed. Model closure is therefore in terms solely of mean cross-sectional and local atmospheric ambient parameters.

The above "algebraic constraints" can be viewed as definitions of, for example, the total mass-flux within the plume, or the area of a circle. It is algebraically convenient to regard these as algebraic equations forming part of a differential/algebraic system. Such a system is then solved by means of the differential/algebraic package SPRINT (Berzins, Dew, and Furzeland 1983; Berzins and Furzeland 1985). Such a formulation allows the somewhat different descriptions of "touchdown" and "slumped" plumes to be incorporated within the same formalism. This results in a computer program HFPLUME, the structure of which is (we suggest) logically segmented, and easily modified and maintained.

§5.6: The Touchdown and Slumped Plume: plume geometry and footprint pressure forces.

Consider next the representation of the plume following first "touchdown". Touchdown occurs at that axial displacement $s > 0$ for which an assumed circular cross-section just touches the horizontal ground surface $z = 0$. It is also the point beyond which the plume footprint width first assumes a non-zero value. The cross-section of a plume following touchdown is modelled not by a circle but rather by a circular segment, the centroid of which lies upon the plume "centre-line". This centroid location will, for a dense plume, continue to fall, so that after some time a semicircular cross section is certain to arise. At this point the plume has passed through a transitional region between circular "airborne" and semi-elliptic "slumped" cross-sections. Further development will, at least initially, be characterised by (transverse) gravity spreading (van Ulden 1974, Raj and Morris 1987), and by air entrainment principally through the "upper" plume surface.

These elements may be assembled within the framework of a "top-hat" model as the differential system:

$$d/ds(dm/dt) = \text{Entr}_{\text{Amb}}^{A(s)};$$

$$d/ds(dP_x/dt) = \text{Drag}_{\text{Amb}}^{A(s)} \cdot \mathbf{e}_x + \text{Shear}_{\text{Amb}}^{A(s)};$$

$$d/ds(dP_z/dt) = \text{Drag}_{\text{Amb}}^{A(s)} \cdot \mathbf{e}_z + \text{Buoy}_{\text{Amb}}^{A(s)} + \text{Foot}_{\text{Amb}}^{F(s)};$$

$$d/ds(dE/dt) = \text{Ener}_{\text{Amb}}^{A(s)}; \quad dx/ds = \cos\phi; \quad dz/ds = \sin\phi;$$

together with the algebraic constraints;

"Touchdown" Plume:

$$A = (D^2/4) [\cos^{-1}(-\eta_c) + \sqrt{(1-\eta_c^2)}];$$

$$dm/dt = A\rho u; \quad dm/dt|_{\text{HF}} = A c u;$$

$$dP_z/dt = dm/dt \cdot u \sin\phi;$$

$$dP_x/dt = dm/dt (u \cos\phi - u_\infty);$$

$$dE/dt = dm/dt (h + (1/2)u^2 - h_\infty - (1/2)u_\infty^2);$$

$$\eta_c = \eta/2 \{ 1 + [1 - (2/3)\eta^2(1-\eta^2)\sqrt{(1-\eta^2)}]^{1/2} \};$$

$$\eta = 2z/D / |\cos\phi|; \quad \eta_c = 2z_c/D / |\cos\phi|.$$

[Notation: A cross-section area (circular segment), D circle diameter, x centroid horizontal displacement, z centroid height, z_c centre height; dm/dt released and entrained mass-flux, $(dP_x/dt, dP_z/dt)$ excess (horizontal, vertical) momentum flux, dE/dt excess energy flux, $dm/dt|_{\text{HF}}$ HF mass-flux; u mean flow-speed, ϕ axis inclination, ρ mean plume density, c mean mass-concentration HF, h specific enthalpy; the suffix " ∞ " denotes ambient conditions at the centroid height. (See Figure 5.4)]

"Slumped" Plume:

$$A = (e\pi/8)D^2; \quad e = (3\pi/2)(z/D)/|\cos\phi|;$$

$$dm/dt = A\rho u; \quad dm/dt|_{HF} = A c u;$$

$$dP_z/dt = dm/dt \, u \sin\phi;$$

$$dP_x/dt = dm/dt \, (u \cos\phi - u_\infty);$$

$$dE/dt = dm/dt \, (h + (1/2)u^2 - h_\infty - (1/2)u_\infty^2).$$

[Notation: A cross-section area (semi-ellipse), D ellipse major-axis length, e ellipse eccentricity, x centriod horizontal displacement, z centroid height; dm/dt released and entrained mass-flux, $(dP_x/dt, dP_z/dt)$ excess (horizontal, vertical) momentum flux, dE/dt excess energy flux, $dm/dt|_{HF}$ HF mass-flux; u mean flow-speed, ϕ axis inclination, ρ mean plume density, c mean mass-concentration HF, h specific enthalpy; the suffix " ∞ " denotes ambient conditions at the centroid height. (See Figure 5.5)]

Note that the differential system is modified in that, in addition to any "airborne" drag forces, we have (generally significant) "ground" drag associated with the strong shear layer at the ground-surface following plume touchdown. A further (pressure) force $Foot_{Amb}^{F(s)}$ is exerted at the ground surface as the result either of the destruction of vertical momentum impacting the impermeable ground, or in response to a pressure build-up associated with the limited (gravity-slumping) rate of transverse plume expansion. These additional forces exist following touchdown and in the slumped plume regime. They have the formal definitions:

$$Foot_{Amb}^{F(s)} = (d/ds) \iint_{F(s)} (p - p_\infty) dA;$$

$$\text{Drag}_{\text{Amb}}^{F(s)} = (d/ds) \iint_{F(s)} (\Sigma_{xz} - \Sigma_{xz}^{\infty}) dA;$$

and are replaced in the actual model HFPLUME by intuitively derived functions which reflect known spreading and impact behaviour.

For the circular segment the cross-sectional area A and centroid height z are not explicitly related but coupled via a single non-linear equation for the geometric centre z_c . In the case of the slumped plume both the area A and centroid height z are related to the eccentricity e of the semi-ellipse; however the eccentricity is given explicitly in terms of known parameters z , ϕ , and D .

§5.7: Closure Assumptions for the "Top-Hat" Model: Prescribing the functions Drag, Drag, Buoy, Shear, Foot, and Ener.

In this section are considered the assumptions, arguments, and simplifications that enable closure of the "top-hat" model: We shall ask: "Which expressions and what coefficient values are appropriate for the formulation of impact forces, drag forces, and buoyancy in each of the three plume regions; airborne, touchdown, and slumped plume?".

Atmosphere-Gradient Induced Forces: Plume Buoyancy:

We begin by considering the simplest of these functions, $\text{Shear}_{\text{Amb}}^{A(s)}$, $\text{Ener}_{\text{Amb}}^{A(s)}$, and $\text{Buoy}_{\text{Amb}}^{A(s)}$, and take first of all the buoyancy force $\text{Buoy}_{\text{Amb}}^{A(s)}$. This has the formal definition,

$$\text{Buoy}_{\text{Amb}}^{A(s)} = \iint_{A(s)} (\rho - \rho_{\infty}) g |J| dA;$$

in which the Jacobian determinant has the value

$$|J| = 1 - r \sin\theta \, d\phi/ds, \quad |J| > 0.$$

Assume that the variation in ambient density is modest over the vertical extent of the plume cross-section $A(s)$, so that ρ_∞ may be replaced to fair accuracy by the first order Taylor expansion about the plume centroid at height z ,

$$\rho_\infty(\zeta) \approx \rho_\infty(z) + (d\rho_\infty/dz)|_z(\zeta - z); \quad D^2/8\rho_\infty \sin^2\phi (d^2\rho_\infty/dz^2)|_z \ll 1.$$

Substitution within the formal definition of the buoyancy force then yields for an airborne plume the (exact) result,

$$\text{Buoy}_{\text{Amb}}^{A(s)} = A(\rho - \rho_\infty)g \left[1 + (1/8)(D \cos\phi \, d\phi/ds)(D/(\rho - \rho_\infty))(d\rho_\infty/dz)|_z \right];$$

in which note the term associated with plume curvature $d\phi/ds$. Should the influence of buoyancy be large this curvature correction is certainly small, although the term $D(d\phi/ds)$ is of unit magnitude. Equally, should the effect of buoyancy be weak, the plume curvature, and hence the curvature correction, is again modest. Whatever the importance of buoyancy for plume development, it is well approximated by the simple expression,

$$\text{Buoy}_{\text{Amb}}^{A(s)} = A(\rho - \rho_\infty)g;$$

a result which extends for expansion about the plume **centroid** for both touchdown and slumped plume.

Analyses and order of magnitude arguments yield analogous results for the functions $\text{Shear}_{\text{Amb}}^{\text{A(s)}}$, and $\text{Ener}_{\text{Amb}}^{\text{A(s)}}$. It follows independently of cross-sectional geometry that

$$\text{Shear}_{\text{Amb}}^{\text{A(s)}} = \text{dm/dt} \sin\phi \, du_{\infty}/dz;$$

$$\text{Ener}_{\text{Amb}}^{\text{A(s)}} = \text{dm/dt} \sin\phi \, (d/dz)[h_{\infty} + (1/2)u_{\infty}^2 + gz].$$

These results are deduced under the assumption of the "top-hat" model that there is no variation within the plume cross-section of the plume density, velocity, or specific enthalpy. We judge such differences no greater than the inconsistency between other aspects of model idealisation and reality: we do not, therefore, introduce further empirically adjustable coefficients such as might pre-multiply these function forms.

Airborne Drag:

Consider next the "drag" function associated with an airborne plume in cross-flow. This function represents the force acting upon the plume as the result of pressure forces created by trailing (wake) vortices. The term "drag" is by analogy to the drag force exerted upon a **rigid** body immersed in a uniform stream. There are, however, major differences between the pressure field of a fluid jet and of a (geometrically similar) rigid body. Firstly there is no sharply defined boundary at which the "no slip" condition may be applied. Secondly the external flow, and hence the boundary integral of pressure, may differ substantially between plume and body. The analogy is therefore weak, so that not only the coefficient magnitudes but also the functional form appropriate to a rigid body may be questioned when applied to a plume in cross-flow. The form and

magnitude of this airborne drag force is therefore particularly uncertain. It is found necessary by some (Ooms 1972, Petersen 1978, Schatzmann 1978), but not by others (Hoot, Meroney and Peterka 1973; Hoult, Fay and Forney 1969; Petersen 1987). A recent study (Coelho and Hunt 1989) of the near-field following release orthogonal to a steady flow found no evidence either experimental or theoretical for a significant "drag" force. Plume deflection was satisfactorily explained by air entrainment alone. We assume (tentatively) that

$$\text{Drag}_{\text{Amb}}^{A(s)} = 0.$$

Plume Impact Forces:

Consider next the pressure forces exerted over the plume "footprint" for a touchdown or slumped plume. These forces arise from two distinct physical mechanisms: the destruction of momentum associated with the impact of a dense plume upon the ground surface; and the pressurization associated with the gravity-limited rate of lateral plume spreading.

Take first the case of a plume impacting the ground surface (Refer Figure 5.10). The assumption of an elastic collision applied to the plume as a whole requires that the impact pressure force be at right angles to the momentary orientation of the centroid axis. This ensures conservation of kinetic energy for a system without entrainment or other disturbing influences such as gravity. Focus next upon that proportion of the descending plume impinging upon level ground in time $dt > 0$. If the footprint is of width ℓ then the impinging momentum flux is correspondingly,

$$dP = dA \rho u (\cos\phi, 0, \sin\phi); dA = \ell u |\tan\phi| dt;$$

in which dA is the sectional area "absorbed" into the ground surface. We assume further that the magnitude of the impact force is such as to destroy completely the momentum-flux impinging at any instant upon the ground. The impact pressure force is therefore,

$$\text{Impact}_{\text{Amb}}^{F(s)} = \ell \rho u^2 |\tan\phi| (\sin\phi, 0, -\cos\phi); \sin\phi \geq 0.$$

This formula differs somewhat from that expected from the control-volume analysis, in that both horizontal and vertical momenta undergo continuous change. The pressure force integral implies a change solely in the vertical momentum. Additionally consideration of the destruction of horizontal momentum yields that flows in the negative x-direction are induced for impact angles in excess of 45° . Certainly, for vertical incidence, the spreading pattern is axisymmetric about the point of impact except inasmuch as this is modified by the ambient wind. For steeply descending plumes, therefore, upwind spreading, vortex formation, and flow separation make a simple transition described in terms of a continuous mean-flow at least difficult. However, for shallow incidence, such upwind spreading is typically absent, so that a "top-hat" transition remains entirely feasible. The form of the impact force $\text{Impact}_{\text{Amb}}^{F(s)}$ implies a transition between "steeply descending" and "shallow incidence" plumes at an angle of descent $\phi = 45^\circ$. This is precisely the value observed experimentally by Karman (1986). We restrict attention, therefore, to plume touchdown at angles ϕ less than 45° . Steeply descending plumes will require either empirical matching of airborne and slumped plumes (Karman 1986), or else matching to a "spreading pool" model, possibly analogous to the area source slumping model HEGABOX (Puttock 1988).

In addition, in the absence of air entrainment or drag forces, such as would describe shallow incidence impact of a liquid jet, the above impact force implies that the mean jet/plume speed remains constant throughout the impact process. This is consistent with a direct application of Bernoulli's theorem, gravity and ground drag being negligible, and is consistent with the impact of a liquid jet on a curved vane (Fox 1974). For this case the horizontal impact force evidently arises from pressure components developed along the curved surface of the deflecting vane. For the actual case of ground impact we may "square the above circle" by regarding the jet/plume as existing above a recirculating flow the common interface of which is the analogue of the physical vane. In the immediate vicinity of first ground impact, therefore, the top-hat model represents not the complete flow but only the non-recirculating portion. Plume impact may then be modelled as a simple (elastic) collision.

Gravity-Slumping Pressure Forces:

Consider next the pressure force induced over the plume "footprint" by the interaction of ("top") entrainment and gravity-"slumping". This pressure arises from the fact that entrainment may increase the cross-sectional mass-flux at a rate incompatible with a prescribed gravity-spreading unless the centre of mass is also raised. Such a raising of the centre of mass against gravity can be accomplished only by means of a pressure force acting over the plume footprint. The absolute magnitude of this pressure is small; its integrated effect significant. Let us begin (refer Figure 5.11) with the gravity-spreading relation (van Ulden 1983, Raj and Morris 1987) for a rectangular, "slumped" jet;

$$(1/2)dD/ds = (k/u)\sqrt{[gh(1-\rho_{\infty}/\rho)]}.$$

[Notation: h plume height, D plume width, g acceleration due to gravity, (ρ, u) mean density and flow-speed, ρ_∞ ambient density, k (0.85-1.20) empirical coefficient, s centre-line displacement.]

We seek a formulation for the vertical momentum equation such that this gravity-slumping behaviour is asymptotically recovered for dense, advected plumes. For such a plume the spatial rate of change of vertical momentum is undoubtedly small, that is the sum of vertical forces is approximately zero. We interpret Raj's formula for gravity spreading as a statement of the approximate balance of a buoyancy force, and the reactive pressure force driven by the interaction of slumping and entrainment. Given, therefore, that the buoyancy force has the form,

$$\text{Buoy}_{\text{Amb}}^{\text{A}(s)} = hDg(\rho - \rho_\infty);$$

we propose a reactive pressure force,

$$\text{Foot}_{\text{Amb}}^{\text{F}(s)} = (1/k^2)D\rho u^2((1/2)dD/ds)^2;$$

proportional to the local footprint width, and to the square of the lateral spreading velocity. In the case of a semi-elliptic cross-section we must reinterpret the lateral spreading velocity, and effective plume height h in terms of the plume width D and centroid height z . The height h is for a rectangular section exactly twice the centroid height which allows the identification $h = 2z$. Additionally the rectangular section has area hD equal to that of a semi-ellipse $(3\pi^2/16)zD$ of centroid z and footprint width D . This results in the final expression, modified for the semi-elliptic geometry,

$$Foot_{Amb}^{F(s)} = (3\pi^2/32)^3 (1/k^2) \ell_{pu}^2 ((1/2) dD/ds)^2, \quad k = 1.15.$$

We follow van Ulden (1983), rather than Raj and Morris (1988) in the choice of the gravity-spreading coefficient. Further work is, however, necessary in order optimally to determine the coefficient value for a semi-elliptic, slumped plume.

This revised formulation will evidently reproduce the gravity spreading behaviour "hard-wired" by Raj and Morris (1988). It is, moreover, physically meaningful for an asymptotically neutral or buoyant plume/jet for which significant departures from gravity-spreading must be expected. In particular the original spreading formula is not defined for a buoyant plume. Initially dense, subsequently buoyant, plumes occur frequently for the release of pressurized liquid HF to ambient atmospheres of moderate humidity (>50%) and temperature (perhaps 20C).

Gravity Current Collapse:

Gravity spreading as formulated by (inter alia) van Ulden (1983) and Puttock (1988) assumes the existence of a (relatively) sharp interface between plume and undisturbed air. Recent experiments by Linden and Simpson (1988) indicate that the leading vortex of such a gravity current is not unconditionally stable but may be disrupted by locally enhanced turbulence. Following gravity current collapse the cloud edge is more diffuse; lateral spreading much reduced.

Study (Chapter 8) of the HTAG ("Heavier than Air Gas") data set (Petersen and Ratcliff 1989), reveals evidence for the existence of such gravity current collapse for uniform ambient turbulence and increasingly weak gravity-head. We propose (Chapter 8) a collapse criterion and post-collapse spreading rate (essentially) as follows:

Ground-surface Drag:

Finally we consider the drag force exerted at the ground surface by an impacting or slumped plume. This force has the formal definition,

$$\text{Drag}_{\text{Amb}}^{F(s)} = (d/ds) \iint_{F(s)} (\Sigma_{xz} - \Sigma_{xz}^{\infty}) dA;$$

and results from differences in the mean horizontal and undisturbed wind speeds in the neighbourhood of the ground surface. The surface stress associated with the wind profile is $\rho_{\infty} u_*^2$, in which u_* is the friction velocity. Equivalently Σ_{xz}^{∞} is proportional to the square of the velocity gradient du_{∞}/dz at the roughness height $z_r > 0$. Profile information regarding the vertical variation in flow-speed within the impacting or slumped plume is therefore necessary in order to estimate the drag force. For an assumed neutrally buoyant plume and a logarithmic velocity profile the friction velocity associated with a plume of velocity $u \cos \phi$ at centroid height z is u/u_{∞} times that of the unperturbed wind. This suggests (for a neutral plume) the drag function

$$\text{Drag}_{\text{Amb}}^{F(s)} = \ell \rho_{\infty} u_*^2 [(u/u_{\infty}) \cos \phi - 1][(u/u_{\infty}) \cos \phi + 1], \quad u_{\infty} > 0,$$

in which ℓ is the footprint width.

For high speed flows we expect the (established) shear profile within a dense gas plume to be governed by surface roughness analogously to that in a neutral boundary layer. The surface stress is simply ρu_*^2 , in which u_* is set by the known (mean) jet velocity at the centroid height. Substitution then yields the drag function in the presence of dense gas effects,

$$\text{Drag}_{\text{Amb}}^{F(s)} = \ell \rho_{\infty} u_*^2 [\sqrt{(\rho/\rho_{\infty})(u/u_{\infty})\cos\phi - 1}] [\sqrt{(\rho/\rho_{\infty})(u/u_{\infty})\cos\phi + 1}].$$

Density stratification damps turbulence and affects both friction velocity and plume drag. The drag force might be presumed proportional to some power of the Richardson number correction $\Phi(Ri_*)$ proposed by Witlox (1988) in the context of heavy-gas entrainment. Now the suppression of entrainment at a dense gas interface is largely due to gravity-driven "recapture" of disturbed dense gas rather than to a lowering of turbulent energies within the system as a whole. This suggests that the influence of density stratification upon ground drag is rather small. We presume the effect negligible.

§5.8: The Entrainment Function: Forms appropriate to airborne, touchdown, and slumped Plumes: jet, cross-flow, passive, gravity spreading, and heavy gas formulae and their interactions.

We consider in this section the form of the entrainment function appropriate to each of the plume regions; airborne, touchdown, and slumped plume. The entrainment function is taken (barring interactions) to be the sum of contributions arising from different physical mechanisms; jet entrainment, cross-wind entrainment, gravity-slumping entrainment, and airborne or heavy-gas passive entrainment. These mechanisms are present to varying degree in each of the plume regions.

Jet Entrainment:

For the discharge of (neutrally buoyant) gas jets to quiescent or coflowing ambient the form and magnitude of the entrainment function is well established

(Briggs 1984; Morton, Taylor and Turner 1956). It assumes for the "top-hat" formulation the symbolic form,

$$\text{Entr}_{\text{jet}} = e_{\text{jet}} \pi D \rho_{\infty} |u - u_{\infty}|, \quad e_{\text{jet}} = 0.08.$$

This form (or related variants) has been found satisfactory in addition for the early release of two-phase propane jets (McFarlane 1988, Cowley and Tam 1988), and for ammonia releases (Wheatley 1987a, 1987b). For dense two-phase jets in cross-flow, we propose the correlation,

$$\begin{aligned} \text{Entr}_{\text{jet}} &= e_{\text{jet}} \eta(\rho/\rho_{\infty}) L_{\text{surface}}^{\text{free}} \rho_{\infty} |u - u_{\infty} \cos \phi|, \\ \eta(\rho/\rho_{\infty}) &= [1 + (4/3)(\rho/\rho_{\infty} - 1)] / [1 + (5/3)(\rho/\rho_{\infty} - 1)]. \end{aligned}$$

Jet entrainment is thus proportional to the absolute difference between the jet speed and the aligned component of the ambient wind. Entrainment takes place over that part of the plume perimeter exposed to the ambient air. The form, excepting the small density correction, has been found satisfactory by several authors (Petersen 1978; Ooms 1972; Hoot, Meroney and Peterka 1973) in combination with various cross-wind formulations for the description of buoyant and dense gas plumes released orthogonal to an imposed wind. It, other than the densimetric correction, is used by Raj and Morris (1987) for their gravity-slumping jet. It is closely analogous (asymptotically equivalent) to a "shear" entrainment formulation based upon Prandtl closure of the turbulent kinetic equation proposed by McFarlane (1988). This formulation showed good agreement with large scale experimental data gathered by Cowley and Tam (1988). This analysis and experimental comparison are set out fully in Appendix 1. It seems uncontroversial to adopt this entrainment formulation to represent "jet" entrainment in each of the three plume regions.

Cross-wind Entrainment:

Crosswind entrainment is associated with the formation in the wake of a rising or falling plume of trailing vortices in response to the deflection by the release plume of ambient air. This mechanism is absent for release to a quiescent atmosphere, or for a wind aligned release, and is (we presume) maximum for releases at right angles to the ambient wind. This suggests immediately the functional form,

$$\text{Entr}_{\text{wind}}^{\text{cross}} = e_{\text{wind}}^{\text{cross}} L_{\text{surface}}^{\text{free}} \rho_{\infty} u_{\infty} |\sin\phi|,$$

(Morton, Taylor and Turner 1956; Hoot, Meroney and Peterka 1973; Hoult, Fay and Forney 1969). By contrast Ooms (1972), and later Petersen (1978,1987) have found good agreement for Gaussian models with the modified form

$$\text{Entr}_{\text{wind}}^{\text{cross}} = e_{\text{wind}}^{\text{cross}} L_{\text{surface}}^{\text{free}} \rho_{\infty} u_{\infty} |\cos\phi \sin\phi|,$$

when used in conjunction with non-zero airborne drag correlation

$$\text{Drag}_{\text{Amb}}^{\text{A(s)}} = e_{\text{Amb}}^{\text{drag-cross}} L_{\text{wind}}^{\text{cross}} \rho_{\infty} u_{\infty}^2 \sin^2\phi (\sin\phi, 0, -\cos\phi).$$

This formulation is reported by Li, Leijdens and Ooms (1986), and by Havens (1988) to be a successful predictor not only of buoyant and neutral plumes, but of dense emissions as well. Several other formulations have been tried (Schatzmann 1979, Spillane 1983, Frick 1984) and are reported as satisfactory in predicting plume rise and lateral spread (Schatzmann and Policastro 1984a, 1984b).

We have encoded various cross-wind entrainment terms within the (ideal-gas) plume model PLUME, and find, following Briggs (1984), that the cases of neutral and buoyant plume rise are adequately represented by the $|\sin\phi|$ correlation and a coefficient value e_{wind}^{cross} of 0.60. By contrast the dense plume data-base of Hoot, Meroney and Peterka is incompatible with **any** uniform choice for the crosswind entrainment coefficient.

Except in the immediate vicinity of the source, plume development is well represented by the Boussinesq approximation (Schatzmann and Policastro 1984b). It follows that rising dense plumes, and descending buoyant plumes should exhibit essentially the same behaviour in response to an imposed cross-wind. This suggests strongly that the same functional form be chosen to represent both dense and buoyant plumes, and that in the limit of great dilution the simple $|\sin\phi|$ dependence be recovered. We find that cross-wind entrainment is weakened by high exit velocities and for rising dense plumes by density excess. Analysis of buoyant (Petersen 1978), and dense (Hoot, Meroney and Peterka 1973) gas-plume data suggests the functional form

$$\begin{aligned} \text{Entr}_{wind}^{cross} &= u_{wind}^{cross} \eta(\rho/\rho_{\infty}, \phi) L_{surface}^{free} \rho_{\infty} u_{\infty} \sqrt{(u_{\infty}/u)} |\sin\phi|, \\ \eta(\rho/\rho_{\infty}, \phi) &= [1 + e_{wind}^{cross} \max(0, (\rho/\rho_{\infty} - 1) \sin\phi)], \\ u_{wind}^{cross} &= 0.60, \quad \rho_{wind}^{cross} = 7.50. \end{aligned}$$

The coefficient ρ_{wind}^{cross} is matched to dense gas maximum rise-height, and the release velocity correction is suggested by an analysis of (early) buoyant plume rise. This expression, when used in conjunction with the above jet entrainment, is a satisfactory predictor of buoyant (Petersen 1978), and of dense plume-rise (both maximum rise-height and its downwind displacement). Plume "touchdown" is also satisfactory, though the validation is complicated by differences between the plume width of a "top-hat" model, and the "visible edge" data presented by

Hoot, Meroney and Peterka (1973). The model adequately reproduces the downward releases of buoyant gas conducted by Li, Leijdens and Ooms (1986), and is of comparable accuracy to the truncated Gaussian model of Ooms and Duijm (1984), and to the similar model proposed by Havens (1988) after Morrow and coworkers (1982).

It should be emphasised that this entrainment term is **empirical**. It is a satisfactory predictor of both dense and buoyant plumes released orthogonal to a laminar cross-wind. Nonetheless it is rather likely that an improved correlation can be developed should plume centre-line touchdown data become available.

Gravity Slumping Entrainment:

By "gravity-slumping" entrainment we intend the absorption of ambient air within a "slumped" plume as the result of lateral expansion in response to density differences between (dense) plume and ambient. This phenomenon was studied by van Ulden (1974) in the context of the initial development of a cylindrical (area) source of dense gas. Van Ulden (1974) proposed the entrainment relation,

$$\text{Entr}_{\text{slump}}^{\text{grav}} = (1/2)e_{\text{slump}}^{\text{grav}}\pi D\rho_{\infty}h(dD/dt), \quad e_{\text{slump}}^{\text{grav}} = 0.05.$$

[Notation: h plume height, D plume diameter, dD/dt slumping rate.]

Entrainment is proportional to the spreading velocity $((1/2)dD/dt)$, to the ambient density (ρ_{∞}) , and to the area (πhD) of the plume "edge". Almost all of the adjacent air is, for such cylindrical slumping, displaced by rather than entrained within the expanding cloud "edge". The analogue of van Ulden's entrainment relation for the (steady) state geometry of the slumped plume is simply,

$$\text{Entr}_{\text{slump}}^{\text{grav}} = e_{\text{slump}}^{\text{grav}} \rho_{\infty} z_u |\cos \phi| (dD/ds),$$

in which we have assumed an equivalent cloud height which is twice that of the plume centroid. We have (provisionally) adopted this formula for the slumped plume.

More recently Puttock (1988), in the computer model HEGABOX, proposed an entrainment coefficient $e_{\text{slump}}^{\text{grav}} = 0.85$, this in accordance with observations on cylindrical collapse conducted at Thorney Island (McQuaid 1984). The coefficient value, $e_{\text{slump}}^{\text{grav}} = 0.85$, may reflect a contribution to entrainment associated with turbulence generated in the cylindrical collapse, turbulence which must decay as the plume is advected downwind. This suggests that the entrainment coefficient $e_{\text{slump}}^{\text{grav}}$ appropriate to a semi-elliptic plume may have a value considerably less than 0.85. Alternatively some dependence of $e_{\text{slump}}^{\text{grav}}$ upon such flow parameters as the local (bulk) Richardson number or upon the local versus initial spreading-rate (Eidsvik 1978) might be investigated.

Conventionally (Ooms 1972, Petersen 1987, Schatzmann 1978, Briggs 1984) such lateral entrainment is absent from the airborne plume: indeed its inclusion results for the approximate equations of motion in an **exponential** growth in plume width. The touchdown plume is physically and geometrically intermediate between airborne and slumped plume. In this region forces are first developed whose interaction with buoyancy results in the subsequent (slumped plume) gravity current. Plausibly gravity current entrainment is weak in this intermediate zone. Certainly this is consistent with the observations of Puttock (1988) who found it necessary to "switch off" gravity-current entrainment for an interval following initial (cylindrical source) release. This delay is required for the formation of a vortex system at the cloud leading "edge". For the touchdown plume, therefore, we propose the interpolated form,

$$\text{Entr}_{\text{slump}}^{\text{grav}} = [1 - 2z_c/D/|\cos\phi|] e_{\text{slump}}^{\text{grav}} \rho_{\infty} z u |\cos\phi| (dD/ds),$$

in which z_c and D denote centre and diameter of the circular segment cross-section. This formulation is of necessity preliminary, and may require modification or "tuning" in the light of subsequent validation or analysis.

Slumped Plume: Heavy Gas Entrainment:

The dilution of a "severely slumped plume" is dominated by "top" entrainment of ambient air in response to ambient turbulence when modified by density stratification. The circumstances of such "severely slumped" plumes are precisely those for which the heavy-gas advection model HEGADAS (Appendix 3, Colenbrander 1980, Colenbrander and Puttock 1988) was designed. As the model HFPLUME is required to merge smoothly with the far-field HEGADAS, it is appropriate to take the "top" entrainment formulation used by the latter, modified to allow for the different cross-sectional geometries. We are led immediately to the entrainment relation,

$$\text{Entr}_{\text{gas}}^{\text{heavy}} = [\Phi(Ri_*)]^{-1} L_{\text{surface}}^{\text{free}} \kappa \rho_{\infty} u_*;$$

$$\begin{aligned} \Phi(Ri_*) = & \begin{cases} 1/\sqrt{(1-3Ri_*/5)} & , Ri_* < 0, \\ 1 & , 0 \leq Ri_* < 189/80, \\ (10/17)\max(Ri_*/7, \sqrt{(1+4Ri_*/5)}) & , Ri_* \geq 189/80, \end{cases} \\ & \text{with } Ri_* = 2gz(\rho/\rho_{\infty}-1)/u_*^2, \end{aligned}$$

The Richardson number correction to the turbulent entrainment is a modification to the HEGADAS formulation suggested by Witlox (1988) following a critical analysis of McQuaid's (1976) wind-tunnel data.

Airborne Plume: Passive Entrainment:

In addition to "jet" and "crosswind" mechanisms, entrainment within the airborne plume is influenced by the state of ambient turbulence. Asymptotically it is this mechanism which is predominant, and which results in the far field in the Pasquill/Gifford correlations for the Gaussian standard deviations (Plate 1982; Stern, Boubel, Turner and Fox 1984) $\sigma_y(x,z)$, and $\sigma_z(x,z)$ as functions of the distance x downwind of release and (Pasquill 1976) of the (effective) plume height z . Additionally the ambient turbulence in the surface layer (Plate 1982; Stern, Boubel, Turner and Fox 1984) is governed (at any rate approximately) by Monin-Obukhov similarity theory, so that the entrainment function should be expressible in terms of the surface roughness, Monin-Obukhov length, and the plume centroid height above the ground surface.

Three approaches seem possible in formulating the passive entrainment function for the airborne plume. First we may attempt direct "matching" from a plume-rise model in which passive entrainment is neglected to a Gaussian Pasquill/Gifford model for the far-field. Conservation of the fluxes of entrained mass, pollutant mass, horizontal momentum excess, prescribe the location of a virtual point source needed by the Gaussian model. This approach has clear computational advantages: it removes the need for the "step by step" downwind integration of a set of ordinary differential equations describing plume motion. It takes advantage of well established empirical correlations for the far-field.

Notwithstanding, we may attempt to introduce within the range of plume rise and fall an approximate passive entrainment function, the effect of which will be to correct somewhat the predictions made in the absence of turbulent diffusion. The range of application will be such that the passive entrainment term is at most of co-magnitude with contributions from "jet" and from "crosswind". Reference

to the literature reveals essentially two procedures for the determination of the passive entrainment function; procedures based upon "matching" to the Pasquill/Gifford correlations (Bloom 1980), and methods based upon an analysis of Monin-Obukhov similarity (Ooms 1972). Of these methods the former class may be criticised in that they rely on function forms constructed from far-field data, yet they are used in the near field when effects of buoyancy and release momentum are yet significant. We prefer the latter class, and in particular propose a (previously unpublished) formulation developed by Disselhorst (1987). The procedure, supporting analysis, and experimental basis, are reproduced in Appendix 2; only the principal results are presented here:

$$\text{Entr}_{\text{turb}}^{\text{amb}} = (1-\ell/D) \pi e_{\text{amb}}^{\text{turb}} \rho_{\infty} \varepsilon^{(1/3)} [\ell_y^{(4/3)} + \ell_z^{(4/3)}];$$

$$\begin{aligned} \ell_y = & \begin{cases} \min[D/2, 0.88(z+z_r)(1-7.4\kappa\zeta)/(1-5\kappa\zeta)], & \text{P/G= \{"A", "B", "C"\}}, \\ \min[D/2, 0.88(z+z_r)] & , \text{P/G= \{"D"\}}, \\ \min[D/2, 0.88(z+z_r)/(1+0.1\zeta)] & , \text{P/G= \{"E", "F"\}}, \end{cases} \end{aligned}$$

$$\begin{aligned} \ell_z = & \begin{cases} \min[D/2, 0.88(z+z_r)(1-7.4\kappa\zeta)/(1-5\kappa\zeta)], & \text{P/G= \{"A", "B", "C"\}}, \\ \min[D/2, 0.88(z+z_r)] & , \text{P/G= \{"D"\}}, \\ \min[D/2, 0.88(z+z_r)/(1+4\zeta)], & , \text{P/G= \{"E", "F"\}}, \end{cases} \end{aligned}$$

$$\begin{aligned} \varepsilon = & \begin{cases} (1-5\kappa\zeta)u_*^3/\kappa/(z+z_r) & , \text{P/G= \{"A", "B", "C"\}}, \\ u_*^3/\kappa/(z+z_r) & , \text{P/G= \{"D"\}}, \\ (1+4\kappa)u_*^3/\kappa/(z+z_r) & , \text{P/G= \{"E", "F"\}}, \end{cases} \end{aligned}$$

$$e_{\text{amb}}^{\text{turb}} = 1.0, \quad \zeta = (z+z_r)/L, \quad L = u_*^3/\kappa/(g/T_g)/(u_*T_g).$$

[Notation: z_r surface roughness, L Monin/Obukhov length, u_* friction velocity, κ von Karman's constant, T_g ground (absolute) temperature, $u_* T_*$ surface/air heat-flux, ε dissipation rate of turbulent kinetic energy, (ℓ_y, ℓ_z) turbulent (transverse horizontal, vertical) eddy length-scales; ℓ plume "base"-length, D plume "diameter", z centroid height; P/G Pasquill/Gifford class.]

This formulation differs from that proposed by Disselhorst in three ways. First the cross-section of an airborne plume is circular and not elliptic: nonetheless the different horizontal and vertical length scales within the atmosphere are represented. Second the atmospheric boundary layer is presumed effectively infinite: this should prove unproblematical for near ground releases of dense gas. Third the entrainment term is in the touchdown region given a linear scaling in $1-\ell/D$ in order to vanish identically at (and beyond) the point of first plume slumping.

Interactions:

Heavy-gas and jet entrainment are **not** independent mechanisms; each modifies the level of turbulence by inducing vertical gradients of velocity. These velocity gradients are (in general) antagonistic; the presence of dense gas requires a positive, of a (strong) jet a negative, gradient at the cloud surface. We take the combined effect of jet and heavy-gas entrainment as the greater of the two contributions when acting in isolation. Further, pursuing the analogy with HEGADAS, we regard the heavy-gas entrainment as taking place across the plume "top", with jet entrainment acting over both "top" and "side". This maximum entrainment is (for reasons of continuity) partitioned amongst heavy-gas and jet

mechanisms in the same proportion as would have arisen from the addition of the contributions Entr_{jet} and $\text{Entr}_{\text{gas}}^{\text{heavy}}$:

$$\text{Entr}_{\text{gas}}^{\text{jet}} = (\ell/L_{\text{surface}}^{\text{free}}) \max(\text{Entr}_{\text{jet}}, \text{Entr}_{\text{gas}}^{\text{heavy}}) + (1 - \ell/L_{\text{surface}}^{\text{free}}) \text{Entr}_{\text{jet}};$$

$$\text{jet} \text{Entr}_{\text{gas}}^{\text{jet}} = [\text{Entr}_{\text{jet}} / (\text{Entr}_{\text{jet}} + \text{Entr}_{\text{gas}}^{\text{heavy}})] \text{Entr}_{\text{gas}}^{\text{jet}};$$

$$\text{heavy} \text{Entr}_{\text{gas}}^{\text{jet}} = [\text{Entr}_{\text{gas}}^{\text{heavy}} / (\text{Entr}_{\text{jet}} + \text{Entr}_{\text{gas}}^{\text{heavy}})] \text{Entr}_{\text{gas}}^{\text{jet}}.$$

The concepts of "top" and "side" require elucidation: we take the "top" to have a length equal to the length ℓ of intersection between cross-section and level ground; the "side" we identify with the balance $L_{\text{surface}}^{\text{free}} - \ell > 0$ of the "free surface" or perimetric length.

The interaction between passive and gravity-slumping entrainment is treated similarly; interaction arises inasmuch as the contribution of passive entrainment induces lateral expansion which itself induces entrainment represented by gravity slumping. Such "feedback" of entrainment is clearly aphysical, and results, for an "airborne" plume, in the exponential increase of plume diameter and dilution. The assumptions are summarised below:

$$\text{Entr}_{\text{grav slump}}^{\text{pass}} = \max(\text{Entr}_{\text{pass}}, \text{Entr}_{\text{slump}}^{\text{grav}});$$

$$\text{pass} \text{Entr}_{\text{grav slump}}^{\text{pass}} = [\text{Entr}_{\text{pass}} / (\text{Entr}_{\text{pass}} + \text{Entr}_{\text{slump}}^{\text{grav}})] \text{Entr}_{\text{grav slump}}^{\text{pass}};$$

$$\text{grav slump} \text{Entr}_{\text{grav slump}}^{\text{pass}} = [\text{Entr}_{\text{slump}}^{\text{grav}} / (\text{Entr}_{\text{pass}} + \text{Entr}_{\text{slump}}^{\text{grav}})] \text{Entr}_{\text{grav slump}}^{\text{pass}}.$$

§5.9: The atmosphere model: relationship to Pasquill/Gifford stability Classes.

The atmosphere is described by a set of temperature, pressure, and wind-speed profiles, each independent of the downwind distance. The pressure gradient is assumed hydrostatic, and is represented by the "lapse rate"

$$dP_{\infty}/dz = -\rho_{\infty}g,$$

the absolute pressure being given at the release height.

The wind-speed profiles have, on the basis of Monin-Obukhov similarity theory (Plate 1982, Wieringa 1980), the standard form

$$[\kappa(z+z_r)/u_*] du_{\infty}/dz = \psi_u(\zeta);$$

$$\psi_u(\zeta) = (1-22\zeta)^{-1/4}, \quad \zeta < 0,$$

$$\psi_u(\zeta) = 1+6.9\zeta, \quad \zeta \geq 0,$$

$$\zeta = (z+z_r)/L, \quad L = u_*^3/\kappa/(g/T_g)/(u_*T_*).$$

L , which is formally infinite for a neutral atmosphere, is the Monin-Obukhov length; T_g the air temperature at the roughness height $z_r > 0$; and u_*T_* the ground to air heat-flux. These forms may be explicitly integrated (Raj and Morris 1987) to yield a standard set of velocity profiles determined by Monin-Obukhov length, surface roughness, and reference wind-speed at a user-specified reference height.

The temperature profile is conventionally expressed as a gradient of "potential" temperature, that is the difference between an adiabatic lapse rate and that observed (correlated) for a given surface roughness and Monin-Obukhov length. This distinction is in practice negligible, the dry adiabatic lapse rate being typically $-9.7^\circ\text{C}/\text{km}$. Reference to standard literature correlations (Plate 1982, Wieringa 1980) yields the forms,

$$[\kappa(z+z_r)/T_*]dT_{\infty}^{\text{pot}}/dz = \psi_T(\zeta);$$

$$\psi_T(\zeta) = 1/\sqrt{1-13\zeta}, \quad \zeta < 0,$$

$$\psi_T(\zeta) = 1+9.2\zeta, \quad \zeta \geq 0.$$

$$\zeta = (z+z_r)/L, \quad L = u_*^3/\kappa/(g/T_g)/(u_*T_*).$$

These differential forms may be explicitly integrated (Raj and Morris 1987)

to yield a complete temperature profile $T_{\infty}(z)$ as a function of Monin-Obukhov length, surface roughness, and a single reference temperature at known height.

It remains to determine the Monin-Obukhov length L based on the Pasquill/Gifford (P/G) stability classes (Plate 1982; Stern, Boubel, Turner and Fox 1984) and surface roughness z_r . The correlation used in HFPLUME is that of Colenbrander (1985), after Irwin (1979), and has the range of validity $1\text{mm} \leq z_r \leq 2\text{m}$:

$$\begin{aligned} L(z_r, P/G) = & \begin{cases} -10.99z_r^{0.0993}, & P/G = \text{"A"}, \\ -13.44z_r^{0.1631}, & P/G = \text{"B"}, \\ -113.5z_r^{0.2946}, & P/G = \text{"C"}, \\ \infty, & P/G = \text{"D"}, \\ 125z_r^{0.3090}, & P/G = \text{"E"}, \\ 26.12z_r^{0.1667}, & P/G = \text{"F"} \end{cases} \end{aligned}$$

In the computer model HFPLUME the above differential equations for the vertical gradients of wind-speed, pressure, and absolute temperature are solved simultaneously with those of the integral-averaged plume/jet model in the modified form

$$dT_{\infty}/ds = \sin\phi \, dT_{\infty}/dz, \quad dP_{\infty}/ds = \sin\phi \, dP_{\infty}/dz, \quad du_{\infty}/ds = \sin\phi \, du_{\infty}/dz,$$

thermal equilibrium being assumed throughout the atmosphere volume.

§5.10: Plume cross-sectional over-lap: curvature limited entrainment, associated model limitations.

The coordinate system used in formulating the "top-hat" model of plume development determines and is determined by the physical interaction of release HF-jet and the ambient wind. The coordinate system is not universal but exists only within a limited distance from the plume axis. Circumstances may arise in which plume curvature, whether in response to strong cross-winds, or to ground impact, results in the predicted "over-lap" of successive plume cross-sections. Such behaviour is certainly rare for gas (including heavy gas) releases, and is largely absent from the wind-tunnel datasets of Hoot, Meroney and Peterka (1973) (dense gases), and of Petersen (1978) (buoyant plumes). Nevertheless, in view of the higher density and lower velocity to be expected in the near-field following release of pressurized liquid HF, it seemed expedient to include provision for such plume "overlap" within the computer algorithm HFPLUME.

This section outlines the method employed by HFPLUME in treating such behaviour: the method adopted is **not** universally effective, but is successful in the clear majority of cases.

We begin by analysing the conditions under which plume overlap occurs in each of the three regions; airborne, touchdown, and slumped plume. Incipient overlap is defined by a geometrical relation in which a representative plume "width" is compared with the axis curvature $d\phi/ds$. The results are as follows:

Airborne Plume:

$$D/2|d\phi/ds| = 1,$$

Touchdown Plume:

$$\begin{aligned} -z/|\cos\phi|d\phi/ds &= 1, \quad d\phi/ds < 0, \\ [D/2 - (z - z_c)/|\cos\phi|]d\phi/ds &= 1, \quad d\phi/ds > 0, \end{aligned}$$

Slumped Plume:

$$\begin{aligned} -z/|\cos\phi|d\phi/ds &= 1, \quad d\phi/ds < 0, \\ [\max(1, e)D/2 - z/|\cos\phi|]d\phi/ds &= 1, \quad d\phi/ds > 0, \\ e &= (3\pi/2)(z/D)/|\cos\phi|. \end{aligned}$$

[Notation: D plume (effective) "diameter", z centroid height, e eccentricity (semi-ellipse), z_c centre height (circular segment), ϕ axis-inclination, s centre-line displacement, $d\phi/ds$ centre-line curvature.]

These conditions define the limits imposed by cross-section geometry upon the interaction of HF-source and ambient atmosphere implied by the conservation laws, and by the (empirically determined) entrainment function. Should these limits be exceeded we are faced with two alternatives: alter the geometry of the cross-section, or modify the entrainment function itself.

Modification of the sectional geometry is the more complex option: we must **simultaneously** satisfy the original entrainment equation and a consistency relation requiring that plume "overlap", while incipient, does not actually occur within the zone of high axis-curvature. Introduction of variable geometry (within the three plume regions already recognized) substantially increases the number and complexity of geometrical transitions that must be represented within a computer based model. Such high curvature regions are, in any case, quite rare,

or have quite limited geometrical extent, so that the need for such an increase in complexity did not seem, a priori, justified.

As an alternative to the modification of plume geometry, we may alter the entrainment function in regions of high curvature so as to prevent the occurrence of plume overlap. Concretely we replace the entrainment relation, $d/ds(dm/dt) = \text{Entr}$, by whichever of the geometrical constraints for incipient plume overlap is appropriate for the present cross-sectional shape. This revised equation system is of necessity geometrically consistent, and may be matched by continuity arguments to the previously existing plume structure. In addition the entrainment rate implied by the geometrical constraint may be calculated as the derivative $d/ds(dm/dt)$. This parameter is then compared with the entrainment rate that would have occurred for the same plume description in terms of sectional mean velocity, density, and the like, from the empirically determined entrainment function Entr . The model reverts to this usual description, should the "curvature limited" entrainment exceed that calculated from the empirical entrainment function. This procedure introduces a minimal change into the basic model consistent with the existence of "curvature limited" behaviour. The procedure rests upon the idea that excessive plume curvature is the result of too rapid air entrainment, and that the reduction of air entrainment to the maximum value compatible with plume geometry will permit integration to continue through the high curvature zone and to recover the basic model at some greater downwind displacement.

The success of this device of "curvature limited" entrainment rests on the ability of the curvature limited model to recover normal entrainment rates. However it may occur that the corollary entrainment rate $d/ds(dm/dt)$ inferred from a curvature limited model actually decreases **more rapidly** than does the associated empirically determined entrainment rate (Entr) for the **same** plume description.

Should this occur termination of the curvature limited zone will occur following detection of the aphysical entrainment step $d/ds(dm/dt) \leq 0$. The computer program HFPLUME terminates with a diagnostic error message.

§5.11: The computer model HFPLUME: algorithmic structure.

This section presents a overview of the computer program HFPLUME. HFPLUME is written entirely in FORTRAN 77. Systems programs, input, output, and diagnostics files are as illustrated in the User Manual.

The model comprises three development regions; the airborne, touchdown, and slumped plume. Each region is represented by a set of 9 (non-linear) algebraic equations and 7 (ordinary) differential equations in the 16 state variables

$$X = (T, y_{HF}, x_1^{HF}, x_{HF}, u, \phi, D, x, z; T_\infty, P_\infty, u_\infty; dm/dt, dP_x/dt, dP_z/dt, dE/dt).$$

These variables describe the plume thermodynamic state, the plume dimensions, centre-line location, and inclination to the horizontal, and the atmosphere state and wind speed at the centroid height z . The equations form a differential/algebraic system whose solution optimally requires a general purpose differential/algebraic solver, developed by numerical analysis specialists, and incorporating automatic ODE "step" determination in the light of prescribed local tolerances.

SPRINT (Software for PRoblems IN Time) is such a solver: it was developed by Shell Research and by Leeds university (Berzins, Dew, and Furzeland 1983; Berzins and Furzeland 1985). SPRINT is effective for the solution of the differential/algebraic system in each plume region. It employs, for the solution of the algebraic constraints, a technique which is efficient for starting values

near to the solution (values as are typically found for successive ODE steps). It may, however, prove inadequate for the determination of the "initial conditions" needed at the release orifice, post flash, at touchdown, or at first plume slumping. Initial values are needed not only for the state vector X , but also and equally importantly, for the 16 first derivatives dX/ds . These derivatives are typically discontinuous at the several model region boundaries, boundaries at which the assumed geometrical shape or phase composition of the developing plume change abruptly.

This difficulty with initial conditions is well known (Berzins, Furzeland and Scales 1988) and (here) thought to reflect the severe non-linearity introduced by the complex thermodynamic interaction of HF and moist air. The "starting" problem, and in particular the calculation of initial derivative values "immediately post transition" may be formulated as a non-linear algebraic problem for which we may employ a "state of the art" non-linear equation solver. Such a solver, NAESOL (Non-lineAr Equation SOLver), has recently been developed at Thornton Research Centre (Scales 1988, 1989). This solver, which incorporates advanced search strategies, and provision for the solution of ill-conditioned or locally singular problems, typically succeeds where SPRINT would fail.

§5.12: Validation studies, entrainment formulae.

Several components of the model encoded as HFPLUME have been subject to independent experimental test. This section summaries the results of these validation studies, noting successes and limitations. Suggestions are made for further work in this area. The model HFPLUME has **not** been tailored to data arising from the Goldfish experiments (Blewitt, Yohn, Koopman and Brown 1987; Blewitt, Yohn and Ermak 1987; Blewitt 1988). or other prototypical data: it has rather

been **assembled** of separately validated models for plume entrainment and thermodynamics. Its success (Chapter 9), when coupled with HEGADAS, in predicting the Goldfish experiments should be viewed in that light.

Jet release: thermal equilibrium:

Initial flow from pressurized liquid HF storage is liquid or two-phase, so that the possibility exists for such phenomena as liquid drop-out and liquid jet break-up (McCarthy and Molloy 1973), rather than prompt atomisation, intimate HF/air mixing, and the rapid formation of a homogeneous equilibrium mixture without interphase "slip". Interest in this initial flow in the context of HF releases focuses upon the possibility of liquid drop-out resulting in evaporating pool formation, and in the influence of early evaporative process on later plume development, especially air entrainment and HF concentration.

We have compared the predictions of an analogous jet model WETJET (Appendix 1, McFarlane 1988) with large scale experimental releases of liquified propane gas. These experiments were conducted jointly by Shell Research Limited and BP International Research Limited at the (former) BP refinery site on the Isle of Grain. We consider a subset (Appendix 1, Table A1.1) of 84 trials comprising steady, unignited, wind-aligned, full-bore (full pipe-diameter) releases of liquid propane. These trials involved the discharge of tonne quantities of liquid propane via a 50mm diameter 100m long pipe placed parallel to and 1m from a specially levelled ground surface.

Figure A1.2 (Appendix 1) illustrates the observed correlation between temperature and C_3H_8 concentration at distances 0.0m, 0.4m, and 0.7m off-axis, and at distances 9m and 14m downwind of the release point. The data is consistent with the assumption of local thermal equilibrium amongst liquid and vapour phases,

the equilibrium conditions for prescribed storage and atmosphere conditions being represented by the single solid line. A large degree of scatter is however evident.

Jet entrainment: Two-phase equilibrium:

Consider next the performance of the simple integral-averaged ("top-hat") model and of the "jet" entrainment function in reproducing observed downwind variation in temperature and (volumetric) concentration C_3H_8 . Figures A1.3 through A1.8 (Appendix 1) illustrate the degree of agreement between theory and momentary point-local values plotted as a function of displacement off plume-axis. Agreement is reasonable as regards jet "width" and mean "subcooling" from ambient. Detailed predictions of centre-line concentrations or temperature, or the displacement off-axis of (say) flammability limits, is beyond the intended model scope. Note the generally large differences that may exist between section-mean and centre-line values of concentration or temperature.

Finally, we consider the derived Gaussian profiles based upon the sectionally averaged predictions of the basic "top-hat" model. These are as illustrated for a downwind displacement of 9m in Appendix 1, Figures A1.3 through A1.8. The agreement is satisfactory, and gives confidence that **local** values of temperature and concentration (both centre-line and off-axis) can be estimated by transformation of sectionally-averaged model predictions.

Buoyant plumes: crosswind entrainment and plume-path:

Petersen (1978) carried out an extensive set of wind tunnel tests in which plume-path and concentration decay were examined as a function of distance downwind of a vertical release into a (near uniform) cross-wind. We consider those (19) experiments conducted for "low" ambient turbulence in the Meteorological (boundary layer) Wind Tunnel at Colorado State University. High temperature air releases were simulated by the (isothermal) release of helium/air mixtures. The plumes were made visible by passing the stack gases over TiCl_4 (titanium tetrachloride) prior to release. The experimental points of Figure 5.12 summarise data initially presented in Petersen's (1978) Figures 6.1-1a through 6.1-4b. The initial conditions are recorded in Table 4.1.3.

We have compared the experimental results obtained by Petersen with model runs in the limit of negligible ambient turbulence and with the entrainment formulation

$$\begin{aligned} \text{Entr} &= (\pi D) [e_{\text{jet}} \eta_{\text{jet}} \rho_{\infty} |u - u_{\infty} \cos \phi| + u e_{\text{wind}}^{\text{cross}} \eta_{\text{wind}}^{\text{cross}} \rho_{\infty} u_{\infty} \sqrt{(u_{\infty}/u)} |\sin \phi|]; \\ \eta_{\text{jet}}(\rho/\rho_{\infty}) &= [1 + (4/3)(\rho/\rho_{\infty} - 1)] / [1 + (5/3)(\rho/\rho_{\infty} - 1)]; \\ \eta_{\text{wind}}^{\text{cross}}(\rho/\rho_{\infty}, \phi) &= [1 + e_{\text{wind}}^{\text{cross}} \max\{0, (\rho/\rho_{\infty} - 1) \sin \phi\}], \\ e_{\text{jet}} &= 0.08, \quad u e_{\text{wind}}^{\text{cross}} = 0.60, \quad \rho e_{\text{wind}}^{\text{cross}} = 7.5. \end{aligned}$$

We compare the experimental rise-heights z_k with those $z(x_k)$ predicted to occur at the experimental (horizontal) displacement x_k downwind of release. The results are summarised in Figure 5.12. Agreement is satisfactory, with the predicted values almost always within 15% of those observed. The function form, and coefficient values for jet and crosswind entrainment are essentially those (0.08

and 0.60) recommended by Briggs (1984) on the basis of extensive data concerning neutral and buoyant plumes released at right angles to an imposed wind.

Dense plumes: crosswind entrainment and plume-path:

Hoot, Meroney and Peterka (1973) conducted experiments in the (boundary layer) wind tunnel at Colorado State University the purpose of which was the characterization of dense plume dispersion. Dense gas was formed by mixing air and Freon 12; releases were directed upwards and at right angles to the ambient wind; plumes were made visible by impinging the premixed (dense gas) jet on the surface of titanium tetrachloride ($TiCl_4$). We consider a series of releases into a laminar crosswind, for which the velocity profile (HMP Figure 4) is essentially constant above 3in from the tunnel floor.

We have compared the experimental results obtained by Hoot, Meroney and Peterka (1973) with predictions obtained in the limit of negligible ambient turbulence. The entrainment formulation is (we recapitulate) as follows:

$$\begin{aligned} \text{Entr} &= (\pi D) [e_{\text{jet}} \eta_{\text{jet}} \rho_{\infty} |u - u_{\infty} \cos \phi| + u_{\text{wind}}^{\text{cross}} \eta_{\text{wind}}^{\text{cross}} \rho_{\infty} u_{\infty} \sqrt{(u_{\infty}/u)} |\sin \phi|]; \\ \eta_{\text{jet}}(\rho/\rho_{\infty}) &= [1 + (4/3)(\rho/\rho_{\infty} - 1)] / [1 + (5/3)(\rho/\rho_{\infty} - 1)]; \\ \eta_{\text{wind}}^{\text{cross}}(\rho/\rho_{\infty}, \phi) &= [1 + \rho_{\text{wind}}^{\text{cross}} \max\{0, (\rho/\rho_{\infty} - 1) \sin \phi\}], \\ e_{\text{jet}} &= 0.08, \quad u_{\text{wind}}^{\text{cross}} = 0.60, \quad \rho_{\text{wind}}^{\text{cross}} = 7.5. \end{aligned}$$

Comparison is made between observed and predicted maximum (centre-line) rise-height, and between (visible leading edge) touchdown and the impact of "top-hat" leading-edge, or extrapolated plume centre-line, the tunnel floor. Initial conditions and observed rise heights and touchdown distances are as

recorded in HMP (Report: Figure 2). In addition, comparison is made with horizontal displacement of maximum plume rise correlated by HMP's formula,

$$x/D_{\square} = (u_{\infty} u_{\square}) / (g D_{\square}) / (\rho_{\square} / \rho_{\infty} - 1).$$

The results of a comparison between the predictions of the PLUME model and HMP data are presented in Figures 5.13 through 5.16. Generally the agreement is good, with (maximum) rise-height fitted to within perhaps 10%, maximum-rise displacement to within 20%. Some systematic error is evident in rise-height displacement.

As regards plume "touchdown" the situation is more complex. Hoot, Meroney and Peterka (1973) measured the horizontal displacement from release of the point of "visible plume edge" touchdown. This differs significantly from (extrapolated) plume centre-line touchdown, and with the touchdown of the integral averaged plume width. It is well known (Briggs 1984) that the "momentum" and "concentration" widths of plume differ significantly. A "top-hat" model, which represents mass and momentum entrainment with a single plume width, cannot accurately predict concentration width. Neither is it possible to identify the "visible plume edge" with any fixed proportion of the equivalent Gaussian (concentration) width. The systematic dilution on the plume centre-line must imply that the "visible edge" is an increasingly small proportion of the Gaussian width. Ultimately, of course, the visible plume must dissipate entirely. In the circumstances we are content to compare "visible edge" data with predicted centre-line (Figure 5.15) and "top-hat" edge displacements at "touchdown" (Figure 5.16). The centre-line displacement is systematically larger, the "top-hat" edge smaller, than visible edge touchdown observed by Hoot, Meroney and Peterka. Considerable scatter is evident: this reflects the sensitivity of plume touchdown to small variations in entrainment taking place in weakly descending (marginally dense) plumes. We consider this comparison satisfactory. Further improvements in the modeled

entrainment must await more accurate experimental data on (extrapolated) centre-line touchdown. This latter could be deducible from photographs of visible plume-path taken (but not published) by Hoot, Meroney and Peterka.

In addition a comparison has been made with the small but well instrumented dataset of Li, Leijdens and Ooms (1986). These authors measured the detailed vertical profiles that resulted from the downward release of heated air into an essentially uniform airsteam. Differences between air and plume density are everywhere small, so that these experiments should be analogous to weakly dense plumes released upwards. The results are presented in Figure 5.17. Agreement is satisfactory, as regards both plume path and width. Accuracy is comparable or better to that achieved by Havens (1988), but is inferior to that of Li, Leijdens and Ooms using their elliptic sectioned Gaussian model. Nevertheless the overall predicative accuracy of the entrainment formulation advanced here is judged sufficient for purpose. Certainly the very large experimental scatter, and range of correlation based predictions should be borne in mind (Petersen 1987).

§5.13: Comparison with the models of Wheatley, Raj and Morris, and Havens.

It is useful to contrast the models of Morris and Raj (1987) for grounded jet, Wheatley (1986) for a two-phase jet, and Havens and Spicer (1988) for a dense gas plume with that here proposed for the representation of HF releases. Each of these models have limitations which restrict, more or less severely, the range of applicability. Certainly none will span the range of release conditions encompassed by HFPLUME.

The free jet model of Wheatley:

This model (Wheatley 1987a, 1987b) was developed in order to predict the downwind distribution of concentration and temperature resulting from a pressurized release of liquid ammonia. The model structure is essentially identical to that of HFJET (Appendix 4): steady state, no atmosphere gradients, (isobaric) thermal equilibrium, entrainment dominated by jet/ambient shear, negligible gravity slumping. Though the model (TRAUMA) was originally "tailored" for liquid ammonia releases, its thermodynamic structure permits the release of several reactive liquids and in particular anhydrous HF. No provision is made for the impact of jet upon the ground, either in respect of induced drag, or of geometrical distortions. Model applicability is thus limited under prototypical conditions (compare Appendix 4) to a downwind range of perhaps 10m, and to HF concentrations in excess of some 1% by volume HF. The model differs from HFJET in that complete "atomization" of the released liquid is not **assumed**, but is rather **checked** against a criterion first developed by Ohnesorge (1936) for thermodynamically stable liquid jets. Maximum stable droplet size and gravitational settlement of droplets (Clift, Grace and Weber 1978) are considered in the context of droplet "rain-out"; a simple (inequality) condition is developed for the absence of droplet rain-out. The analysis takes no account of droplet evaporation. The restricted downwind range of Wheatley's model make it suitable for the near-field prior to plume touchdown. No provision is made for other than horizontal releases. Overall the accuracy and range of validity of this model (comparable to HFJET) is, we judge, insufficient for a confident "matching" to either heavy gas or passive dispersion models in the far field.

The grounded jet model of Morris and Raj:

Raj and Morris (1987) proposed a "top-hat" (sectionally averaged) model for a ground affected (rectangular) jet. The range of validity extends from (plume) touchdown through momentum dominated jet, towards heavy gas dispersion. The model structure takes account of wind shear and atmospheric stability, and incorporates ground drag and gravity slumping effects. The cross-section is vertical. The equation system comprises horizontal momentum, conservation of pollutant mass-flux, a (differential) entrainment relation, and a gravity spreading law. Thermal equilibrium is assumed throughout. The entrainment relation is proportional to the mean difference (over "top" or "side") between ambient wind-speed and jet velocity. Entrainment is further proportional to the ambient density and to a dimensionless entrainment coefficient which on the basis of gas jets has an anticipated magnitude $e \approx 0.08$. This is analogous to the formulations in HFJET and HFPLUME, except that all parameters are referred in these latter cases to the centroid height. The drag force comprises two parts, a shear force exerted at the "top" surface, and a "drag" at the ground. Drag on either surface is assumed proportional to the square of the difference at the bounding surfaces between jet velocity and wind speed. Account is taken of density differences inasmuch as the drag at the jet "top" is assumed proportional to the ambient density, whereas that at the ground is linear in the jet mean density. This model is strongly empirical, however, in that both ground and atmosphere drag are assigned adjustable coefficients for matching with experimental data. Additional entrainment terms, representing ambient atmosphere entrainment, and lateral spreading entrainment (Puttock 1988) are entirely absent. The several empirically adjustable coefficients are obtained (and the model tuned) by comparison of model predictions against an extremely small dataset, the Desert Tortoise 4 Ammonia Release (Ermak, Chapman, Goldwise, Gouveia and Rodean 1987).

In spite of these limitations it seems likely that the model of Raj and Morris represents a significant improvement on that of Wheatley for a free jet. The key difference rests in the explicit representation of gravity slumping in the formula,

$$dD/ds = (k/u)\sqrt{gh(\rho/\rho_\infty - 1)}, \quad k = 1.15.$$

This permits a reasonable description of gravity slumping for a near horizontal release in which horizontal and vertical motions are largely decoupled. Entrainment is dominated by jet/atmosphere shear. The structure is, however, incompatible with existing integral-averaged plume models, and cannot represent the early interaction between impacting plume and ground that accompanies "touchdown". Neither can the early (airborne) jet be followed, so that for predictions near the source a "free" jet model, such as HFPLUME, HFJET (Appendix 4), or TRAUMA, must be matched to that of Raj and Morris (1988).

The problem, mathematically, is that a gravity slumping formula has replaced the vertical momentum equation in the limit of horizontal jet flow: the solution (§5.7) is to introduce pressure forces, acting at the ground surface, such as allow recovery of gravity slumping and plume descent in the appropriate asymptotic limits. Such a formulation we expect to be of comparable or greater accuracy for horizontal pressurized releases, whilst permitting extrapolation to vertical releases, and releases inclined to the ambient wind. The formulation of the drag forces at upper and lower jet edge is complex, and highly empirical. Formulations based on an analysis of the turbulent averaged equations of motion lead rather directly (§5.7) to a drag force expressed in terms of ambient parameters at the centroid height, the form of which introduces no empiricism beyond that required for heavy gas (ambient) entrainment. The formulation of HFPLUME is therefore consistent throughout the free jet, touchdown, and slumped plume regions, and

contains entrainment mechanisms relevant to all. HFPLUME is (we expect) uniformly valid from point of release to far within the heavy gas advection regime.

The atmosphere plume model of Havens and Spicer:

Havens and Spicer (Havens 1988) have proposed that the model of Ooms, Mahieu, and Zelis (1974) be used for the representation of dense gas releases prior to plume touchdown. The model is a variant of the simple integral average models in that a truncated Gaussian ("similarity") profile is imposed upon velocity, density, and concentration within the developing plume. The model also includes an initial zone model, in which are adopted empirical correlations spanning the region prior to the establishment within the plume of (approximately) Gaussian conditions. This initial zone model is uncertain, even in the context of gaseous releases (Keffer and Baines 1963, Kanotani and Greber 1972); it is doubtful whether this additional complexity is necessary or desirable.

Specific comments may be made regarding such (truncated Gaussian) formulations. The centre-line concentration is artificially heightened by the process of profile "cut-off" whereby the mass in the Gaussian "tail" is redistributed toward the plume centre. The use of a cut-off is not necessary for such a self-similarity theory and may be eliminated by a reformulation of the integral equations of motion (Schatzmann 1978, McFarlane 1988).

Li, Leijdens and Ooms (1986) employed a "drag" force in order to reproduce the observed plumepath for a set of 3 buoyant jets released downwards: the use of such a drag force is controversial (Briggs 1984); the data set severely limited. Coefficient values and the functional form of the entrainment function are uncertain (Petersen 1978, Schatzmann 1978); there is considerable scatter in the experimental data (Petersen 1987).

The benefits of truncated Gaussian over simpler "top-hat" models seem to us unproven, even in the context of gas plumes. For reactive, initially two-phase releases, solution of such models requires numerical integration of the energy equation at each downwind advance of the discretized differential system for plume motion; it is not possible to introduce the several simplifications to the system thermodynamics that allow explicit integration of the enthalpy excess over the plume cross-section (Havens 1987). For complex reactive flows, and in particular for pressurized releases of anhydrous HF, the computational cost of a Gaussian model seems prohibitive. Additionally the model requires initial zone information appropriate to pressurized gas or two-phase, or atomized liquid phase releases.

In practical terms what is required is a model prior to plume touchdown passing integral averaged information to a grounded jet model (Raj and Morris 1987), a slumping pool model (Raj and Morris 1987), or (perhaps) a heavy gas advection model (Colenbrander and Puttock 1988). Details of concentration behaviour off-axis cannot readily be passed from model to model; nor is this information likely to be accurate. A sectionally-averaged or "top-hat" model seems to us a reasonable compromise between computational complexity and predicative accuracy. Development of the energy equation for such a model presents no difficulty (Davidson 1986); neither are problems found with the inclusion of reaction chemistry (Forney and Droescher 1985).

The touchdown model of Havens and Spicer has the merit of simplicity:

"The Ooms model" ... "is terminated when the lower edge of the plume impinges the ground. The resulting downwind distance, plume centre line concentration and temperature, and plume radius ($b_j\sqrt{2}$) are used as input to DEGADIS. The ground level gas source input to DEGADIS is a circular area source with radius $b_j\sqrt{2}$ and concentration and temperature equal to the centre-line values output from Ooms model." (Havens 1988a, 1988b)

Insufficient detail is given to permit full consideration of the touchdown assumptions. We presume however that the DEGADIS circular source has an

"evaporation rate" such as to conserve mass- and excess-enthalpy flux at the plane of transition. No account is taken of the momentum excess in either horizontal or vertical direction developed in the course of plume rise and fall. Substantial vertical velocities must imply enhanced (impact) spreading; differences in horizontal velocity between plume and wind imply transition to a grounded jet model, or to some intermediate touchdown model. It seems essential to take some account of these velocity (momentum) differences in the vicinity of plume touchdown. We suggest transition to a spreading pool model (fed from above) or to a slumped plume model in the manner of HFPLUME. Alternatively some empirical correlation between plume and heavy-gas advection might be developed.

For releases which result in much delayed plume touchdown, (>1km, say) we agree with Havens that the use of Ooms model is compromised by the much earlier touchdown of the leading plume edge. A possible solution is to include an "image" plume as a model of the (horizontal) ground. However dilution is likely to be such that plume behaviour more closely approximates passive dispersion than that appropriate to heavy-gas advection models such as DEGADIS or HEGADAS. We suggest that for these cases transition should be made to a Gaussian far-field dispersion model (Hanna 1982) based upon asymptotic matching of plume and Pasquill/Gifford standard deviations σ_y and σ_z . Discussion of "image" plume dynamics illustrates the additional complexity imported with Gaussian rather than "top-hat" models in plume touchdown.

§5.14: Conclusions.

Indications are that HFPLUME (and HFJET) are satisfactory predictors of the early dispersion behaviour of anhydrous HF. "Matching" of HFPLUME to the heavy

gas advection model HEGADAS (Chapter 7), or to the passive dispersion model PGPLUME (Chapter 6) allows prediction of the far-field.

References:

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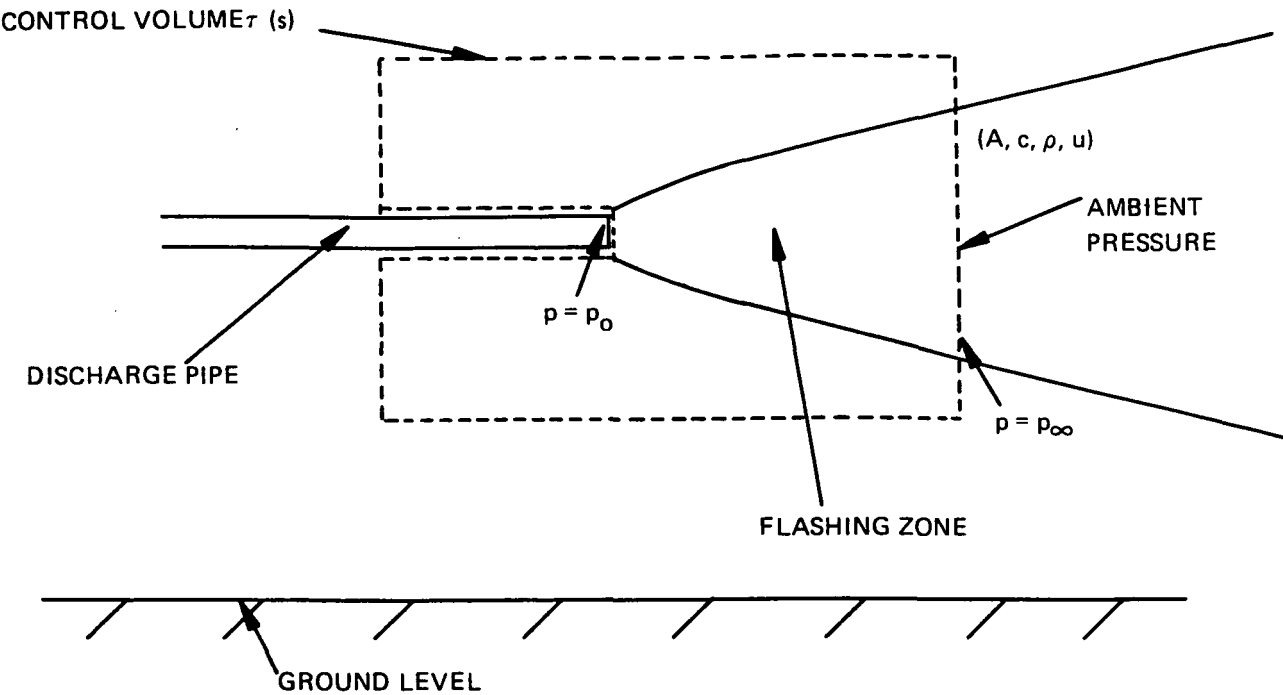


FIG. 5.1 – The zone of external flashing. On release, fluid expands to ambient pressure. Thermal equilibrium assumed. Entrainment and interphase slip taken to be negligible.

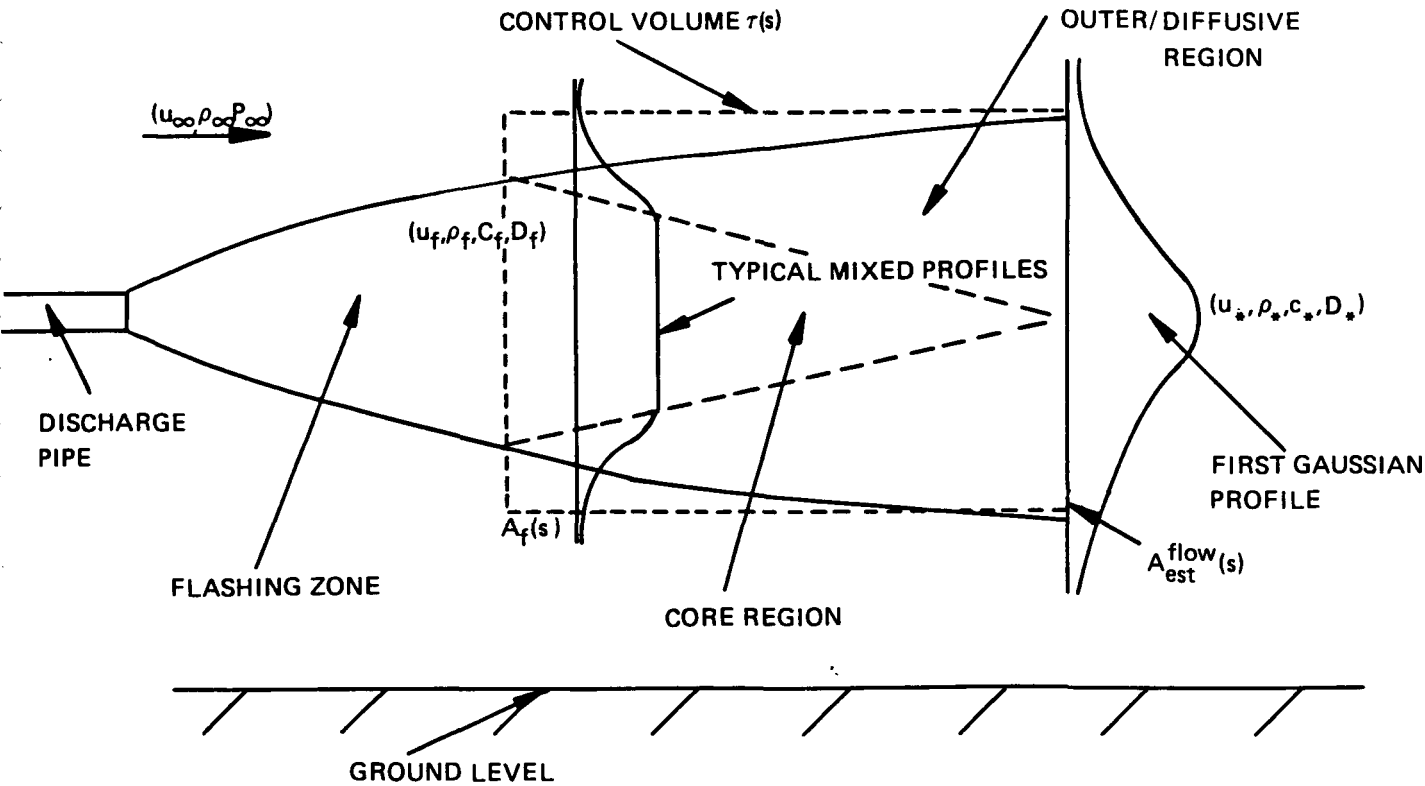


FIG. 5.2 – The zone of flow establishment. Transition region in which initially “top-hat” profiles are eroded by entrainment into outer region. Zone ends when undisturbed inner core region disappears to leave Gaussian profiles and self-similar flow.

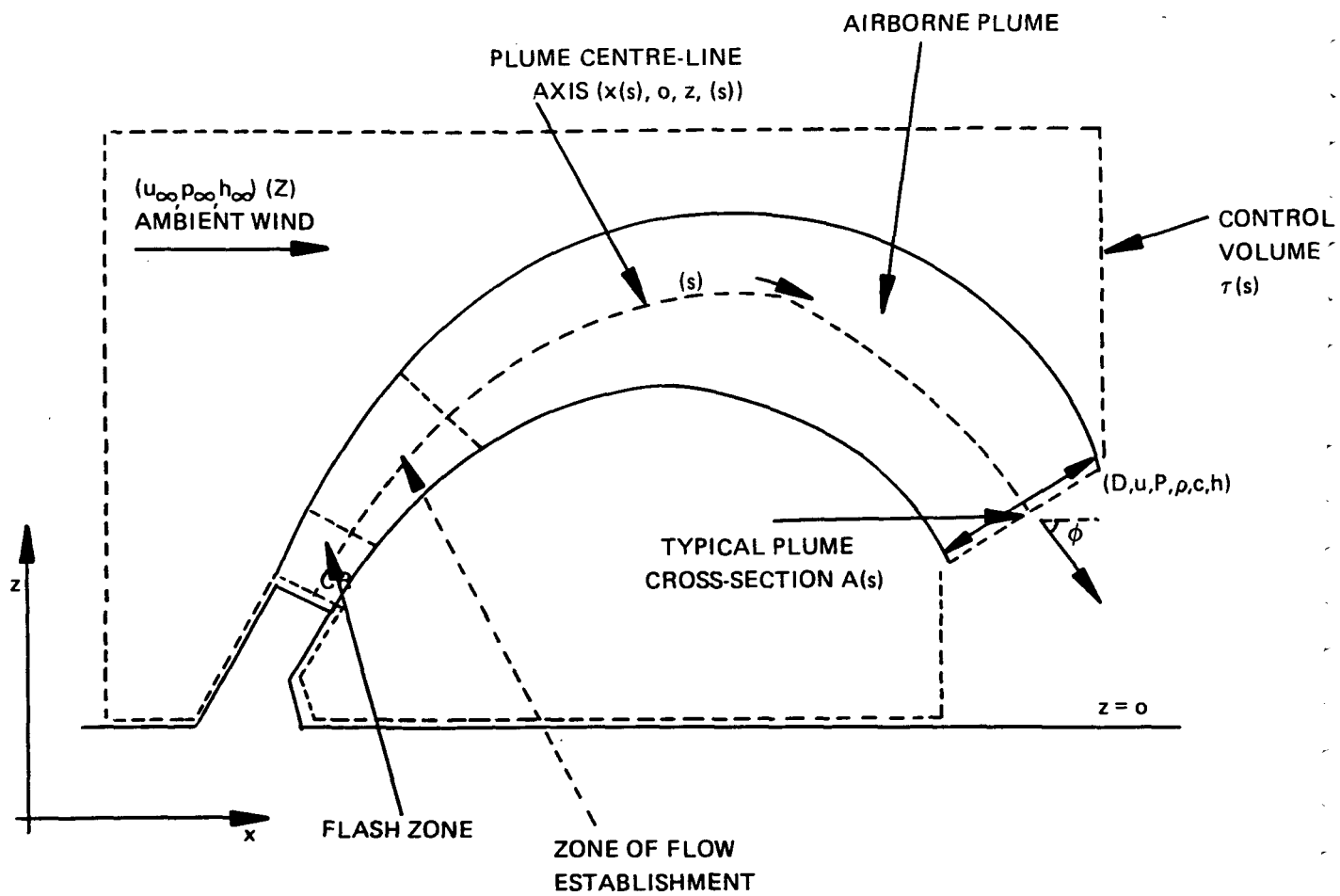


FIG. 5.3. — The airborne (established) plume. Negligible ground effect. Radial symmetry about plume centre-line.

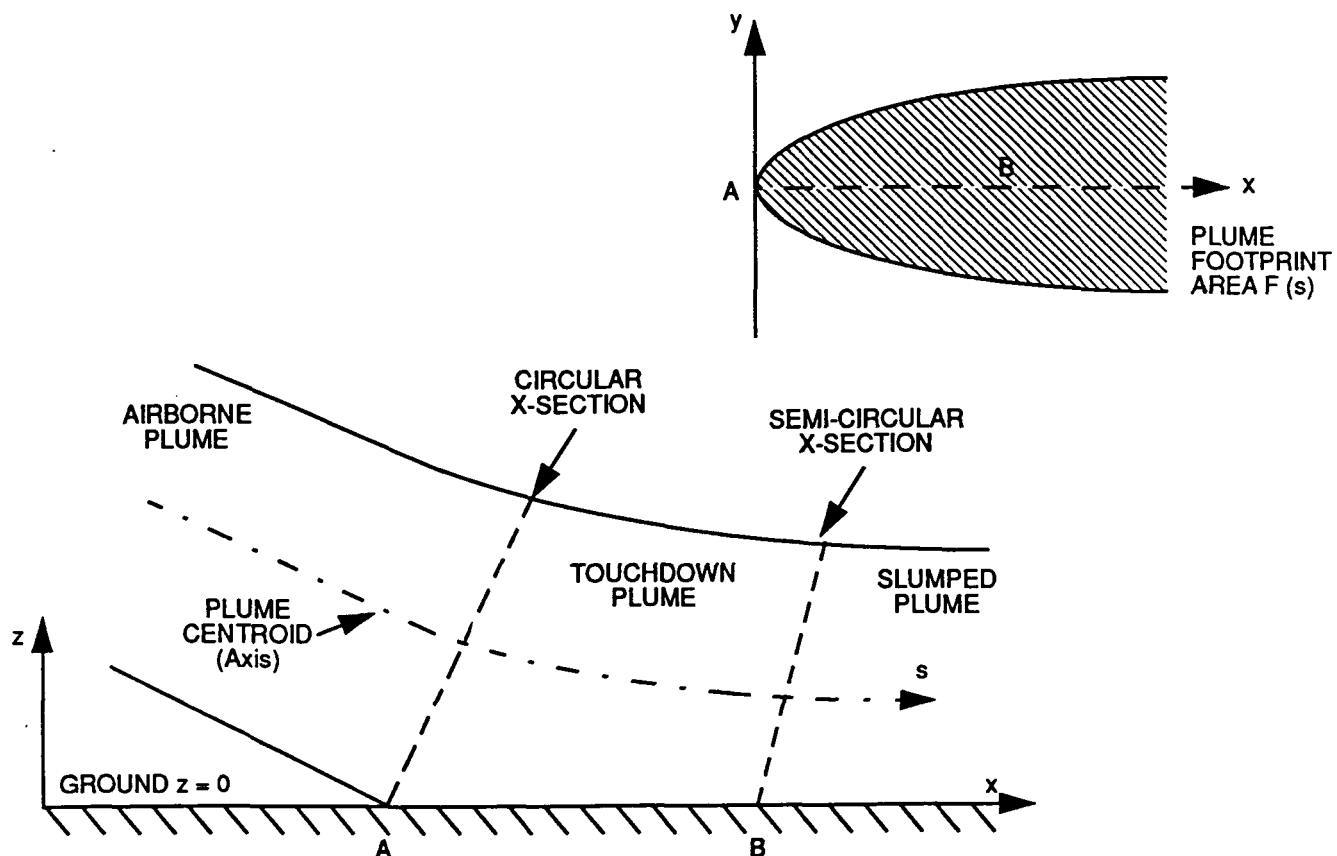


FIG. 5.4 - The touchdown plume. Transition of plume from circular X-section to semi-circular X-section in the touchdown region

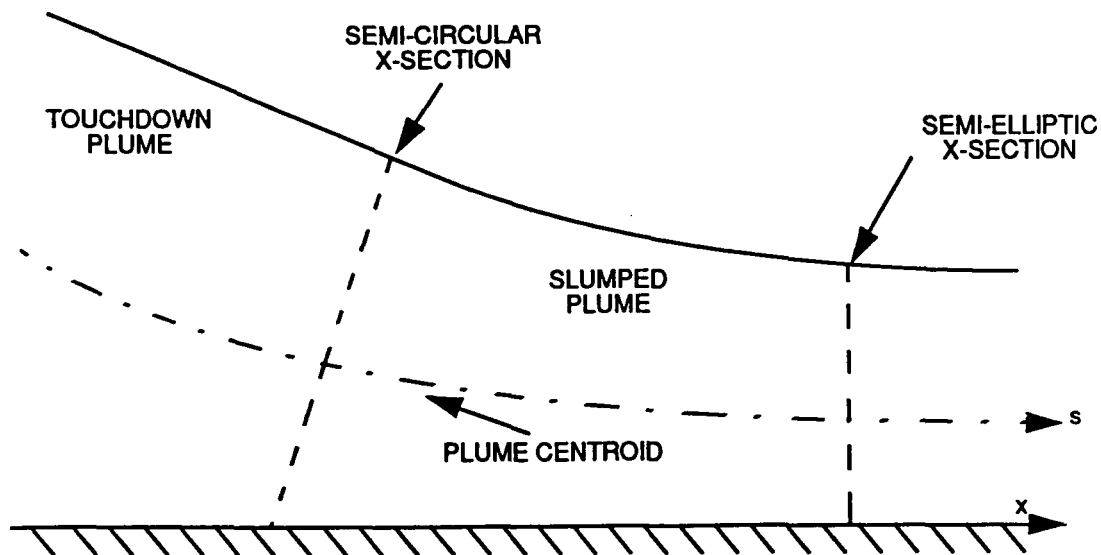


FIG. 5.5 - The slumped plume. Semi-elliptic X-section due to lateral gravity spreading

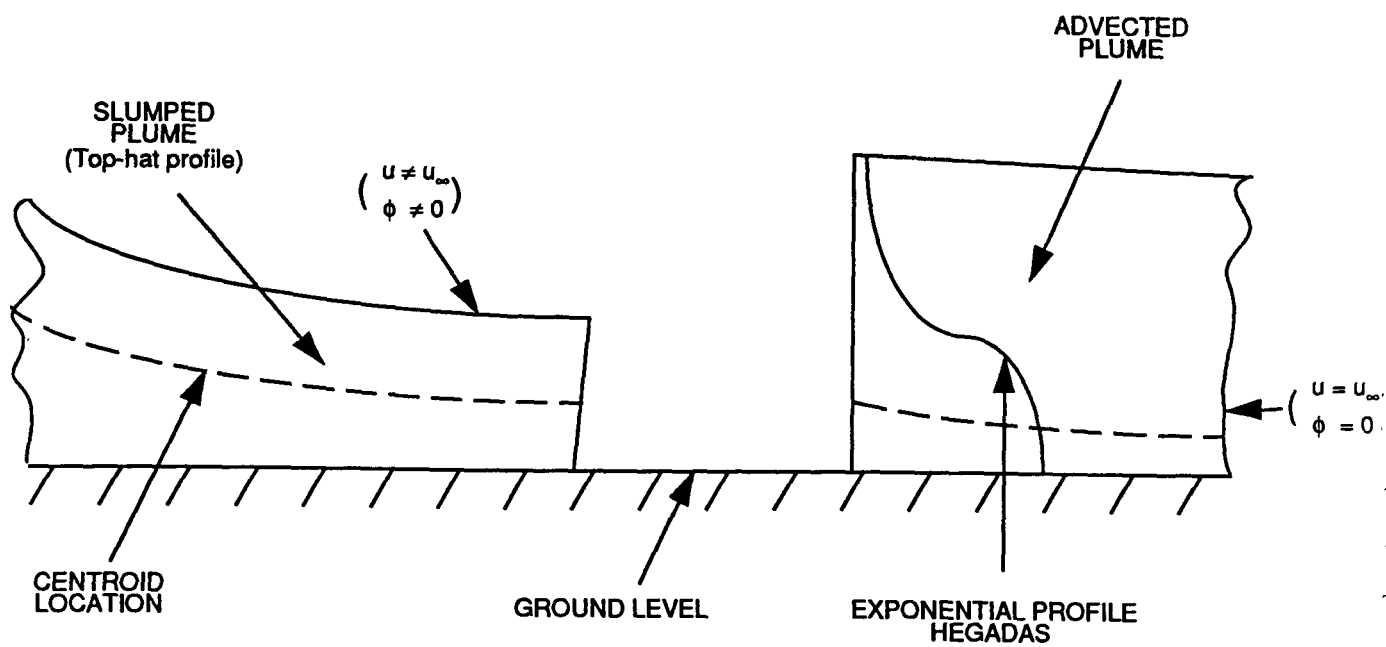


FIG. 5.6 - Transition to advected dense gas plume (HEGADAS). Criteria for transition are small plume excess velocity over ambient, and small jet entrainment

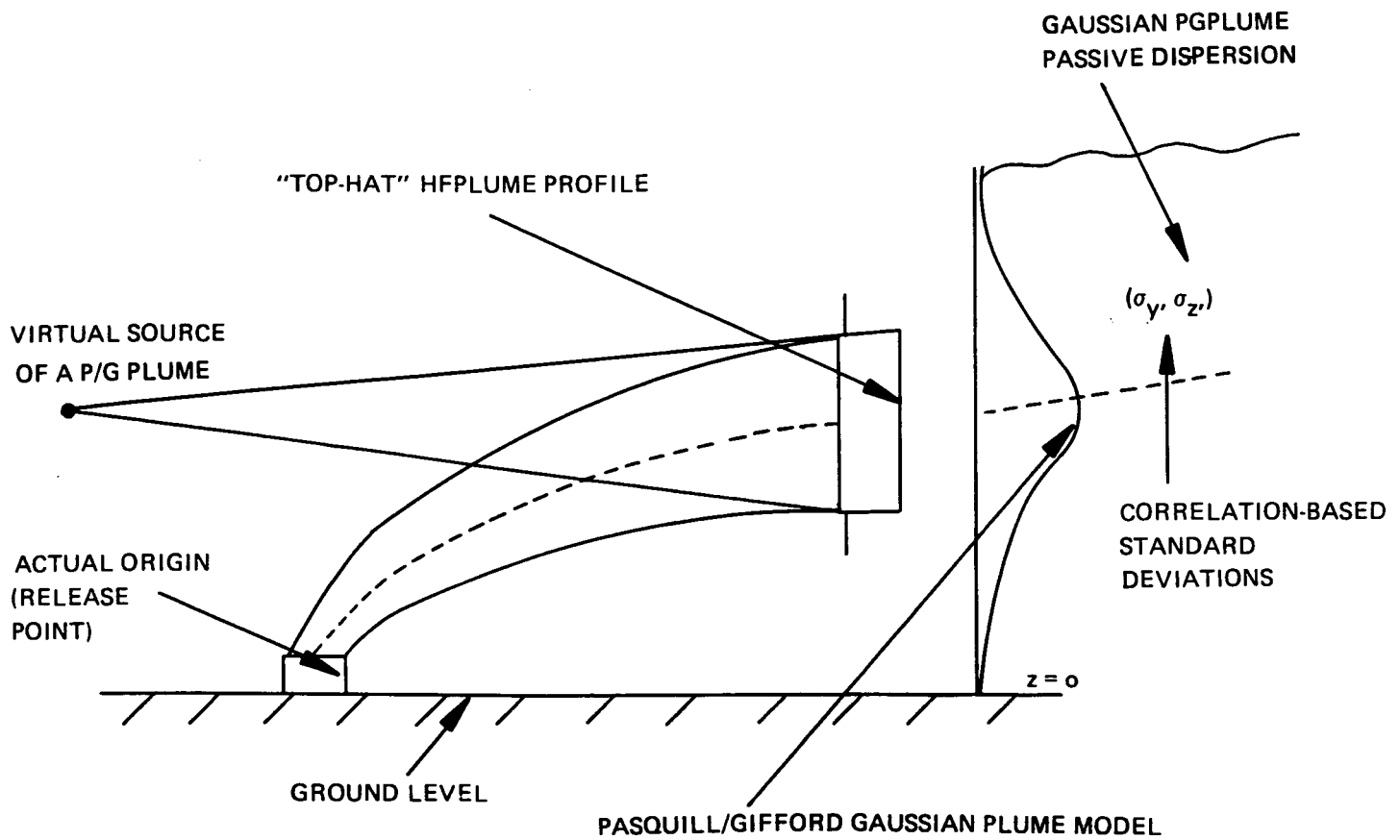


FIG. 5.7. — Transition to passive dispersion as an elevated Gaussian plume, when velocity excess over ambient is small and buoyancy/shear entrainment weak compared with passive entrainment.

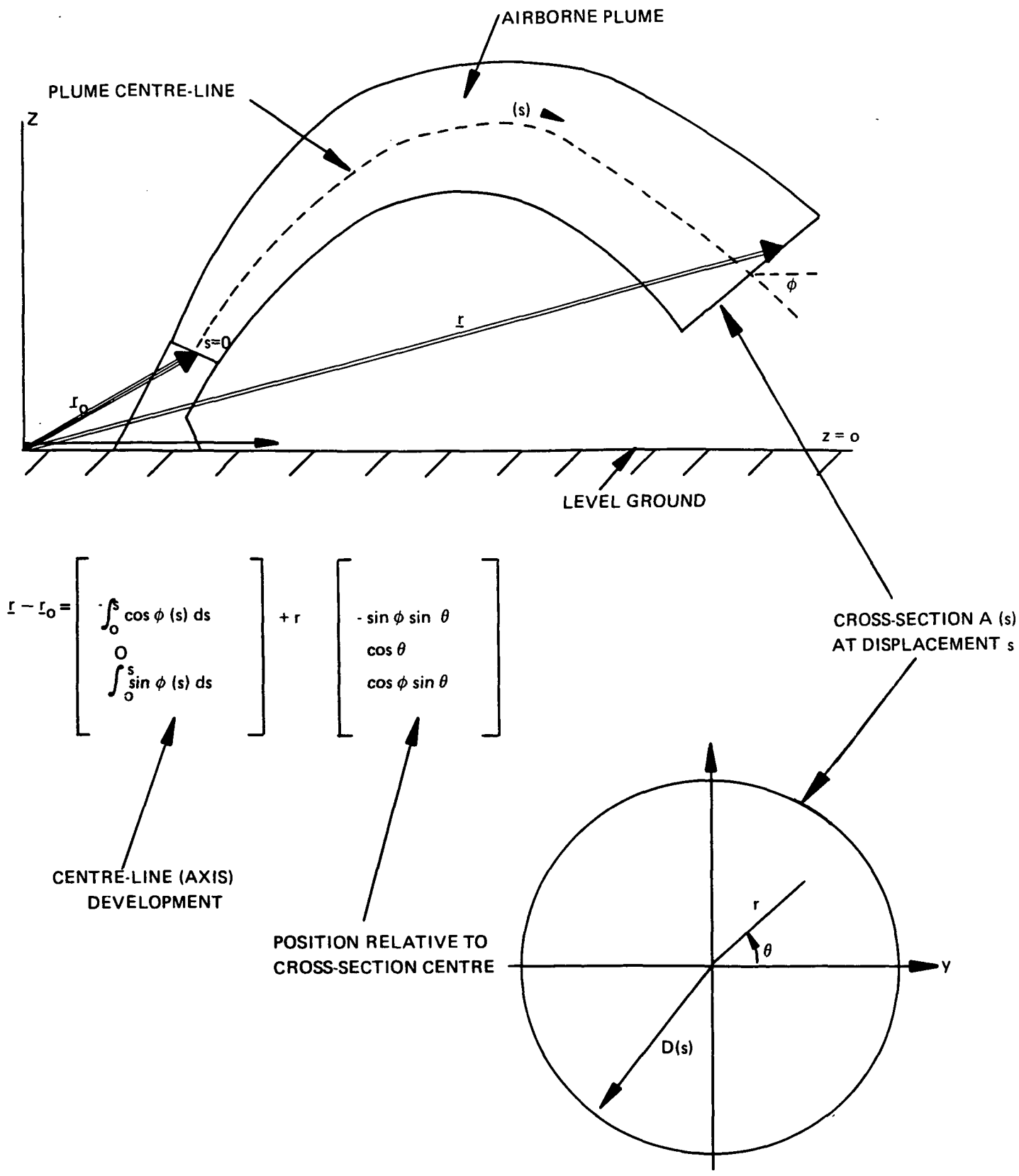
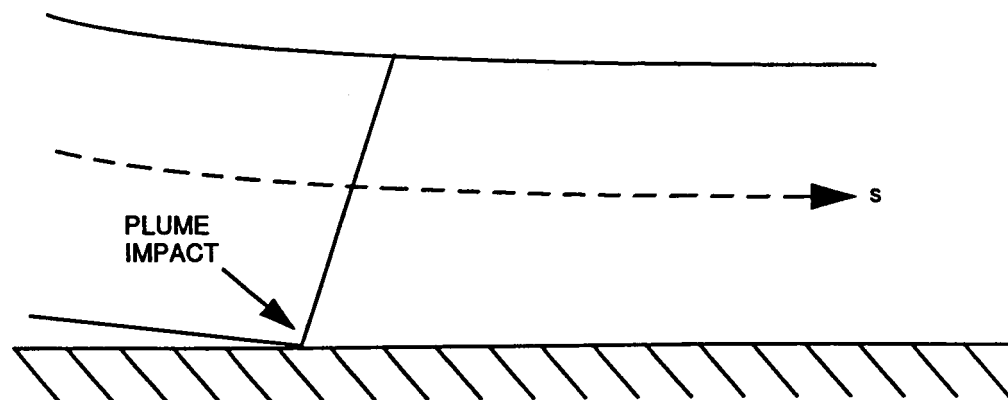


FIG. 5.9. — The plume coordinate system.



MOMENTUM FLUX
 $\underline{dP} = dm \, u (\cos \phi, 0, \sin \phi)$

IMPACT FORCE
 $= l u^2 |\tan \phi| (\sin \phi, 0, -\cos \phi)$

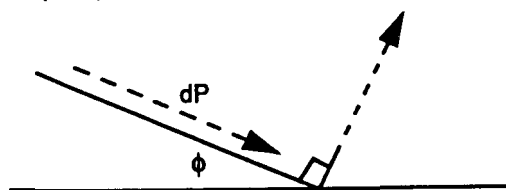


FIG. 5.10 - Plume Impact Pressure Forces. Fluid momentum impacting the ground is destroyed, exerting force per unit axis length of $l u^2 |\tan \phi|$. Kinetic energy conserved in elastic impact

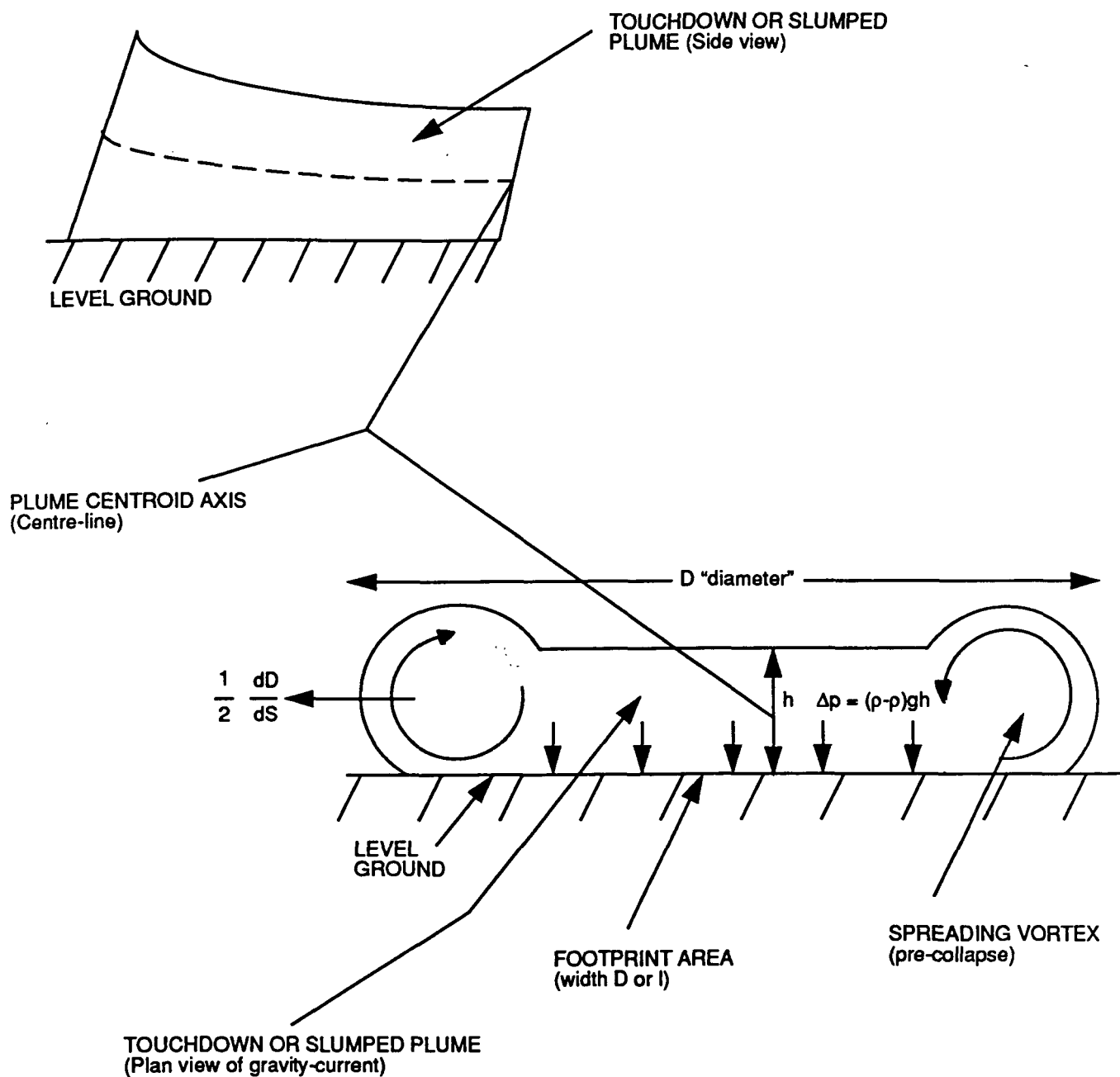


FIG. 5.11 - Gravity slumping and footprint area pressure forces. Lateral gravity spreading of heavy gas dominates slumping of plume

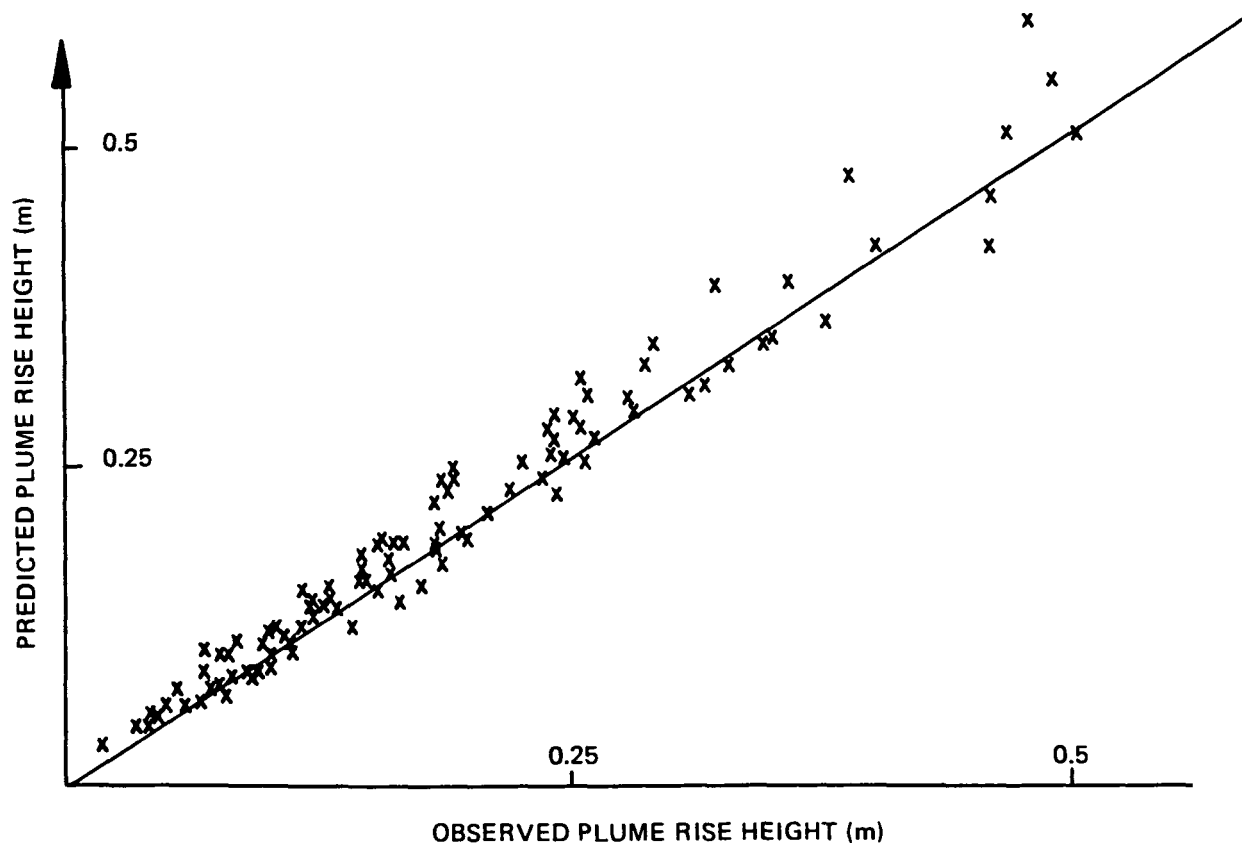


FIG. 5.12. — Comparison of the predicted plume rise height of buoyant plumes with the experimental data of Petersen (1978).

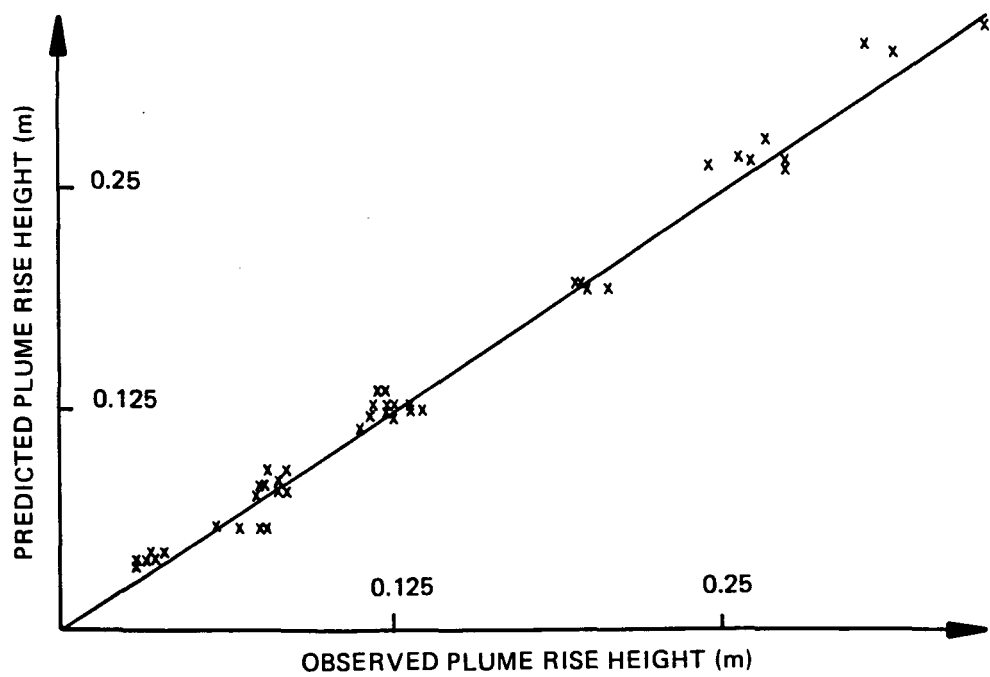


FIG. 5.13. — Comparison of the predicted plume rise height with experimental dense gas wind-tunnel data of Hoot, Meroney and Peterka (1973).

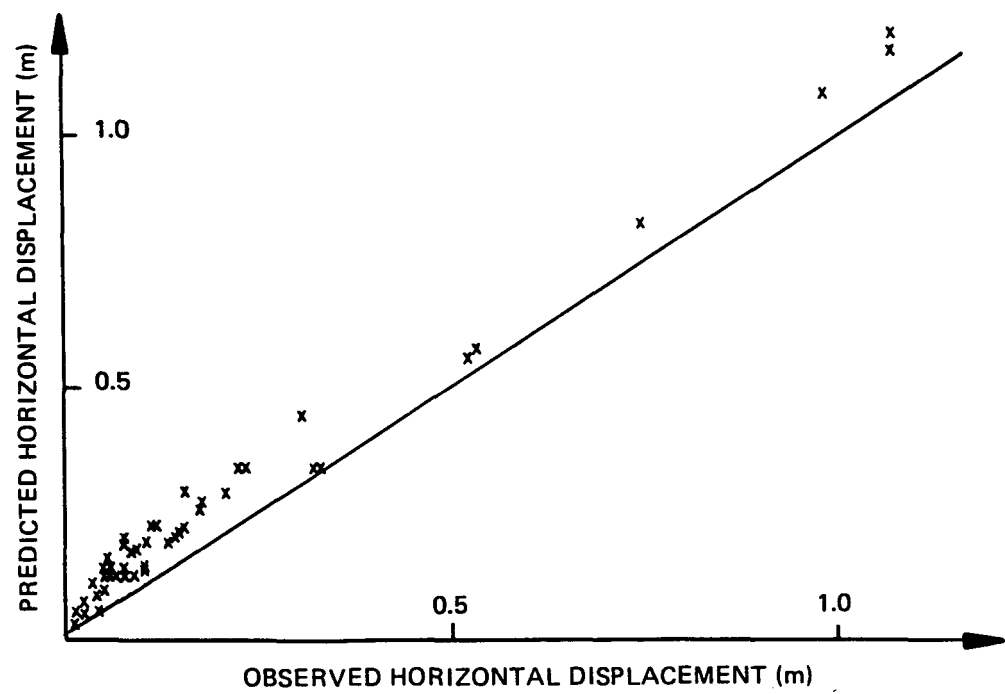


FIG. 5.14. — Comparison of the predicted location of maximum plume rise with experimental dense gas wind-tunnel data of Hoot, Meroney and Peterka (1973).

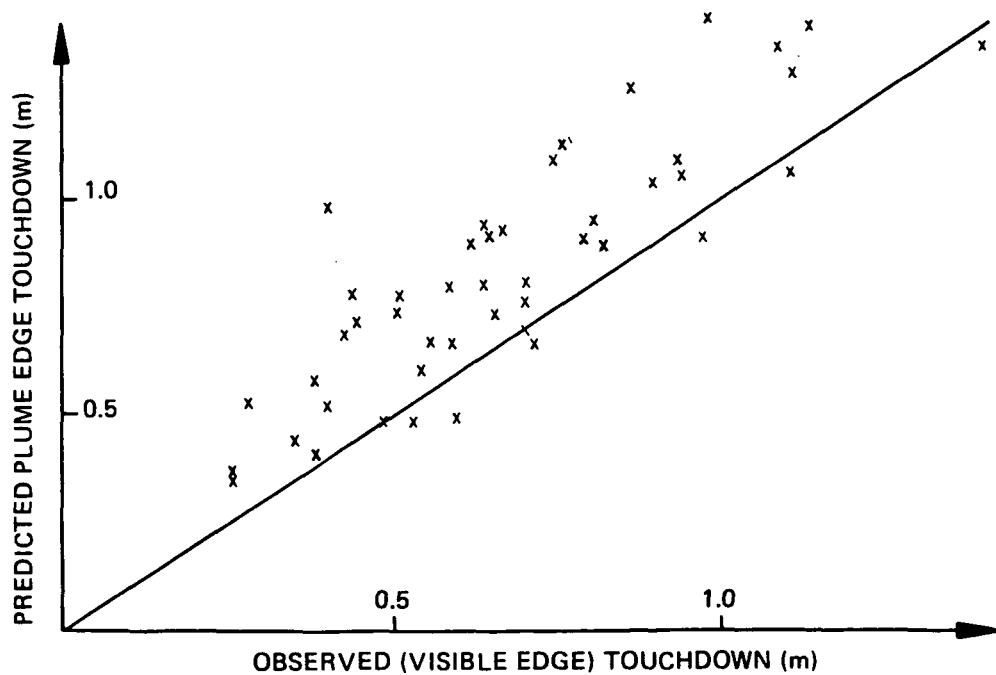


FIG. 5.15. — Comparison of the predicted point of plume touchdown with experimental (visible edge) touchdown of Hoot, Meroney and Peterka (1973).

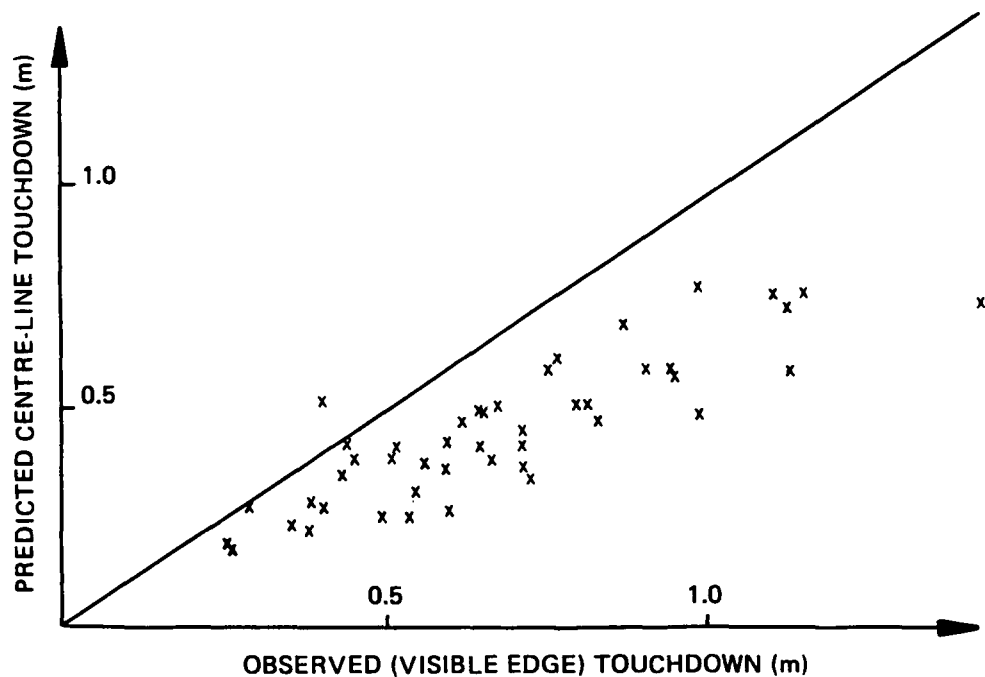
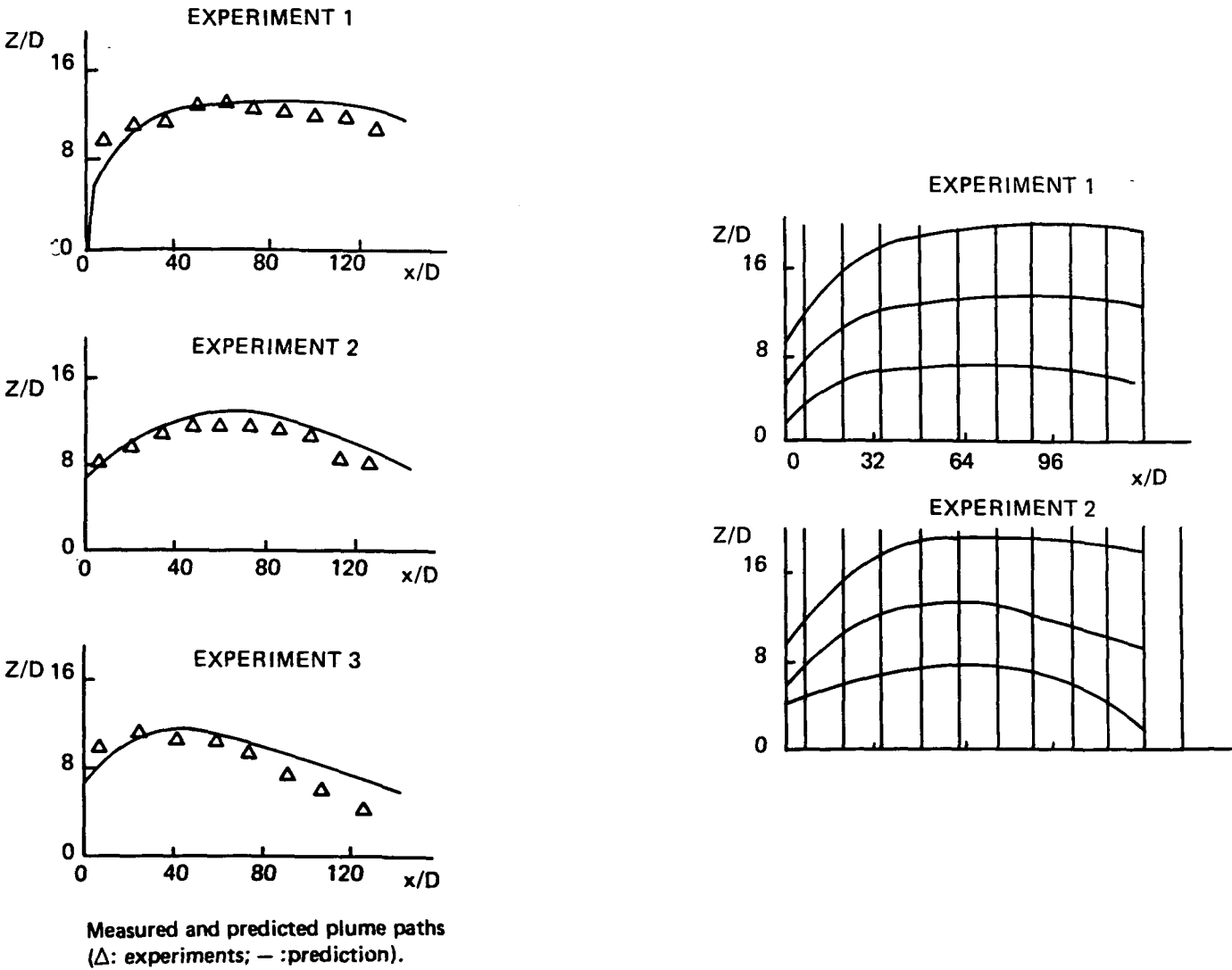


FIG. 5.16. — Comparison of predicted Centre-line touchdown with experimental Visible Edge touchdown data of Hoot, Meroney and Peterka (1973).



Experimental conditions (T_a : tunnel temperature; T_c stack plume exit temperature)

	D (m)	U_a (m s ⁻¹)	U_c (m s ⁻¹)	T_a (K)	T_c (K)	Re	Fr
Experiment 1	0.025	0.92	5.16	293	353	8600	3.45
Experiment 2	0.025	0.97	5.75	292	393	9580	3.84
Experiment 3	0.020	0.85	3.68	291	393	4900	3.68

D orifice diameter
 U_a ambient wind speed
 U_c centre-line speed
x horiz. distance
z (downward) vertical distance

FIG. 5.17. — Comparison of predicted centre-line plume trajectory and plume width with data from experiments 1, 2 and 3 of Li Leijdens and Ooms (1986).

6. Far-field Dispersion: Matching to Pasquill/Gifford Curves

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§6.1: Introduction.

The influence upon plume dispersion of release conditions and of complex reaction dynamics decreases with increasing downwind distance, and becomes negligible when compared with ambient turbulence in the far-field. Inasmuch as the formulation of ambient turbulence within HFPLUME is rather uncertain, it is inappropriate to extrapolate HFPLUME far downwind of release.

For the regime of passive advection considerable (empirical) success has been obtained by means of a Gaussian plume/"image"-plume model. Local concentrations are prescribed in terms of horizontal and vertical standard deviations, each expressed as a function of distance downwind of the source. Atmosphere stability is described by the familiar Pasquill/Gifford classes 'A' through 'F'. The correlations apply properly to extended and level terrain (Pasquill 1961, Gifford 1975). More recent developments allow correction of the standard correlations for surface roughness (Hanna 1982), for concentration averaging time (plume meander) (Hanna, Briggs and Hosker 1982), for release duration (Blewitt, Yohn, and Ermak 1987), and for the influence of the nearby ground (Pasquill 1976).

We may choose either to modify the entrainment function within HFPLUME, or else to link HFPLUME to the well established Pasquill/Gifford Gaussian plume model. Modifications might incorporate the Pasquill/Gifford standard deviations into the entrainment function (Bloom 1980; Petersen and Cermak 1980); or else represent surface layer structure implied by observation and Monin-Obukhov similarity (Ooms 1972; Schatzmann 1978; Disselhorst 1984; HFPLUME, Chapter 5). in such a way as to reproduce observed farfield behaviour.

The choice of method is governed by computational efficiency and by the need to ensure **accurate** reproduction of well-known farfield effects. We link HFPLUME

to a Pasquill/Gifford farfield model by asymptotic matching, in which a virtual source for a Pasquill/Gifford model is located by requiring the continuity of mass, momentum, and energy fluxes between near and farfield descriptions at a (given) matching plane. Subsequent dispersion is then obtained by function evaluation, rather than by the numerical solution of a set of ordinary differential equations. The matching procedures are broadly analogous to those proposed in the context of heavy gas dispersion by Raj and Morris (1987).

§6.2: Far-field Dispersion: Pasquill/Gifford Models.

The dispersion of a trace contaminant from a ground or an elevated point source over flat homogeneous terrain is well described by an (essentially empirical) plume/"image"-plume model of the general form (Stern, Boubel, Turner and Fox 1984; Hanna 1982; Hanna, Briggs and Hosker 1982):

Point-local concentration:

$$c(\Delta x, y, z)/c_* = \psi(y, z; \sigma_y, \sigma_z, z_{PG}); \quad c_* = dm/dt|_{HF} / [2\pi u_\infty \sigma_y \sigma_z];$$

$$\psi(y, z; \sigma_y, \sigma_z, z_{PG}) = \exp(-y^2/2\sigma_y^2) [\exp(-(z-z_{PG})^2/2\sigma_z^2) + \exp(-(z+z_{PG})^2/2\sigma_z^2)];$$

$$\sigma_y, \sigma_z = (\sigma_y, \sigma_z)(\Delta x = x_{PG} - \langle x \rangle, z_{PG}; \tau, z_{cm}, z_r);$$

$$0 \leq z; \Delta x \geq 0; -\infty < y < \infty, z_{cm}, z_{PG}; \sigma_y, \sigma_z \geq 0.$$

[Notation: Δx , displacement downwind of a (virtual) point-source of pollutant (HF) mass-flux $dm/dt|_{HF}$ at coordinates $(x_{PG}, 0, z_{PG})$; c_* , "centre-line" mass-concentration at displacement Δx ; $(x_{PG} + \Delta x, y, z)$, coordinates of a general point within the Pasquill/Gifford plume a distance z above ground, and a

(horizontal) distance y off-axis; (σ_y, σ_z) , standard deviations in horizontal and vertical directions; u_∞ mean wind-speed.]

Pollutant is **advected** at the (vertical-mean) wind-speed u_∞ . Cross-wind dispersion is described by vertical and horizontal standard deviations, σ_z and σ_y respectively. Each standard deviation depends on the atmosphere stability (class), distance downwind of the source (Gifford 1976), the chosen concentration averaging time (Pasquill 1976, Hanna 1982), the surface roughness (Hanna and Briggs 1984), and the mean plume (centroid) "height" (Pasquill 1976).

The standard Pasquill/Gifford standard deviations based upon a surface roughness $z_r^{PG} = 3\text{cm}$, ground-level source, and an averaging time $\tau_{PG} = 10$ minutes (Hanna, Briggs and Hosker 1982) were given graphically for distances less than some 10-50km downwind of release. These correlations were given numerical form by Turner and Busse (1973), who proposed for σ_y^{PG} the dimensioned form (Stern, Boubel, Turner and Fox 1984),

Horizontal Standard Deviation:

$$\sigma_y^{PG} = 465.116(\Delta x/10^3) \tan(\theta\pi/180) ;$$

$$\begin{aligned} \theta(\Delta x, PG) = & \begin{cases} 24.167 - 2.5334 \ln(\Delta x/10^3), & PG = 'A'; \\ 18.333 - 1.8096 \ln(\Delta x/10^3), & PG = 'B'; \\ 12.500 - 1.0857 \ln(\Delta x/10^3), & PG = 'C'; \\ 8.3333 - 0.72382 \ln(\Delta x/10^3), & PG = 'D'; \\ 6.2500 - 0.54287 \ln(\Delta x/10^3), & PG = 'E'; \\ 4.1667 - 0.36191 \ln(\Delta x/10^3), & PG = 'F'; \end{cases} \end{aligned}$$

$$0 \leq \Delta x < 100\text{km}; \quad PG = \{'A', 'B', 'C', 'D', 'E', 'F'\}.$$

[Notation: Δx , downwind distance (m); PG, Pasquill/Gifford stability class; σ_y^{PG} , standard (Pasquill/Gifford) horizontal standard deviation (m).]

In addition the vertical standard deviation σ_z^{PG} is assigned for each stability class a piece-wise power-law form (Turner and Busse 1973; Stern, Boubel, Turner and Fox 1984).

Vertical Standard Deviation:

$$\begin{aligned}
 \sigma_z^{A'} = & \begin{cases} 122.80\Delta x^{0.9447} \text{ m}, & \Delta x < 100\text{m}; \\ 158.08\Delta x^{1.0542} \text{ m}, & 100\text{m} \leq \Delta x \leq 150\text{m}; \\ 170.22\Delta x^{1.0932} \text{ m}, & 150\text{m} < \Delta x \leq 200\text{m}; \\ 179.52\Delta x^{1.1262} \text{ m}, & 200\text{m} < \Delta x \leq 250\text{m}; \\ 217.41\Delta x^{1.2644} \text{ m}, & 250\text{m} < \Delta x \leq 300\text{m}; \\ 258.89\Delta x^{1.4094} \text{ m}, & 300\text{m} < \Delta x \leq 400\text{m}; \\ 346.75\Delta x^{1.7283} \text{ m}, & 400\text{m} < \Delta x \leq 500\text{m}; \\ 346.75\Delta x^{1.7283} \text{ m}, & 400\text{m} < \Delta x \leq 500\text{m}; \\ 453.85\Delta x^{2.1166} \text{ m}, & 500\text{m} < \Delta x \leq 3.11\text{km}; \\ 5000\text{m}, & \Delta x > 3.11\text{km}; \end{cases} \\
 \sigma_z^{B'} = & \begin{cases} 90.673\Delta x^{0.93198} \text{ m}, & \Delta x < 200\text{m}; \\ 98.483\Delta x^{0.98332} \text{ m}, & 200\text{m} \leq \Delta x \leq 400\text{m}; \\ 109.30\Delta x^{1.09710} \text{ m}, & 400\text{m} \leq \Delta x \leq 35\text{km}; \\ 5000\text{m}, & \Delta x > 35\text{km}; \end{cases} \\
 \sigma_z^{C'} = & \begin{cases} 61.141\Delta x^{0.91465} \text{ m}, & 0\text{m} < \Delta x; \end{cases} \\
 \sigma_z^{D'} = & \begin{cases} 34.459\Delta x^{0.86974} \text{ m}, & \Delta x < 300\text{m}; \\ 32.093\Delta x^{0.81066} \text{ m}, & 300\text{m} < \Delta x \leq 1\text{km}; \\ 32.093\Delta x^{0.64403} \text{ m}, & 1\text{km} < \Delta x \leq 3\text{km}; \\ 33.504\Delta x^{0.60486} \text{ m}, & 3\text{km} < \Delta x \leq 10\text{km}; \\ 36.650\Delta x^{0.56589} \text{ m}, & 10\text{km} < \Delta x \leq 30\text{km}; \\ 44.053\Delta x^{0.51179} \text{ m}, & \Delta x > 30\text{km}; \end{cases}
 \end{aligned}$$

$$\begin{aligned}
\sigma_z^{E'} = & \begin{cases} 24.260\Delta x^{0.83660}_m, & \Delta x < 100m; \\ 23.331\Delta x^{0.81956}_m, & 100m \leq \Delta x \leq 300m; \\ 21.628\Delta x^{0.75660}_m, & 300m \leq \Delta x \leq 1km; \\ 21.628\Delta x^{0.63077}_m, & 1km \leq \Delta x \leq 2km; \\ 22.534\Delta x^{0.57154}_m, & 2km \leq \Delta x \leq 4km; \\ 24.703\Delta x^{0.50527}_m, & 4km \leq \Delta x \leq 10km; \\ 26.970\Delta x^{0.46713}_m, & 10km \leq \Delta x \leq 20km; \\ 35.420\Delta x^{0.37615}_m, & 20km \leq \Delta x \leq 40km; \\ 47.618\Delta x^{0.29592}_m, & 40km \leq \Delta x; \end{cases} \\
\sigma_z^{F'} = & \begin{cases} 15.209\Delta x^{0.81558}_m, & \Delta x < 200m; \\ 14.457\Delta x^{0.78407}_m, & 200m \leq \Delta x \leq 700m; \\ 13.953\Delta x^{0.68465}_m, & 700m \leq \Delta x \leq 1km; \\ 13.953\Delta x^{0.63227}_m, & 1km \leq \Delta x \leq 2km; \\ 14.823\Delta x^{0.54503}_m, & 2km \leq \Delta x \leq 3km; \\ 16.187\Delta x^{0.46490}_m, & 3km \leq \Delta x \leq 7km; \\ 17.836\Delta x^{0.41500}_m, & 7km \leq \Delta x \leq 15km; \\ 22.651\Delta x^{0.32681}_m, & 15km \leq \Delta x \leq 30km; \\ 27.074\Delta x^{0.27436}_m, & 30km \leq \Delta x \leq 60km; \\ 34.219\Delta x^{0.21716}_m, & \Delta x > 60km; \end{cases}
\end{aligned}$$

$$0 \leq \Delta x < 100km; \quad PG = \{ 'A', 'B', 'C', 'D', 'E', 'F' \}.$$

[Notation: Δx , downwind distance (km); PG, Pasquill/Gifford stability class; σ_z^{PG} , standard (Pasquill/Gifford) horizontal standard deviation (m).]

Plume standard deviations derive ultimately from the spectrum of turbulence within the ambient atmosphere. Short averaging times correspond to diffusion associated with small scale eddies: long averaging times are dominated by plume meander. The distributions of vertical and horizontal turbulence differ, with the vertical turbulence materially influenced by the proximity of the ground. Turbulent kinetic energy is further influenced surface roughness: greater roughness implies greater turbulent energy, and greater eddy diffusivity.

Hanna (1982), following Smith (1973, 1977) and McDonald (1978), suggested for σ_z a surface roughness effect $(z_r/z_r^{PG})^{0.2}$. Now surface roughness governs the friction velocity u^* (say), and the Monin-Obukhov length L , with the distribution of turbulence in horizontal (σ_u/u^* , and σ_v/u^*) and vertical (σ_w/u^*) directions universal functions of the scaled height z/L (Arya 1982). Plausibly the influence

of surface roughness applies equally and proportionately to the horizontal standard deviation σ_y of a dispersing plume. However, Roberts (Chapter 5), analysing extensive meteorological data (Draxler 1984), discerned **no** significant effect of surface roughness upon σ_y . Certainly for longer averaging times the dominant influence upon σ_y is plume meander, which is essentially uncorrelated with (local) surface roughness; we follow observation and take σ_y independent of the surface roughness.

The influence upon horizontal standard deviation of plume meander and concentration averaging time effect has the form of the power law $(\tau/\tau_{PG})^{0.2}$ (Hanna 1982). Vertical spectra differ from horizontal as the result of the geometrical influence of the ground, so that for long averaging times no further increase in σ_z with averaging time is to expected. For such times the vertical spectrum is fully active in determining turbulent diffusion. Equally for very short averaging times turbulent diffusion is dominated by small-scale eddies, the distribution of which is roughly homogeneous. This suggests that for short averaging times the functional dependence of both σ_z and σ_y on averaging time τ should be identical, whereas, near the ground, or for long averaging times, σ_z should be independent of τ . We propose, following Hanna (1982) and Pasquill (1976), the dimensioned forms:

Effects of surface roughness, plume centroid height, and concentration averaging-time:

$$\begin{aligned}\sigma_y &= \sigma_y^{PG} (\tau/\tau_{PG})^{0.2}; \\ \sigma_z &= \sigma_z^{PG} (z_r/z_r^{PG})^{0.2} \{\min[\tau, (z_{cm}/100)\tau_{PG}, \tau_{PG}]/\tau_{PG}\}^{0.2}; \\ z_r &> 0; \quad z_{cm} > \geq 0; \quad \tau \geq \tau_{match} > 0.\end{aligned}$$

[Notation: z_{cm} , plume-section centroid height (m); τ , concentration averaging time (s); $\tau_{match} \approx 19s$, effectively "instantaneous" averaging time (TNO 1990); $z_r > 0$, ground surface roughness.]

§6.3: Local versus Integral Average Properties: Near/Far field Matching.

The nearfield model HFPLUME is idealised particularly in respect of the shape of the cross-wind profiles of concentration and temperature. Predictions are made not of point-local but of average behaviour within each plume cross-section, and take properly into account the several effects of source momentum, orientation, and dense gas dispersion in determining air entrainment and the development of the plume trajectory. Farfield dispersion is similarly idealised. Predictions are made of local (particularly ground-level) concentrations; no account is taken of near source effects influencing plume trajectory. The far-field dispersion of plumes is independent of release conditions except inasmuch as they determine the downwind displacement, height above ground, and strength of an equivalent point source.

Consider an asymptotically neutral or marginally buoyant release downwind of release. In the near-field predictions are available of entrained air mass-flux, released mass-flux HF, and the excess (above ambient) fluxes of momentum and total energy. Sufficiently far from the source the conditions for passive dispersion of an inert pollutant are well met: chemical reaction has all but ceased; the influences of release buoyancy and initial momentum largely spent. At such distances the sectional-average predictions supplied by HFPLUME (say) correspond closely to those of a matched Pasquill/Gifford (Gaussian) plume. Equating fluxes deduced from Gaussian far-field and "top-hat" near-field models will then furnish a set of non-linear integral equations for the virtual source

location, and will define the Pasquill/Gifford plume at the transitional or "matching" plane and at greater distances downwind of release.

Matching Equations:

$$\langle dm/dt \rangle|_{HF} = \int_0^\infty dz \int_{-\infty}^{+\infty} dy \, cu ;$$

$$\langle dm/dt \rangle|_{N_2O_2} = \int_0^\infty dz \int_{-\infty}^{+\infty} dy \, [(\rho - c)u - \rho_\infty u_\infty] ;$$

$$\langle dP_x/dt \rangle = \int_0^\infty dz \int_{-\infty}^{+\infty} dy \, \rho u(u - u_\infty) ;$$

$$\langle dE/dt \rangle = \int_0^\infty dz \int_{-\infty}^{+\infty} dy \, [h + (1/2)u^2 - h_\infty - (1/2)u_\infty^2] \rho u .$$

[Notation: $\langle dm/dt \rangle|_{HF}$, mass-flux of HF pollutant $\langle dm/dt \rangle|_{N_2O_2}$, mass-flux of entrained air $\langle dP_x/dt \rangle$, mass-flux excess (horizontal) momentum $\langle dE/dt \rangle$, mass-flux excess above ambient total-energy; (c, ρ, h, u) , point-local mass-concentration HF, total density, specific enthalpy, and (horizontal) velocity; $(\rho_\infty, h_\infty, u_\infty)$, ambient air density, ambient air specific enthalpy, and wind-speed. The notation "<...>" refers to a sectional-average value such as is predicted by the near-field model HFPLUME.]

The equations express the invariance between plume descriptions of $\langle dm/dt \rangle|_{HF}$, the HF mass-flux, $\langle dm/dt \rangle|_{N_2O_2}$, the entrained air mass-flux, $\langle dP_x/dt \rangle$, the excess horizontal momentum, and $\langle dE/dt \rangle$, the excess above ambient of total energy. The pressure P_∞ within the plume is essentially that (hydrostatic) value within the undisturbed atmosphere.

Pasquill/Gifford Profiles:

The assumption of a Gaussian plume/"image"-plume description of the far-field dispersion yields for the mass-concentration, and for the excess velocity the explicit profiles:

$$\begin{aligned}
 c/c_{\star} &= \psi(y,z;\sigma_y,\sigma_z,z_{PG}); \\
 (u-u_{\infty})/(u_{\star}-u_{\infty}) &= \psi(y,z;\varepsilon\sigma_y,\varepsilon\sigma_z,z_{PG}); \\
 \psi(y,z;\sigma_y,\sigma_z,z_{PG}) &= \exp(-y^2/2\sigma_y^2) [\exp(-(z-z_{PG})^2/2\sigma_z^2) + \exp(-(z+z_{PG})^2/2\sigma_z^2)]; \\
 \sigma_y, \sigma_z &= (\sigma_y, \sigma_z)(\Delta x=x_{PG}-\langle x \rangle, y=0, z_{PG}; \tau=\tau_{match}, z_{cm}=\langle z \rangle, z_r). \\
 0 \leq z, \quad x \geq 0, \quad -\infty < y < \infty, \quad \langle z \rangle, \sigma_y, \sigma_z &\geq 0.
 \end{aligned}$$

[Notation: ε^2 , turbulent Schmidt number; $u_{\star}-u_{\infty}$, "centre-line" excess of horizontal velocity $\langle z \rangle$, near-field centroid height; τ_{match} , "instantaneous" (concentration) averaging-time z_r , level ground surface roughness.]

The averaging time appropriate to the standard deviations σ_y and σ_z must be chosen for comparability with the near-field description underlying the entrainment assumptions of (say) HFPLUME. Such an averaging time is certainly short, and may be regarded as effectively "instantaneous". Reference to TNO (1990) yields for an "instantaneous" average the effective averaging time $\tau_{match} \approx 19s$. Note that in addition to the expected profile for the mass concentration $c(x,y,z)$, a second related profile has been introduced for the excess-velocity $(u-u_{\infty})(x,y,z)$. This reflects the broad comparability of density and velocity differences in the near-field, and the desire to assign both influences equal weight in the criteria of matching. The velocity profile is identical in form to the Gaussian image system proposed for concentration; the standard deviations are scaled by the far-field turbulent Schmidt number ($\varepsilon^2 = 1.35$) to reflect the

different rates of mass and momentum diffusion (Rouse, Yih and Hyumphreys 1952; Ooms 1972).

Local Thermal Equilibrium:

The assumption of thermal equilibrium allows the **point-local** thermodynamic relation

$$(h+(1/2)u^2-h_{\infty}-(1/2)u_{\infty}^2)=(c/\rho)(\langle dE/dt \rangle / \langle dm/dt \rangle |_{HF}),$$

to be developed. This equation may be motivated as follows: First consider the integral-averaged plume description, and in particular the total energy-flux $\langle dE/dt \rangle$ passing a given cross-section. The mean-flow may be assumed to result from the uniform mixing of a pure HF stream of mass-flux $\langle dm/dt \rangle_{HF}$ with an ambient air stream of mass-flux $\langle dm/dt \rangle_{N_2O_2}$. The pure HF stream has therefore the specific enthalpy $\langle dE/dt \rangle / \langle dm/dt \rangle_{HF}$ above ambient values. Next abstract unit mass of HF/moist-air mixture from within a plume cross-section. The sample possesses a definite mass-fraction c/ρ of HF: it results from the intimate mixing of two parcels of material; the one (pure HF) of mass c/ρ , the specific energy content of which (relative to the ambient air) is $(\langle c \rangle / \langle \rho \rangle)(\langle dE/dt \rangle / \langle dm/dt \rangle_{HF})$; the other air of mass $1-c/\rho$ and **zero** specific energy. The mixture specific total energy is correspondingly $h-h_{\infty}+(1/2)u^2-(1/2)u_{\infty}^2$. The point local relationship follows from energy conservation. The non-linear equation

$$\langle dE/dt \rangle = \int_0^{\infty} dz \int_{-\infty}^{+\infty} dy (h+(1/2)u^2-h_{\infty}-(1/2)u_{\infty}^2)\rho u ;$$

is then satisfied identically. The equation system for near/far-field matching then provides a set of three non linear equations in the "centre-line"

concentration c_* , the centre-line velocity-excess $u_* - u_\infty$, and in the virtual origin location $(x_{PG}, z_{PG} \geq 0)$. An additional equation is therefore needed to close the equation system.

Model Closure: Centroid, Buoyant Potential Energy, and Angular Momentum.

Recall the importance of the plume centroid or "centre of mass" in model formulation: this suggests that the plume centroid height be invariable between the near and far-field descriptions. The matching equation then becomes

$$\langle z \rangle = \left[\int_0^\infty dz \int_{-\infty}^{+\infty} dy \, z(\rho - \rho_\infty) \right] / \left[\int_0^\infty dz \int_{-\infty}^{+\infty} dy \, (\rho - \rho_\infty) \right].$$

This equation is straightforward; it accurately reflects the systematic rise in the Pasquill/Gifford centroid height with increasing downwind distance, a variation not followed by the virtual source. It differs significantly in functional form from the other matching conditions, which represent the invariance between near and far-field descriptions of the material **fluxes** whether of HF, entrained air, excess (horizontal) momentum, or excess total-energy. We suggest that the final (closure) equation should express the invariance of some physically based flux. Such considerations lead, rather naturally, to the invariance of the buoyancy potential-energy flux,

$$\langle dB/dt \rangle = \int_0^\infty dz \int_{-\infty}^{+\infty} dy \, gz(1 - \rho_\infty/\rho)\rho u.$$

Equally some account should be taken of residual differences between plume and ambient velocities at the plane of matching; this in addition to the (hydrostatic) "centre of gravity" effects governed by density differences alone. We suggest that the excess above ambient values of plume **angular momentum** be conserved.

Taking moments from the point of the matching plane of maximum ground-level concentration yields the equation,

$$\langle dL_y/dt \rangle = \int_0^\infty dz \int_{-\infty}^{+\infty} dy \, z(u-u_\infty)\rho u .$$

Matching is not influenced by the choice of origin for L_y . This equation has the form of a physically derived flux, and is, in the limit of negligible velocity difference, equivalent to centroid invariance. Account is now taken of velocity differences on a equal footing with density differences analogously to the remaining conservation equations.

It is, however, **impossible** simultaneously to satisfy buoyant-energy and angular-momentum flux conservation. This illustrates a general problem of matching, that only a limited number of physical invariants can be transferred between matched models, the limit (here) being set by the Pasquill/Gifford far-field. Introducing a velocity profile allows a rather better transfer of momentum related information than would otherwise have been possible; however it does not seem possible to introduce sufficient degrees of freedom to encompass $\langle dL_y/dt \rangle$ and $\langle dB/dt \rangle$ invariance. In the circumstances we must **choose** which invariant will be conserved. Inasmuch as the buoyancy flux occurs explicitly as a major determinant of near-field behaviour, whereas the angular momentum is only implicitly calculated, we prefer $\langle dB/dt \rangle$ invariance for the calculation of the far-field.

Existence of Matched (Far-field) Solutions:

It is a general feature of non-linear equations that physically appropriate solutions may not exist for certain ranges of the input parameters. Certainly,

circumstances may arise under which the matching of a near-field description and a far-field Pasquill/Gifford model may be inappropriate: source momentum may be significant; heavy gas effects may predominate. Even under near passive conditions sufficient "memory" of earlier (heavy gas, say) dispersion may be retained to prevent physically sensible matching: the solution space, in terms of the matching variables $\langle dm/dt \rangle|_{HF}$, $\langle dm/dt \rangle|_{N_2O_2}$, $\langle dP_x/dt \rangle$, $\langle dB/dt \rangle$ needs to be examined. This discussion is deferred until an appropriate asymptotic analysis of the non-linear system has been carried out.

§6.4: System Asymptotics: the Limit of Great Dilution.

Inasmuch as the Pasquill/Gifford formulation applies to **passive** dispersion, significant departures between plume and ambient atmosphere at the plane of transition are inappropriate. It is not necessary to solve the matching equations in full generality; it suffices to examine the solution space in the limit of great plume dilution.

First order expansion about the ambient state $(\rho_\infty, T_\infty; P_\infty)$ yields estimates of the enthalpy and temperature excess above ambient, together with estimates of the centre-line concentration and velocity-excess. Vertical variation within the plume is neglected, with the wind-speed and ambient density assigned (mean) values $\langle u_\infty \rangle$ and $\langle \rho_\infty \rangle$ evaluated at the (near-field) centroid height $\langle z \rangle$.

First Order Approximation:

$$(h-h_\infty)/(c_p^\infty T_\infty) = (T/T_\infty - 1);$$

$$1 - T/T_\infty = (\rho/\rho_\infty - 1) + (\mu_\infty/\mu_{HF} - 1)c/\rho_\infty;$$

$$c_*/\rho_\infty = (\beta/2/\pi)(\langle c \rangle/\rho_\infty); \quad \beta = \langle A \rangle/(\sigma_y \sigma_z);$$

$$u_*/u_\infty - 1 = (\beta \epsilon^2/2/\pi)(\langle u \rangle/u_\infty - 1);$$

$$\langle z \rangle = (1/\sqrt{\pi}) \exp(-\eta^2) + (1/2) \eta \operatorname{erf}(\eta); \quad \eta = z_{PG}/(\sigma_z \sqrt{2});$$

$$|\langle \rho \rangle/\rho_\infty - 1| \ll 1, \quad |\langle c \rangle/\rho_\infty| \ll 1,$$

$$|\langle u \rangle/u_\infty - 1| \ll 1, \quad |u_\infty^2/(2c_p^\infty T_\infty)| \ll 1.$$

[Notation: $\operatorname{erf}(\eta) = (2/\sqrt{\pi}) \int_0^\eta e^{-\xi^2} d\xi$, standard error function (Abramowitz and Stegun 1972); c_p^∞ , ambient (moist) air (isobaric) specific heat μ_∞ , ambient air (mean) molecular weight μ_{HF} , molecular weight HF-monomer; $\langle z \rangle, \langle A \rangle$ near-field plume centroid height and (effective) cross-sectional area; $\langle c \rangle, \langle \rho \rangle$ near-field (integral-average, HF mass-concentration and total-density; $\langle u \rangle$, near-field (mean) flow-velocity; $(u_\infty, \rho_\infty, T_\infty)$ mean wind-speed, atmosphere density, and (absolute) temperature; (ρ, c, h, T) , point-local density, concentration, specific enthalpy, and absolute temperature; h_∞ , atmosphere specific enthalpy.]

Note that the virtual origin is not located by first order matching; the quantity $\langle A \rangle/(\sigma_y \sigma_z)$ being undetermined. Second order asymptotic analysis yields the required equation,

Second Order Closure:

$$\langle A \rangle/(\sigma_y \sigma_z) = 4\pi [\Delta^2 h + 2h_\rho \delta_u (\delta_\rho + \delta_u)] / [I(1,1) \Delta^2 h + 2h_\rho \delta_u (I(1,\epsilon) \delta_u + I(\epsilon,\epsilon) \delta_\rho)];$$

$$\Delta^2 h = h_{\rho\rho} \delta_\rho^2 + 2h_{\rho c} \delta_\rho \delta_c + h_{cc} \delta_c^2 + 2h_\rho \delta_\rho^2 + 2h_c \delta_\rho \delta_c;$$

$$I(\epsilon, \mu) = 2\epsilon^2 \mu^2 / (\epsilon^2 + \mu^2) \{ 1 + \exp[-2\epsilon^2 \mu^2 / (\epsilon^2 + \mu^2) (z_{PG}/\sigma_z)^2] \};$$

$$h_\rho = \rho_\infty / (c_p^\infty T_\infty) \partial(h - h_\infty) / \partial \rho|_c; \quad h_c = \rho_\infty / (c_p^\infty T_\infty) \partial(h - h_\infty) / \partial c|_\rho;$$

$$h_{\rho\rho} = \rho_{\infty}^2 / (c_p^{\infty} T_{\infty}) \partial^2 (h - h_{\infty}) / \partial \rho^2 |_c; \quad h_{cc} = \rho_{\infty}^2 / (c_p^{\infty} T_{\infty}) \partial^2 (h - h_{\infty}) / \partial c^2 |_p;$$

$$h_{\rho c} = \rho_{\infty}^2 / (c_p^{\infty} T_{\infty}) \partial^2 (h - h_{\infty}) / \partial \rho \partial c; \quad \delta_{\rho} = \langle \rho \rangle / \rho_{\infty} - 1; \quad \delta_c = \langle c \rangle / \rho_{\infty}; \quad \delta_u = \langle u \rangle / u_{\infty} - 1;$$

together with the consistency constraints,

$$|\langle u \rangle / u_{\infty} - 1| |4\pi - \beta \varepsilon^2 I(1, \varepsilon)| < 4\pi, \quad \beta = \langle A \rangle / (\sigma_y \sigma_z),$$

$$|(\langle u \rangle / u_{\infty} - 1)[4\pi - \beta \varepsilon^2 I(1, \varepsilon)] + (\langle \rho \rangle / \rho_{\infty} - 1)[4\pi - \beta I(\varepsilon, \varepsilon)]| < 4\pi.$$

The virtual origin is then located relative to the matching plane $x = \langle x \rangle$ at such height z_{PG} above ground, and such horizontal displacement $\Delta x = x_{PG} - \langle x \rangle$ that the (leading order) area and centroid matching satisfies the equation set:

Virtual Origin Location:

$$\langle z \rangle = (1/\sqrt{\pi}) \exp(-\eta^2) + (1/2) \eta \operatorname{erf}(\eta); \quad \eta = z_{PG} / (\sigma_y \sigma_z);$$

$$\langle A \rangle / (\sigma_y \sigma_z) = 4\pi [\Delta^2 h + 2h_{\rho} \delta_u (\delta_{\rho} + \delta_u)] / [I(1, 1) \Delta^2 h + 2h_{\rho} \delta_u (I(1, \varepsilon) \delta_u + I(\varepsilon, \varepsilon) \delta_{\rho})];$$

$$\Delta^2 h = h_{\rho\rho} \delta_{\rho}^2 + 2h_{\rho c} \delta_{\rho} \delta_c + h_{cc} \delta_c^2 + 2h_{\rho} \delta_{\rho}^2 + 2h_c \delta_{\rho} \delta_c;$$

$$I(\varepsilon, \mu) = 2\varepsilon^2 \mu^2 / (\varepsilon^2 + \mu^2) \{1 + \exp[-2\varepsilon^2 \mu^2 / (\varepsilon^2 + \mu^2) (z_{PG} / \sigma_z)^2]\};$$

$$\sigma_y, \sigma_z = (\sigma_y, \sigma_z) (\Delta x = x_{PG} - \langle x \rangle, z_{PG}; \tau = \tau_{\text{match}}, z_{cm} = \langle z \rangle, z_r).$$

[Notation: $\langle x \rangle$, downwind distance from release of the plane of matching; $\langle z \rangle$, near-field plume centroid at matching; τ_{match} , "instantaneous" matching time; ε^2 , turbulent Schmidt number; $\langle u \rangle$, near-field (mean horizontal) velocity.]

This non-linear system, though complex, has (plausibly) a **unique** solution for assumed monotone increasing standard deviations σ_y and σ_z and for $x_{PG} \leq \langle x \rangle$, **provided** only that $\langle z \rangle / \sigma_z \geq \sqrt{(2/\pi)}$; otherwise **no** solution exists. In the absence

of a solution we presume a ground-level (virtual) source, and solve for the (demonstrably) **unique** root of the second order equation in $\langle A \rangle / (\sigma_y \sigma_z)$, $z_{PG} = 0$.

The solution is regular in the limit of passive dispersion, and where matching is dominated by densimetric or velocity differences: second order matching then yield the results,

$$\begin{aligned}\langle A \rangle / (\sigma_y \sigma_z) &\rightarrow 4\pi/I(1,1), \quad \langle u \rangle \rightarrow u_\infty; \\ \langle A \rangle / (\sigma_y \sigma_z) &\rightarrow 4\pi/I(1,\varepsilon), \quad \langle \rho \rangle \rightarrow \rho_\infty. \\ \langle A \rangle / (\sigma_y \sigma_z) &= 4\pi/I(1,1), \quad \langle \rho \rangle = \rho_\infty, \quad \langle u \rangle = u_\infty, \quad \langle c \rangle \neq 0.\end{aligned}$$

Certain consistency conditions need be imposed on the quantities $\langle \rho \rangle$ and $\langle u \rangle$ at matching. The empirical form of σ_y is severely "pathological" for $0 < \langle x \rangle - x_{PG} \ll 1\text{mm}$ and for $\langle x \rangle - x_{PG} \gg 10\text{km}$, that is outside the correlated range $10\text{m} < \langle x \rangle - x_{PG} < 10\text{km}$, say. Aphysical solutions so arising are very unlikely to intrude upon asymptotic matching.

§6.5: Prediction of (Steady) Far-field Dispersion.

Having located the virtual origin, it remains only to evaluate for each downwind displacement $x \geq \langle x \rangle$ the Pasquill/Gifford standard deviations σ_y and σ_z associated with the required concentration averaging-time $\tau \geq \tau_{\text{match}}$. Note that the vertical standard deviation σ_z depends implicitly upon the local centroid height z_{cm} via the equation

$$z_{cm} = (1/\sqrt{\pi})\exp(-\eta^2) + (1/2)\eta\text{erf}(\eta); \quad \eta = z_{PG}/(\sigma_z\sqrt{2}).$$

The solution for the pair $(\sigma_z, z_{cm} \geq 0)$ is (demonstrably) **unique**. Note that for displacements for which $z_{cm} > 100\text{m}$ the dependence of σ_z upon z_{cm} is ended, and explicit calculation recovers first σ_z and then (if required) z_{cm} . Armed with the "width" parameters σ_y , and σ_z the local concentration at downwind distance $x > \langle x \rangle$, height $z \geq 0$, and (horizontal) off-axis distance y is to leading order,

$$c(x,y,z)/c_* = \psi(y,z;\sigma_y,\sigma_z,z_{PG}); \quad c_* = dm/dt|_{HF}/[2\pi u_\infty \sigma_y \sigma_z];$$

$$\psi(y,z;\sigma_y,\sigma_z,z_{PG}) = \exp(-y^2/2\sigma_y^2) [\exp(-(z-z_{PG})^2/2\sigma_z^2) + \exp(-(z+z_{PG})^2/2\sigma_z^2)];$$

$$0 \leq z; \quad x_{PG} < \langle x \rangle \leq x; \quad -\infty < y < \infty; \quad z_{PG}, \sigma_y, \sigma_z \geq 0.$$

The local velocity excess is calculated similarly.

§6.6: Transient Effects: Releases of Limited Duration.

Thus far we have presumed that steady state conditions either exist or will develop throughout the asymptotic farfield. In practice, however, spill duration may be a few minutes; whereas the establishment of steady conditions at kilometer distances requires tens of minutes or even hours. Such disparate timescales are especially significant for high consequence, low probability events, for example catastrophic storage vessel failure: steady-state predictions are in such cases not merely conservative, but unrealizably large. There is, therefore, a practical need for "best estimate" values reflecting (more or less accurately) the influence of release duration upon peak concentrations in the farfield.

Downwind Diffusion:

Limited duration, "puff", releases disperse both perpendicular and parallel to the ambient wind: dispersion occurs in response not only to eddy diffusion, but also (Hanna 1982) to the cumulative effect of wind-shear. We follow Ermak (1986, 1989), and Blewitt, Yohn, and Ermak (1987), in representing downwind dispersion (in the context of a Gaussian plume model) in terms of the plume standard deviation σ_x . The (time/meander-averaged) standard deviation attributable to downwind diffusion is taken to be (essentially) equal to the standard deviation σ_y , horizontal and perpendicular to the ambient wind. The effect of wind-shear is represented after Smith (1965), except that attention has been given to elevated as well as ground-level sources. The proposed formulation is as follows:

$$\sigma_x^2 = \sigma_y^2 + [2/(3\pi)] \sigma_z^2 \left\{ \left(du_\infty/dz \right) \Big|_{z_{cm}} \left(\Delta x/u_\infty \right) \Big|_{z_{cm}} \right\}^2.$$

Note that the gradient du_∞/dz is evaluated at the plume centroid height z_{cm} rather than at Smith's (1965) reference height of $\sigma_z/2$. This choice is representative of the (mean) wind-shear not only for grounded but also for elevated plumes. The coefficient $[2/(3\pi)]$ multiplying the wind-shear term ensures predictions identical to Smith (1965) for grounded plumes and neutral stability.

Prediction of Peak Concentrations

Gaussian plume modeling is based upon the (**steady-state**) solution of the diffusion equation for a fixed point-source, uniform wind, and constant (eddy-) diffusivities. This (naive) formulation suggests the Gaussian form upon which the highly successful Pasquill/Gifford model is constructed. Perhaps encouraged by this success, Ermak (1986) formulated a transient release model based upon the general solution of the above diffusion equation in the (Green's function) form:

$$\begin{aligned}
c(x,y,z;t) &= \int_{-\infty}^{+\infty} d\tau \, (dm/dt)(\tau) G(x,y,z;t-\tau); \\
G(x,y,z;\tau) &= G_x(x;\tau) G_y(y) G_z(z); \\
G_x(x;\tau) &= [\sqrt{(2/\pi)/\sigma_x}] \exp[-(x-x_{PG}-u_{\infty}\tau)^2/(2\sigma_x^2)]; \\
G_y(y) &= 1/[\sqrt{(2\pi)\sigma_y}] \exp[-y^2/(2\sigma_y^2)]; \\
G_z(z) &= 1/[\sqrt{(2\pi)\sigma_z}] \{ \exp[-(z-z_{PG})^2/(2\sigma_z^2)] + \exp[-(z+z_{PG})^2/(2\sigma_z^2)] \}; \\
\sigma_x(\tau) &= \sqrt{(2K_x\tau)}; \quad \sigma_y(\tau) = \sqrt{(2K_y\tau)}; \quad \sigma_z(\tau) = \sqrt{(2K_z\tau)}.
\end{aligned}$$

[Notation: dm/dt (momentary) mass release-rate (kg/s); $(x_{PG},0,y_{PG})$ location of the fixed (point) source (K_x,K_y,K_z) eddy diffusivities parallel and perpendicular to the ambient wind; (x,y,z,t) coordinates and time following first release at which the (mass-) concentration c is to be evaluated.]

Formally the plume standard deviations $(\sigma_x, \sigma_y, \sigma_z)$ are functions of the elapsed **time** from the moment of release. We nevertheless follow Ermak (1986) in interpreting σ_x, σ_y , and σ_z as known (above specified) functions of the **distance** (x) downwind of a fixed source. The (reinterpreted) solution $c(x,y,z;t)$ forms a "template" for a transient (Pasquill/Gifford) model of farfield diffusion. The solution $c(x,y,z;t)$ is further simplified by presuming a **steady** source of **limited** duration. The source function $dm/dt(t)$ assumes the form,

$$\begin{aligned}
dm/dt(t) &= \begin{cases} 0, & -\infty < t < 0, \\ (dm/dt)|_{\infty}, & 0 < t < \tau_{\infty}, \\ 0, & \tau_{\infty} < t < \infty, \end{cases}
\end{aligned}$$

with corresponding farfield concentration,

$$c(x,y,z;t)/[G_y G_z (dm/dt)|_{\infty}] = (1/2) \operatorname{erf}\left\{ \eta/(\sigma_x \sqrt{2}) \right\} \Big|_{\eta=\Delta x - u_{\infty} \min(0, t - \tau_{\infty})}^{\eta=\Delta x - u_{\infty} t}.$$

[Notation: $\Delta x = x - x_{PG}$ distance downwind of the (virtual) point source $dm/dt|_{\infty}$ (sustained) mass release-rate $\text{erf}(\eta) = (2/\sqrt{\pi}) \int_0^{\eta} e^{-\xi^2} d\xi$, standard error function (Abramowitz and Stegun 1972).]

For each downwind distancement (x) the time (t) at which occurs the maximum concentration corresponds to the (unique) root of the (turning point) equation $\partial c / \partial t = 0$. The maximum concentration at distance x downwind of release is therefore (Ermak 1986),

$$c_{\max}(x, y, z) / [G_y G_z (dm/dt)|_{\infty}] = (1/2) \text{erf}\left\{ (1/\sqrt{2}) [\min(\Delta x, (1/2) u_{\infty} \tau_{\infty}) + \eta] / \sigma_x \right\} \Big|_{\eta=0}^{\eta=u_{\infty} \tau_{\infty}},$$

with the steady-state value recovered in the limit of infinite release duration. Release maximum and steady-state concentrations are then related by the (dimensionless) factor,

$$c_{\max} / c_{\text{state}}^{\text{steady}} = \text{erf}\left\{ \sqrt{2} [\min(\Delta x, (1/2) u_{\infty} \tau_{\infty}) + \eta] / \sigma_x \right\} \Big|_{\eta=0}^{\eta=u_{\infty} \tau_{\infty}} / \{1 + \text{erf}[\Delta x / (\sigma_x \sqrt{2})]\},$$

which provides an **approximate** correction for the combined effects of downwind diffusion and of release duration. The correction acts upon steady-state values estimated from asymptotic matching and by the straightforward use of standard Pasquill/Gifford formulae.

§6.7: Computer Implementation; Conclusions.

In the far-field the calculation of plume dispersion by means of an entrainment based (intergal-averaged) description is both highly uncertain and seriously inefficient. Such models as exist currently (Bloom 1980) derive

entrainment from an analysis of observed dispersion behaviour summarized in the Pasquill/Gifford curves; any satisfactory formulation of entrainment must, in the far-field, recover the observed results.

Such far-field performance is best achieved by means of (asymptotic) "matching"; that is by preserving at some matching plane a set of physically derived fluxes generated in the near-field by an integral-averaged model. This results in the identification of a virtual (point) source, such that a Pasquill/Gifford plume at the matching plane is, as regards several physical fluxes, identical to that predicted near the actual source. Beyond the matching plane, dispersion behaviour is taken to be that derived for a Pasquill/Gifford model. Approximate correction may be made for limited duration releases and for downwind diffusion using an (error function) correction suggested by Ermak (1986). The formulation, though tentative, should provide an estimate of the "conservatism" inherent in assigning steady-state predictions to high consequence, short duration releases of anhydrous HF.

Matching is achieved in the limit of large dilution, for which buoyancy effects, mis-alignment of plume and wind, and the influence of release momentum are all but negligible. Matching takes proper account of differences in vertical and horizontal diffusion, and of the influence upon these of concentration averaging times, and the proximity of the ground. Once the virtual source is located concentrations, may be predicted for **any** required averaging time, and for any point downwind of the plane of matching.

A FORTRAN 77 (Monro 1982) computer program PGPLUME has been written incorporating the above (asymptotic) theory. Information derived (presumably) from the near-field dispersion model HFPLUME (Chapter 5) is used by PGPLUME in order to locate the virtual origin of a far-field equivalent Pasquill/Gifford point-source. Thereafter PGPLUME returns (source duration corrected)

Pasquill/Gifford predictions of dispersion behaviour in the far-field. The analysis of far/near field matching is independent of the thermodynamic behaviour of hydrogen fluoride, inasmuch as the analysis is carried out in the (unassociated monomer) limit of great HF dilution. PGPLUME is, in effect, a "post-processor" to HFPLUME (or indeed PLUME) to be used beyond the limits of PLUME/HFPLUME when the near-field dispersion remains "airborne", or at least does not credibly merge into a heavy-gas advected plume in the manner of HEGADAS (Appendix 3, Colenbrander and Puttock 1988).

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7. NEW FEATURES IN THE HEAVY-GAS-DISPERSION PROGRAM HEGADAS

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7.1. INTRODUCTION

7.1.1. General introduction

This section describes the dispersion model HEGADAS. This model can be used in the HGSYSTEM software package after the models EVAP, HFFLASH, or HFPLUME. There are two versions of the HEGADAS model, i.e. HEGADAS-S for steady-state releases and HEGADAS-T for transient or finite duration releases. HEGADAS-T should be used for situations where the travel time to a distance of concern is greater than the release duration.

This section describes a revised version of HEGADAS, called HEGADAS-5. HEGADAS was developed for modelling heavy gas dispersion around area sources. The model was originally formulated by Colenbrander (1980) for both cases of steady-state and transient releases (versions called HEGADAS-1 and HEGADAS-2). In a later stage the model was extended to include heat and water vapour effects (versions called HEGADAS-3 and HEGADAS-4). A detailed technical description of the public-release version HEGADAS-4 (Witlox (1988)) of the program HEGADAS is given in Appendix 3 and the basic concepts of the program HEGADAS are summarised in Section 7.1.2.

The revised program HEGADAS-5 is a considerably extended version of the previous HEGADAS-4 program. The goals in enhancing the HEGADAS model were

- to provide an HF-thermodynamics option in addition to simulating the thermodynamics of ideal gases
- to improve the crosswind-spreading formulation for dense-gas clouds
- to improve the formulation of along-wind-diffusion effects for transient or finite-duration releases
- to improve the formulation describing the spreading and evaporation of the gas pool (gas-blanket formulation) for transient or finite-duration releases
- to be able to simulate heavy-gas-dispersion over terrain with varying surface roughness
- to improve the user-friendliness of the model

- to provide interfaces with other HGSYSTEM programs, i.e. the pool evaporation program EVAP and the near-source programs HFFLASH and HFPLUME

An overview of the enhancements in HEGADAS is given in Section 7.1.3. A detailed description of the enhancements is given in Sections 7.2, 7.3, 7.4, 7.5, 7.6 and 7.7.

The physics or fundamentals of the HEGADAS model was developed using experimental laboratory data. Parameters which quantify a particular physical process have been determined, where possible, from laboratory experiments which study that process in isolation. The model was then validated against independent field data to ensure that it correctly describes the effect of these various physical processes in combination. Thus an independence is maintained between the model formulation and the data which is used to verify the model (i.e. HEGADAS is not tuned to any particular field data set). By using this approach, greater confidence can be given to the predictions from the HEGADAS model when it is applied to the simulation of an accidental release. Verifications of the new HEGADAS-5 model are presented in Chapter 8 and 9.

7.1.2. Basic concepts of HEGADAS model

The basic concepts of the heavy-gas-dispersion model HEGADAS are summarised below (see Appendix 3 for details).

1. VELOCITY AND CONCENTRATION PROFILES

For the steady-state version HEGADAS-S, the program adopts a power-law fit of the ambient wind speed for the velocity u (z_0 is a reference height at which the velocity is u_0 ; α is a fitting parameter),

$$u = u_0 \left[\frac{z}{z_0} \right]^\alpha$$

and a similarity profile for the concentration c ,

$$c(x,y,z) = c_A(x) \exp \left[- \left[\frac{z}{S_z(x)} \right]^{1+\alpha} \right], \quad |y| < b$$

$$c(x,y,z) = c_A(x) \exp \left[- \left[\frac{|y| - b(x)}{S_y(x)} \right]^2 - \left[\frac{z}{S_z(x)} \right]^{1+\alpha} \right], \quad |y| > b$$

In the above formulas x, y, z are Cartesian coordinates with the x -, y - and z - directions corresponding to the downwind, crosswind and vertical directions, respectively. The release of the gas is at a rectangular ground-level area source located at $-L < x < L$, $-B < y < B$, $z=0$, with L being the source length and B the source half-width.

Figure 1 in Appendix 3 illustrates the above concentration profile, which is expressed in terms of the following four unknowns:

- the centre-line ground-level concentration c_A , kg / m^3

- the vertical dispersion coefficient S_z (m) defining the decay of the concentration in the vertical direction
- the crosswind dispersion coefficient S_y (m) defining the decay of the concentration along the Gaussian flanks of the crosswind concentration profile
- the half-width b of the middle part of the crosswind profile (along which the ground-level concentration equals c_A), m; as S_y increases, b eventually becomes zero and the crosswind profile is purely Gaussian.

These four unknowns are determined from the following four equations.

- An empirical entrainment law describing the vertical entrainment of air into the gas cloud. This law gives the entrainment velocity as a continuous, decreasing function of the bulk Richardson number $Ri_*(x)$; Ri_* is proportional to the density difference between the gas cloud and the air, and reduces to zero in the far-field, passive-dispersion region.
- A continuity equation describing the conservation of gas mass through a plane $x = \text{constant}$.
- An empirical law describing the gravitational spreading of the gas cloud in the cross-wind direction. In this spreading law the following phases are distinguished:
 - o initial gravitational spreading governed by Van Ulden's spreading law
 - o neglect of gravity spreading downwind of the point at which the crosswind profile becomes purely Gaussian, i.e. the gravity-spreading law is applied for $b > 0$ only.
- An empirical law describing passive diffusion in the crosswind direction. The rate of increase of S_y is related to the lateral growth

of a passive plume (σ_y), with σ_y being related to the downwind distance via a power-law.

2. TIME-DEPENDENT EFFECTS

For the transient version HEGADAS-T the solution is obtained via the following observer concept.

- Observers are released at a series of times upwind of the pool. These observers travel with the wind.
- The pool data observed by each observer are determined.
- For each observer, the observed concentration is computed via steady-state HEGADAS calculations adopting the observed pool data. Thus, by calculating the position of each observer at a given time t , the concentrations are determined at time t for a number of downwind distances from the pool.
- At a given time t the actual concentration is determined from Gaussian integration with respect to the downwind distance x of the above observer concentrations. This Gaussian integration involves a downwind dispersion coefficient σ_x , by means of which longitudinal diffusion is taken into account.

3. HEAT AND WATER VAPOUR EFFECTS

In HEGADAS heat and water vapour effects are included by adding a surface-heat transfer relation and a water-vapour relation for the two additional unknown quantities, i.e.

- the heat H_g added from the surface, Joule / mole of mixture
- the water-vapour y_{w3} added from the surface, mole / mole of mixture

In the thermodynamics of the mixing of the dense gas with the humid ambient air it is assumed in HEGADAS-4 that the mixture components (gas,

air, water) behave as ideal gases with constant specific heats and that the gas is non-reactive.

7.1.3. Enhancements to HEGADAS model

This section gives an overview of the new features in the extended version HEGADAS-5 of the heavy-gas-dispersion program HEGADAS. Details on the use of the steady-state (HEGADAS-S) and transient (HEGADAS-T) versions of HEGADAS are contained in the User's Manual, while further details of the program are given in the System's Manual.

The following presents an overview of the enhancements made to the HEGADAS model.

1. HF-THERMODYNAMICS OPTION

A HF-thermodynamics option is included in addition to ideal-gas thermodynamics. The thermodynamics for HF is complex because of:

- the formation of polymers $(\text{HF})_2$, $(\text{HF})_4$, $(\text{HF})_6$, $(\text{HF})_8$,
- the depolymerisation of the HF to a monomer state (an endothermic reaction), and
- the exothermic reaction of HF with water vapour in the ambient air.

The thermodynamic behaviour of HF has been modelled by Schotte (1987, 1988). This model has been incorporated into HEGADAS. See Chapter 2 and Appendix 5 for further details of this model. Section 7.2 describes the implementation of this model in HEGADAS.

2. IMPROVED CROSS-WIND DISPERSION FORMULATION; TREATMENT OF SURFACE ROUGHNESS; LATERAL GRAVITY SPREADING

The empirical crosswind diffusion power-law relationship adopted in HEGADAS for the crosswind dispersion coefficient S_y may be inaccurate at large distances downwind of the source. Section 7.3.1 presents a generalised formulation, which allows for the use of the formula by Briggs (1973) for the crosswind diffusion.

Previous verifications of HEGADAS and other dense gas dispersion models have been made using field experiments in which the surface roughness was very small, i. e. typically 0.00006 to 0.003m. (Ermak et al., 1988). To study the application of HEGADAS to higher roughness environments, in the absence of relevant field data, wind tunnel data on dense and trace gas releases (Petersen and Ratcliff, 1989) have been used. A major finding from this is that, for releases in a turbulent boundary layer which are strongly affected by gravity-spreading, the organised structure of the gravity current can "collapse" at some stage. Subsequently the gravity-driven lateral spreading is much reduced. This phenomenon was also found in suitable experiments at low surface roughness. Section 7.3.2 describes a modification to the gravity-spreading law which takes this effect into account.

After the inclusion of this modification, the existing entrainment formulation in HEGADAS was found empirically to give reasonable predictions for high surface roughness (uniformly distributed obstacles), and this formulation has not been changed.

3. IMPROVED DOWNWIND SPREADING FORMULATION FOR TRANSIENT OR FINITE DURATION RELEASES

The formula adopted in HEGADAS for the downwind dispersion coefficient σ_x was not based on well-established data. It was a direct function of the downwind distance x , but did not account for the wind shear near the ground and therefore was not dependent on atmospheric stability.

Section 7.4 includes a literature review of along-wind-diffusion formulations. Formulations from Chatwin (1968), Wilson (1981) and Ermak (1986) have been implemented in adapted form in HEGADAS as new options for evaluating σ_x :

- In an adapted Ermak/Wilson formulation σ_x is a direct function of x , which depends only on the stability class and the exponent α in the power-law fit to the ambient logarithmic wind-speed profile.

- In an adapted, more rigorous Chatwin/Wilson formulation σ_x is not a simple, direct function of x , but it is proportional to the ambient friction velocity u_* and the travel time t_{obs} of the observers. Notice that through u_* and t_{obs} , σ_x depends on the ambient wind speed and the stability class. In this formulation along-wind-diffusion is neglected in high-density cloud regions in which the bulk Richardson number is high.

4. IMPROVED GAS-BLANKET FORMULATION FOR TRANSIENT OR FINITE DURATION RELEASES

In Section 7.5 an improved gas-blanket formulation without oscillatory behaviour previously observed in HEGADAS-4 is introduced. This formulation has been implemented as the default option in HEGADAS-T.

5. BREAKPOINT FACILITY

Section 7.6.2 describes the extended breakpoint capabilities of HEGADAS-S. HEGADAS-S now allows for a 'full' breakpoint, whereby the HEGADAS run is started at a specified distance downwind of the source (breakpoint) and gas-blanket calculations are not performed. This facility is used to interface HEGADAS to the near-field models HFPLUME and PLUME.

The program also allows for multiple breakpoints (at several distances downwind of the source). This facility can be used to simulate dispersion over terrain with a varying surface roughness.

Section 7.6.3 describes the new breakpoint facility in HEGADAS-T, in which all required time-dependent data are given at a breakpoint located at a certain specified distance downwind of the source. The breakpoint data may also be interpreted as corresponding to a time-dependent vertical source. The HEGADAS-T calculations are started from this breakpoint.

Section 7.6.4. describes the original, simplified type of breakpoint in HEGADAS-T (partial breakpoint).

6. IMPROVED EFFICIENCY AND USER-FRIENDLINESS; NEW POST-PROCESSORS

The revised version of HEGADAS has an option for the calculation step size to increase in the downwind direction, which can reduce the calculation time considerably. Input to the program has been made more user-friendly and input error checks have been included. The HEGADAS output has been improved, and new interactive post-processors HSPOST (for HEGADAS-S) and HTPOST (for HEGADAS-T) have been developed. Thus the user can quickly print and/or develop data to plot concentration data. See Section 7.7 for further details.

7. INTERFACES WITH NEAR-SOURCE PROGRAMS

See Chapter 4 and the EVAP user's guide (Chapter 5 in the User's Manual) for a description of the interface of HEGADAS with the pool evaporation program EVAP. The program EVAP outputs the (steady-state or time-dependent) pool data, which are required by (the steady-state or transient version of) HEGADAS.

Section 7.8.2 describes the HF-flash calculation program HFFLASH. This program produces as output the post-flash data required by the program HEGADAS (in the form of HEGADAS input panels).

Section 7.8.3 describes the interface of the program HEGADAS with the near-source programs HFPLUME and PLUME (see Chapter 5). HFPLUME/PLUME is first run up to a transition point at a certain downwind distance from the pool, which is derived from appropriate termination criteria. The HFPLUME/PLUME data at the transition point are then converted into corresponding HEGADAS breakpoint data by means of appropriate matching criteria. Subsequently the HEGADAS calculations are started from the transition point.

8. AUTOMATION OF RELEASE OF OBSERVERS FOR TIME-DEPENDENT SOURCES

In HEGADAS-4 the user needed to provide the time interval Δt_{obs} with which observers were released. This procedure required know-how by the user of the observer concept (see Section 7.1.2), since selection of a too large time step lead to inaccurate concentration predictions at the specified output times.

In HEGADAS-5 Δt_{obs} is determined internally in the program to ensure accurate predictions. Section 7.9 discusses in detail the automated release of observers in HEGADAS-T.

7.2. New HF-THERMODYNAMICS OPTION

The reader is referred to Chapter 2 and Appendix 5 for a detailed description of the HF thermodynamics model and a validation of the model with experimental data. This section describes the implementation of this model into the HEGADAS program. First an explanation is provided on how the HF-thermodynamics calculations are carried out in HEGADAS. Secondly the coupling of the HF-thermodynamics with the dispersion calculations is discussed.

HF-Thermodynamics calculations in HEGADAS

In HEGADAS the thermodynamics calculations are performed by the subroutine THERMO. In THERMO, calculations for the cases of normal thermodynamics (for ideal gases) and HF thermodynamics are carried out by calls to the subroutines THRMNO and THRMHF, respectively.

The input and output data to the subroutine THRMHF are described in Appendix 5. Apart from input data which are constant throughout a HEGADAS analysis (ambient humidity and temperature, post-flash data for HF), THRMHF requires as input the solution variables y_{HF} (HF molar fraction) and H_e (added heat from surface), which are a function of the downwind distance. The data to be output are the mixture temperature T , the mixture volume V_m , and the ratio ρ_m/ρ_{amb} of mixture density to ambient air.

The algorithm adopted in the subroutine THRMHF for solving the nonlinear thermodynamic equations is described in Section 2 of Appendix 5. THRMHF solves the thermodynamic equations by calling the subroutine NAESOL. The NAESOL software has been developed by Scales (1989) for the solution of systems of nonlinear algebraic equations. The nonlinear thermodynamic equations to be solved by NAESOL are specified in the subroutine HFVEC. Several precautions are taken in HFVEC to avoid instability in NAESOL and unphysical values for variables, e.g. molar fractions being negative or larger than one.

Coupling of HF-thermodynamics with dispersion calculations

One might consider to calculate the thermodynamic data in HEGADAS by means of a look-up table. As described above these data are a function of both y_{HF} and H_e . Thus a two-dimensional look-up table is required with data given at sufficiently small incremental steps of y_{HF} ($0 \leq y_{HF} \leq 1$) and H_e ($0 \leq H_e \leq H_e^{max}$; H_e^{max} is upper-bound for H_e). The generation in HEGADAS of this look-up table would involve many unnecessary calls to THRMHF and a considerable CPU-time. Instead, the routine THRMHF is called in HEGADAS whenever thermodynamic data are required for specific values of y_{HF} and H_e .

The most frequent calls to the thermodynamics subroutine THERMO (and hence THRMHF) in HEGADAS are made during the numerical integration of the 5 differential equations for S_z , S_y , b , D and y_{w3} in the downwind direction x . This integration is performed by the subroutine STINTS developed by Prothero and Robinson (1973). STINTS solves a set of first-order differential equations by means of an implicit, first-order, A-stable one-step method. STINTS selects a larger step size Δx in the downwind direction if the solution to the differential equations becomes more 'smooth' (i.e. less variation in the derivatives to x of the solution variables), and it selects a smaller value of Δx if it becomes less 'smooth'.

During the development of HEGADAS-5 it was found that STINTS did not adapt quickly enough to the highly nonlinear HF thermodynamic behaviour. This resulted in ill-conditioned Jacobian matrices in NAESOL and/or failure to reach convergence within a specified maximum number of iterations.

In STINTS (solution of differential equations) it was found necessary to take into account the convergence behaviour of NAESOL (solution of algebraic thermodynamic equations) in the selection of the size (Δx) for the next incremental step in the downwind direction. Let ITR be the maximum number of iterations corresponding to all NAESOL calls during a downwind step Δx of STINTS. ITR will be larger for a larger value of Δx . If ITR is too large, the CPU-time required for thermodynamic calculations is high relative to that for the other STINTS calculations. In this case the step size selected in HEGADAS is decreased to reduce the CPU-time required for

the next step (and also the CPU-time required for the entire HEGADAS run) and to avoid failure of convergence in this step.

STINTS allows the next incremental step to be half, equal, or the same as the previous incremental step. The following modifications to the STINTS algorithm have been applied in case of HF-thermodynamics.

- The step size is always halved if ITR is larger than the maximum number of iterations MAXITR, i.e. for $ITR > MAXITR$
- Doubling of the step size is only allowed if ITR is smaller than the minimum number of iterations MINITR, i.e. for $ITR < MINITR$ (with $1 < MINITR < MAXITR$)
- If a failure of convergence in NAESOL occurs during a step Δx , an automatic restart of the step is initiated with a halved step size. The user does not need to specify any data controlling convergence, since the change in step size is controlled by the program itself.

The values MAXITR=12 and MINITR=4 are presently chosen in STINTS. From several trial runs it was found that these values seemed to lead to stable behaviour of HEGADAS and a minimum of CPU-time.

The above procedure has reduced the CPU-time required by HEGADAS considerably. It is noted that the major part of the CPU-time is needed for the dispersion calculations near the source. In this region the thermodynamic solution variables f_1, T, x defined in Appendix 5.2 vary rapidly, which forces the selection of small steps in the STINTS subroutine. Also the very first call of THERMO (e.g. corresponding to the gas blanket or a breakpoint) may lead to many NAESOL iterations, if the initial guess for f_1, T, x is not sufficiently close to the solution root.

7.3. MODIFIED CROSS-WIND DISPERSION AND GRAVITY SPREADING FORMULATION

7.3.1. Equation for cross-wind dispersion coefficient S_y

7.3.1.1. Empirical formulae for cross-wind dispersion coefficient

Original HEGADAS formula for σ_y

Various formulae have been proposed for the dependence of the lateral dispersion coefficient σ_y against x in passive dispersion. These formulae are generally not consistent with a constant lateral diffusivity K_y , but with a K_y which changes as σ_y increases. The reason for this is that, as the plume width increases, successively larger scales of turbulence contribute to the turbulent spread of the plume. In dense gas dispersion the width of the plume can be increased greatly by gravity spreading. HEGADAS does not assume that S_y (the width of the Gaussian edges) is the same function of x as for σ_y . Instead, the assumption taken is that the (turbulent) rate of spread is related to the current width of the plume in the same way as the rate of spread of the passive plume relates to its width. The derivation is described in Appendix 3, Section 4.1.

In the original HEGADAS program the formulae used for σ_y are of the form of a power law in x ,

$$\sigma_y = \delta x^\beta \quad (7.1)$$

where δ and β are dependent on the stability class and the averaging time as given in Table 7.1.

Effects of surface roughness on σ_y

It has been suggested that σ_y should also be taken to be dependent on surface roughness since lateral diffusion is caused by turbulence and the turbulent intensity increases with increasing surface roughness length, being approximately proportional to u_* . As an initial hypothesis, it might

appear reasonable to take σ_y , or particularly δ , proportional to u_* , by analogy with the vertical diffusion parameter, S_z , which increases in proportion to u_* at low Richardson number.

We have examined the experimental evidence which might support a change to a roughness-dependent formula for σ_y using the summary of large scale diffusion experiments compiled by Draxler as our data source. (Draxler, 1984). These data correlations, from experiments with surface roughness lengths between about 0.01 and 1 m, have been compared with the consequential change in σ_y of adopting the above hypothesis (Puttock, 1989).

The experimentally determined dependence of σ_y on surface roughness was found to be much weaker than changes in u_* , especially under unstable conditions, as shown in Figures 7.1-7.4. The experimental results indicated in these figures are quoted best fit lines and these are superposed upon hypothetical curves for 0.001, 0.01, 0.1, and 1.0 m roughness lengths. These match to the HEGADAS values at a z_R of 0.03 m.

Examination of the data from Draxler shows that two studies have been most often used to define σ_y , Prairie Grass and St Louis. The Prairie Grass measurements are described by the Pasquill-Gifford curves which are plotted here. The measurements are for low roughness, 0.01 m, and for distances smaller than 1000 m. The St Louis experiments, analysed by McElroy and Pooler, are for surface roughness values greater than .5 m and for distances of 500 - 5000 m. The latter experiments used one hour sampling times. In Figures 7.1-7.4 the values of σ_y are reduced from a one hour average to a 10 minute average by adopting the common empirical approach that σ_y is proportional to (averaging time)^{0.2}. Briggs (1973) fitted expressions of the form:

$$\sigma_y = \delta x / (1 + \beta x)^{.5} \quad (7.2)$$

to these data classified into "open country" and "urban" categories for the two data sets. For D stability in particular, if the urban results are extrapolated to small distances x , then a larger σ_y is predicted compared

with the open country results. If the open country results are extrapolated above 1 km then similar σ_y values to the urban results are found. The data upon which the Briggs urban correlations are based is rather scattered and does not suggest that extrapolation can be attempted with any confidence.

Other data in Draxler is provided by experiments at Julich, $z_R=1.8$ m, which seem good for stability classes B,C and D. Stable experiments were badly affected by plume meander. The averaging time and range of validity is not known but measurements extended to 10 km. These seem generally to agree with (extrapolated) P-G results. Data from Brookhaven National Laboratory have a probable roughness length between 0.1 and 1.0 m. The data is generally closer to the P-G correlation than to the McElroy Pooler results.

There would seem to be no compelling evidence based on these limited data bases to support the inclusion of a surface roughness dependent expression for σ_y into HEGADAS. In the experiments there is little evidence to support a consistent dependence of σ_y on surface roughness. It is possible that for small averaging times σ_y could be affected by z_R as suggested by Wilson (1990). Data taken over high roughness tends to be longer range than that taken over low roughness. There is a trend for the exponent β to decrease as surface roughness increases. This is anticipated by the Briggs formulation (Briggs, 1973) which has β asymptotically decreasing from a value of 1 in the near field to 0.5 in the far field.

Generalised formula for σ_y in HEGADAS

The expression for σ_y originally in HEGADAS gave values, on the whole, very close to the Pasquill-Gifford curves, with a range of validity up to about 1 km. At greater distances the HEGADAS formulation is likely to give an overestimate of the plume width. If HEGADAS calculations are to be carried out to larger distances, the Briggs formulation is more appropriate. In the following section a generalised formulation for the evaluation of the crosswind dispersion coefficient is introduced, which allows for both the original HEGADAS power-law and Briggs formula. The latter formulation has been implemented as an additional option in HEGADAS.

7.3.1.2. Generalised formulation for calculation of S_y

The derivation of the differential equation for the crosswind dispersion coefficient S_y is given in Section 4.1 of Appendix 3 for the original version HEGADAS-4 of the dense-gas-dispersion program HEGADAS. This derivation is based on an empirical formula for the non-dense crosswind dispersion coefficient σ_y . In HEGADAS-4 this formula is restricted to a power-law dependence of σ_y on the downwind distance x . Thus it does not allow for e.g. Briggs formula (7.2), which as discussed in the previous section is more physically reasonable in the far-field.

In this section a generalised theoretical formulation for the evaluation of S_y is introduced. This formulation allows for any arbitrary empirical function $\sigma_y = \sigma_y(x)$, provided this function can be inverted to $x = x(\sigma_y)$. In this section first the general formulation is given. Secondly the formulation is applied to two specific formulas for σ_y , i.e. the original HEGADAS power-law and Briggs formula. The latter two formulae are presently included as options in HEGADAS.

General formulation

BASIC EQUATIONS AND ASSUMPTIONS

The following basic equations and assumptions are adopted.

1. The crosswind concentration distribution used to describe passive dispersion

$$c = c_A \exp \left\{ -\frac{1}{2} \left(\frac{y}{\sigma_y} \right)^2 \right\} \quad (7.3)$$

is considered, in which c_A is the centre-line concentration and σ_y the crosswind dispersion coefficient.

2. The crosswind dispersion coefficient σ_y is assumed to be known as an invertable, empirical function of the downwind distance x ,

$$\sigma_y = \overline{\sigma_y}[x] \quad (7.4)$$

with the inverse

$$x = \overline{x}[\sigma_y] \quad (7.5)$$

3. The concentration profile (7.3) satisfies the simple two-dimensional diffusion equation

$$u_x \frac{\partial c}{\partial x} = \frac{\partial}{\partial y} (K_y \frac{\partial c}{\partial y}) \quad (7.6)$$

in which u_x is the horizontal wind speed (independent of x and y) and K_y the crosswind diffusion coefficient. K_y is assumed to be proportional to u_x , with the proportional factor k_y being a (to be determined) function of the cloud half-width $W = (\pi/2)^{1/2} \sigma_y$,

$$K_y = u_x k_y = u_x \overline{k_y}[W] \quad (7.7)$$

REDUCED DIFFUSION EQUATION

Upon insertion of equations (7.3) and (7.7) the diffusion equation (7.6) reduces to

$$\frac{1}{c_A} \frac{\partial c_A}{\partial x} + \frac{y^2}{\sigma_y^3} \frac{\partial \sigma_y}{\partial x} = \overline{k_y}[W] \left\{ \frac{y^2}{\sigma_y^4} - \frac{1}{\sigma_y^2} \right\} \quad (7.8)$$

Since the above equation should apply for all y , we deduce the following two equations by equating powers of y ,

$$\frac{1}{c_A} \frac{\partial c_A}{\partial x} = - \overline{k_y}[W] \frac{1}{\sigma_y^2} \quad (7.9)$$

$$\sigma_y \frac{\partial \sigma_y}{\partial x} = \overline{k_y} [W] \quad (7.10)$$

The continuity equation

$$\int_0^\infty c u_x dy = \text{constant} \quad (7.11)$$

is by use of eq. (7.3) easily seen to lead to $c_A u_x \sigma_y = \text{constant}$. Thus it can be shown that the system of equations (7.9), (7.10) is equivalent to the set of equations (7.11), (7.10). Hence equation (7.9) is not considered further, but attention is restricted to the differential equation (7.10) for σ_y .

By inserting eq. (7.4) into eq. (7.10), the dependence of k_y on the cloud half-width W can be determined,

$$k_y = \overline{k_y} [W] = \sigma_y \frac{\partial \overline{\sigma_y}}{\partial x} [\overline{x}[\sigma_y]], \quad \text{with} \quad \sigma_y = \left(\frac{2}{\pi}\right)^{1/2} W \quad (7.12)$$

EQUATIONS FOR THE CROSSWIND DISPERSION COEFFICIENT S_y ADOPTED IN HEGADAS

The derivation of equation (7.10) for the non-dense crosswind dispersion coefficient σ_y is based on the "pure Gaussian" crosswind concentration profile (7.3). In the heavy-gas-dispersion program HEGADAS, the crosswind dispersion coefficient S_y corresponds to $2^{1/2} \sigma_y$. It is noted, however, that in HEGADAS the concentration c is uniform in a middle part of half-width b and it exhibits Gaussian decay for $|y| > b$ only; see eq. (7.2) in Appendix 3. Therefore in the calculation of S_y in HEGADAS-5 a generalisation of eq. (7.10) is adopted for $b > 0$,

$$S_y \frac{\partial S_y}{\partial x} = 2 \overline{k_y} [B_{eff}] \quad (b > 0) \quad (7.13)$$

with $B_{eff} = b + W = b + \pi^{1/2} S_y / 2$ being the effective half-width of the cloud.

The differential equation (7.13) is applied in HEGADAS for distances downwind of the pool with the middle part of the concentration profile $b > 0$. Let $x = x_t$ be the downwind distance at which b becomes 0. The following equation is adopted to evaluate S_y for $x > x_t$,

$$S_y(x) = 2^{1/2} \overline{\sigma_y}[x + x_v] \quad (b=0) \quad (7.14)$$

in which x_v is determined from

$$x_t + x_v = \overline{x}[2^{-1/2} S_y(x_t)] \quad (7.15)$$

Power-law and Briggs formula for σ_y

In HEGADAS, the general formulation given above is presently applied to two specific types of empirical formulae for σ_y , i.e. a power-law in the downwind distance x (formerly adopted in HEGADAS) and Briggs formula.

POWER-LAW FOR σ_y

The power-law and its inverse are given by

$$\sigma_y = \overline{\sigma_y}[x] = \delta x^\beta, \quad x = \overline{x}[\sigma_y] = (\sigma_y / \delta)^{1/\beta} \quad (7.16)$$

Insertion of eq. (7.16) into (7.12) leads to

$$\overline{k_y}[W] = \beta \delta^{1/\beta} \left\{ \frac{2}{\pi} W^2 \right\}^{1-1/2\beta} \quad (7.17)$$

For the option of the power-law for σ_y , the equations adopted in HEGADAS for S_y now follow by insertion of eqs. (7.16), (7.17) into eqs. (7.13) and (7.14).

BRIGGS FORMULA FOR σ_y

Briggs formula and its inverse are given by

$$\sigma_y = \overline{\sigma_y}[x] = \frac{\delta x}{(1 + \beta x)^{1/2}}, \quad x = \overline{x}[\sigma_y] = \frac{\sigma_y^2 \beta}{2\delta^2} \{1 + [1 + (\frac{2\delta}{\beta \sigma_y})^2]^{1/2}\} \quad (7.18)$$

Insertion of eq. (7.18) into (7.10) leads to

$$\overline{k_y}[W] = \frac{2\delta^2}{\beta} (S^{-1} - S^{-2}) \quad \text{with } S = \overline{S}[W] = 1 + \{1 + 2\pi(\frac{\delta}{\beta W})^2\}^{1/2} \quad (7.19)$$

For the option of Briggs formula, the equations adopted in HEGADAS for S_y now follow by insertion of eqs. (7.18), (7.19) into eqs. (7.13) and (7.14).

7.3.1.3. Averaging times for transient releases

In predicting the hazards associated with accidental releases of toxic gases, there is a need to provide predicted concentrations averaged over some period of time. The averaging time may be as long as one hour. This contrasts with hazard analysis for flammable gas releases, where estimates of near-instantaneous concentrations are required.

Even if the release rate of gas is constant over a long period of time and the distances of concern are small, so that the steady-state model can be used, predictions are still dependent on averaging time since the plume meanders. Meandering is due to random changes in wind direction, or, equivalently, low frequencies in lateral turbulence. Thus, the longer one observes a "steady" plume, the wider is the area swept out by meandering and the lower the average peak concentration. This is accounted for in trace gas modelling by making the lateral plume spread parameter σ_y dependent on averaging time.

In HEGADAS-S the equivalent parameter is S_y (see eq. (7.13) and (7.14) for the relationship between S_y and σ_y). The values used currently for σ_y are taken to be proportional to (averaging time)^{0.2}; see Tables 7.1 and 7.2. This is a common empirical approach, which is frequently used but which is an area where additional research is still needed.

For time-dependent dispersion predictions (releases of varying rate and finite duration), there are two issues. First, even in the absence of meander (i.e. a non-varying wind), the predictions of concentration at any given location are a function of time. It is thus necessary to average these predictions over the desired averaging time.

For this situation it is also necessary to take into account the meander of the plume. Suppose that we are interested in the exposure at a location downwind of a ten minute release of gas, and that the hourly-averaged concentration is required. Clearly, meandering of the plume during the ten minutes while it is passing over the desired location will reduce the average concentration. But changes of wind direction during the remaining

fifty minutes will not affect the average concentration. To take account of the meander during the ten minutes of the release, it is appropriate to use ten-minute σ_y 's, but not one-hour values. However, to take account of the short duration of the release the predicted concentrations must be averaged over one hour to obtain the desired results.

The time-dependent model HEGADAS-T uses the appropriate values of S_y (σ_y) consistent with the averaging time. The averaging of the time-dependent predicted concentrations is done after other calculations are complete. This is accomplished by using the post-processor HTPOST to HEGADAS-T, which provides an option to average concentrations over any given period of time; see Section 8.6.2 in the User's Manual.

In performing such calculations, the user should not take an inappropriately long averaging time in HEGADAS-T. For a steady release of limited duration, the maximum would be the duration of the release. For more complex time-dependent releases, we suggest using the effective release time (Wilson and Zelt, 1990) as a maximum:

$$t_s = \frac{2 \int_0^{\infty} E(t) t \, dt}{\int_0^{\infty} E(t) \, dt}$$

where t_s is the mass-release weighted sampling or averaging time for the entire event, and t is the local time at which the release rate equals $E(t)$. Note that for a constant finite-duration release t_s equals the duration time.

7.3.2. Gravity-spreading

The comparison of HEGADAS predictions of wind tunnel dense gas dispersion experiments, described in Chapter 8, revealed an important difference between the predicted and the measured cloud width. The experimental data showed that the clouds effectively stopped spreading at a downwind position where concentrations were still large enough (about 10% volume fraction) for the cloud to be considered dense. HEGADAS predicted plume width well up to this transition point, as shown in Figure 8.3, but thereafter the calculated plume width was too great and consequently concentrations were too low.

The gravity-spread formulation originally used in HEGADAS, and other dense gas models, is based on gravity current flows into still air and is considered well founded (Van Ulden, 1984). It has been successfully used to predict gravity dominated flows such as the experiments at THORNEY ISLAND. It has been successful in predicting cloud shapes from continuous area sources, in particular those for the SHELL MAPLIN SANDS experiments, where the comparison was based on the visible cloud. In the MAPLIN LPG experiments, however, the visible cloud outline was essentially an iso-concentration contour mapping the high, $> 9\%$ v, concentration region of the cloud. As such it corresponds to the pre-transition regime in the wind tunnel experiments where the HEGADAS predictions were good.

In all but one of the MAPLIN LPG experiments the region of the cloud strongly affected by gravity spreading was quite small. The HEGADAS model concentration predictions were not sensitive to the gravity spreading description and were in good agreement with data. The exceptional case was Spill 54, a continuous release of LPG into a low wind speed, where HEGADAS-4 significantly underpredicted the distance to LFL. This result was not understood but is consistent with the revised gravity-spreading relationship in HEGADAS-5. A comparison is presented in Figure 8.3 between experimental data for Maplin 54 and model predictions by HEGADAS-5 and HEGADAS-4. As indicated by this figure the revised HEGADAS-5 model now simulates the observed cloud in this experiment.

Laboratory experiments by Linden and Simpson (1986, 1988) offer an explanation of the wind tunnel data and Maplin Spill 54. They compared the advance of a gravity current into an otherwise still fluid with its advance into a fluid with continuously generated turbulence. They found that, in the turbulent environment, the characteristic leading edge of the gravity current was destroyed by vertical mixing and subsequently the rate of advance of the dense fluid was slowed by up to a factor of 8. In experiments where the turbulence generation was turned off the gravity current reformed.

Taken together these results suggest that boundary layer turbulence is able to cause a collapse of the edge of a dense gas cloud and slow down its rate of lateral spread. A description of this process is needed to predict dispersion in cases where the gas cloud is dense over large distances. The GOLDFISH experiments are an example of such a case.

To develop a model for the conditions under which gravity current collapse occurs, and to derive an expression for the rate of spread after this transition, we apply the reasoning of Linden and Simpson (1986, 1988) to a boundary layer flow.

We first consider conditions following collapse of the leading edge of the gravity current. After collapse, the step change in density which marked the edge of the gravity current has been destroyed and the dense and ambient fluids are separated by a region across which the density changes smoothly. There is then a lateral pressure gradient across this region balanced by turbulent diffusion:

$$\frac{d}{dz} K \frac{du}{dz} = - \frac{g'(H-z)}{L} \quad (7.20)$$

where H is the depth of the dense gas layer, L the lateral extent of the interface and K is the turbulent diffusivity. To solve this equation we need to identify the turbulent diffusivity for momentum appropriate to the small, gravity driven, secondary flow perpendicular to the wind direction.

In a neutrally stratified, rough wall, boundary layer flow the turbulent diffusivity for momentum is given by:

$$K = k u_* z \quad (7.21)$$

where $k = 0.41$ is von Karmans constant. The exact dependence of K on stratification, parameterized by the bulk Richardson number, Ri_* , is uncertain. If we assume that the effect of stable stratification on K is the same as the effect on the turbulent diffusivity for mass transfer within the cloud, then:

$$K = \frac{k u_* z}{(1 + 0.8 Ri_*)^{0.5}} = \frac{k u_* z}{\Phi(Ri_*)} \quad (7.22)$$

Equation (7.20) is to be solved according to the boundary conditions:

$$u(H) = u(\epsilon) = 0 \quad (7.23)$$

where ϵ is a small distance from the ground. The speed of the cloud is given by the average velocity over the cloud depth:

$$u = \frac{1}{(H-\epsilon)} \int_{\epsilon}^H u(z) dz \quad (7.24)$$

Equation (7.20) has been solved subject to the conditions (7.23) and integrated according to equation (7.24). For finite ϵ the result is algebraically complex, however, in the limit as ϵ tends to zero:

$$\frac{u}{u_*} = \frac{1}{3k} Ri_* (1 + 0.8 Ri_*)^{0.5} \frac{H}{L}$$

where $Ri_* = g'H/u_*^2$. We have made a great number of assumptions in deriving this equation and, in particular, have not identified the characteristic length-scales H or L . However, if we assume that the appropriate vertical

and horizontal scales are proportional to the HEGADAS cloud height, H_{eff} , and cloud half-width, B_{eff} , then we obtain:

$$\frac{u}{u_*} = \frac{1}{3kC_D} R_i (1 + 0.8 Ri_*)^{0.5} \frac{H_{eff}}{B_{eff}} \quad (7.25)$$

where C_D is the constant of proportionality.

We now turn to the conditions determining transition between the two gravity spreading regimes. The sudden change in cloud spreading rate seen in Figure 8.3 points to a catastrophic breakdown of the leading gravity head of the cloud. In this case spreading up to the transition point would be described by the gravity current equation:

$$u = u_* C_E Ri^{0.5} \quad (7.26)$$

After collapse of the gravity current, spreading will be described by the diffuse cloud equation, (7.25).

We do not know what event causes breakdown of the gravity current. We suspect that it is an instability in the flow, possibly in the case of the HTAG experiments an interaction with vortices shed from the roughness elements. As such it is difficult to understand how to predict transition. In Linden and Simpson's experiments the ratio of velocities before/after transition appears to be almost constant. In our case the ratio of velocities (7.26) to (7.25) is proportional to:

$$\frac{B_{eff} / H_{eff}}{(R_i (1 + 0.8 Ri_*))^{1/2}} = A_t ,$$

where all quantities are evaluated at the transition point.

We have identified transition conditions for the HTAG database by estimating the downwind position at which the rate of spread of the dense gas plumes appears to diverge significantly from that predicted by HEGADAS. Assuming that the gravity current equation applies up to this point, and

hence that HEGADAS predicts dispersion correctly, we are able to calculate the parameters H_{eff} , B_{eff} , Ri and Ri_* at transition. These values, together with the ratio A_t and the ratio B_{eff}/H_{eff} , are given in the following table for the area source experiments described in Chapter 8. We observe that the transition ratio, A_t , is remarkably constant compared to the variation in cloud aspect ratio and to the variation in the Richardson number and has an average value of 6.5.

RUN No	Est. Trans'n Point m	H_{eff} m	B_{eff} m	Ri_* -	Ri -	A_t -	B_{eff}/H_{eff} -
HT139	70	1.09	29.1	3.69	3.55	7.12	27
HT140	80	0.68	49.9	13.80	10.88	6.46	74
HT142	50	3.45	28.0	0.77	0.76	7.32	8
HT143	35	1.48	44.4	5.30	4.39	6.25	30
HT48	----- RUN NOT USED -----						
HT49	130	0.81	93.6	23.80	17.49	6.18	116
HT51	60	3.54	38.7	1.50	1.46	6.09	11
HT52	60	1.87	80.1	8.01	6.42	6.21	43

Thus we can use the ratio of the spreading velocities as a transition criterion which becomes:

$$\frac{B_{eff} / H_{eff}}{(R_i (1 + 0.8 Ri_*))^{\frac{1}{2}}} = A_t = 6.5 \quad (7.27)$$

We assume that when the criterion (7.27) is reached conventional gravity current spreading stops. Further increases in cloud width proceed at a rate given by equation (7.25) until dispersion is essentially passive and the cloud width increases at a rate $d\sigma_y/dx$. We introduced a constant of proportionality $1/C_D$ into equation (7.25) to give the post-transition spreading velocity in terms of the HEGADAS cloud height and width parameters. The post transition dispersion predictions are not very sensitive to the value of C_D , as discussed in Appendix A to section 8, and we found a value $C_D = 5$ gave the best fit to the HTAG measurements.

The criterion (7.27) and the value of u ($u = dB_{eff}/dt$) calculated from equation (7.25) have been incorporated into HEGADAS-5 and an extra input variable C_D defined. The sensitivity of the calculations to C_D is discussed in Appendix A to Chapter 8.

To summarize, we find that it is possible for turbulence to disrupt the initial rapid gravity-current spreading characteristic of dense gas releases, a process we have termed transition. The conditions at which transition occurs can be predicted accurately. Post-transition the rate of lateral spread of the cloud is slow and comparable in magnitude to the lateral diffusive spreading of a neutrally buoyant cloud. We have introduced an empirical constant, C_D , into the post-transition gravity-spread equations to account for this slow spread. A value of 5 is indicated by matching to the HTAG experiments.

7.4. MODIFIED ALONG-WIND-DIFFUSION FORMULATION FOR TRANSIENT RELEASES

7.4.1. Introduction

The original downwind spreading formulation adopted for the transient version HEGADAS-T of HEGADAS is discussed in detail in Section 6.2 in Appendix 3. In this formulation the centre-line ground-level concentration $c_A = c_A(x, t)$ is calculated as a function of time t and distance x downwind of the source by means of Gaussian integration of the observer concentration $C_A(\xi)$ at ξ ,

$$c_A(x, t) = \int_0^{\infty} \frac{C_A(\xi)}{(2\pi)^{1/2} \sigma_x(\xi)} \exp \left[- \frac{(x-\xi)^2}{2\sigma_x^2(\xi)} \right] d\xi \quad (7.30)$$

In the above equation ξ is the position at time t of an observer travelling with the wind in the downwind direction. At this position the observer observes the concentration $C_A(\xi)$, where $C_A(\xi)$ is calculated from a steady-state HEGADAS solution based on zero along-wind diffusion. In (7.30) along-wind diffusion is taken into account by assuming that the concentration $C_A(\xi)$ spreads out around ξ according to a Gaussian distribution with a downwind dispersion coefficient $\sigma_x = \sigma_x(\xi)$.

Note that the position ξ of the observer in eq. (7.30) corresponds to the observer position AFTER the cloud shape correction for gravitational spreading in the wind direction has been applied. This correction is described in detail in Appendix C contained in Appendix 3 to this report.

The dispersion coefficient σ_x is usually considered to consist of two statistically independent components σ_{xs} and σ_{xt} ,

$$\sigma_x = (\sigma_{xs}^2 + \sigma_{xt}^2)^{1/2} \quad (7.31)$$

The component σ_{xs} is the spread induced by vertical wind shear and σ_{xt} is the turbulent spread caused by downwind-direction velocity fluctuations.

Increasing the wind shear du/dz increases the relative speed at which the top and bottom of the cloud are advected, and so increased shear du/dz results in increased spread σ_{xs} . From the formula of the wind speed $u(z)$ given by eq. (B.1) in Appendix 3, it follows that the shear component changes as a function of stability. Thus the spread σ_{xs} increases with stability. This is confirmed by the experimental data of Nickola (1971) depicted in Figure 7.5.

In the original HEGADAS-T formulation the formula $\sigma_x = \sigma_x(\xi)$ did not take into account the change of wind shear and hence the formula is not altered as a function of the stability class. As a result of this a literature review of along-wind-diffusion formulations was conducted to examine if a more appropriate treatment of σ_x could be included into HEGADAS-T.

In Section 7.4.2 the along-wind-diffusion formulation in the original HEGADAS-T program is described. The results of the literature review are given in Section 7.4.3. Section 7.4.4.1 describes the along-wind-diffusion formulations which have been implemented in the new HEGADAS-T program. Section 7.4.4.2 compares and validates these formulations by means of an example problem involving a finite-duration steady-state release. In Section 7.4.5 the major conclusions are summarised and recommendations are given for the selection of the appropriate along-wind-diffusion formulation in the new HEGADAS-T program.

7.4.2. Along-wind-diffusion formulation in original HEGADAS program

See Section 6.2 in Appendix 3 for details on the original along-wind-diffusion formulation in the program HEGADAS-T (Version 4). In this formulation σ_x is given by the power-law

$$\sigma_x(\xi) = a [\max(0, \xi - x_{br})]^b \quad (7.32)$$

In the above equation a, b can be specified by the user; the default values are $a = 0.13$ and $b = 1.00$. Furthermore x_{br} is the distance of the

breakpoint downwind from the pool; $x_{br} = 0$ if no breakpoint is applied. Eq. (7.32) implies zero along-wind dispersion ($\sigma_x = 0$) upwind of x_{br} .

The above power-law is not based on well-established data. Note that in this law σ_x is directly related to the downwind distance ξ and is not altered as a function of the stability class.

7.4.3. Literature review of along-wind-diffusion formulations

The following provides an overview of the literature review conducted on along-wind-diffusion formulations. See also Hanna (1982) for a short review on σ_x -formulations.

Formula for σ_{xs} by Smith (passive flow)

Smith (1965) analysed theoretically the problem of shear diffusion of puffs released in the surface layer. Using the method of moments he arrived at the following formula for σ_{xs} (source at ground level)

$$\sigma_{xs} = \sigma_{xs}(\xi) = 12^{-1/2} (du/dz) t_{obs} \sigma_z \quad (7.33)$$

Here t_{obs} is the travel time of the puff from (the middle part of) the pool to the present puff position $x = \xi$, σ_z the vertical dispersion coefficient, and du/dz the vertical gradient of the horizontal wind speed $u(z)$.

Formula for σ_{xs} by Chatwin (neutrally stratified, passive flow)

Chatwin (1968) studied the passive dispersion of a puff in a neutral atmosphere. He arrived at the following formula for the downwind dispersion coefficient σ_{xs} ,

$$\sigma_{xs} = \sigma_{xs}(\xi) = 0.596 u_* t_{obs} / k \quad (7.34)$$

Here $k=0.41$ is the Von Karman constant and u_* the ambient friction velocity.

The derivation of Eq. (7.34) by Chatwin is based on the following two basic assumptions,

- a a logarithmic formula for the ambient wind speed u valid for neutrally stratified flow only: $u = (u_*/k) \ln[z/z_R]$, with z being the height above ground and z_R the surface roughness
- b the linear formula $K = k u_* z$ for the vertical diffusivity valid for passive gases only

The above two assumptions are not satisfied in the program HEGADAS. HEGADAS adopts a more general formula for the wind speed for stratified flow and a heavy-gas, non-passive extension of the formula for the vertical dispersion coefficient; see eqs. (B.1) and (3.3) in Appendix 3.

The analytical derivation of eq. (7.34) by Chatwin consists of two parts. In the first part the velocity $d\xi/dt$ and position ξ of a puff (frozen puff, moving with the wind) as a function of the travel time t_{obs} is calculated (see eq. (23) in Chatwin (1968)),

$$d\xi/dt = (u_*/k) \ln[e^{-0.577} k u_* t_{obs}/z_R] \quad (7.35)$$

$$\xi = (u_* t_{obs}/k) \ln[e^{-1.577} k u_* t_{obs}/z_R] \quad (7.36)$$

The extension of this calculation to stratified, heavy-gas flow can be done relatively easily. See Chaudry and Meroney (1972) for an extension of this calculation to stratified flow.

In the second part σ_{xs} is calculated by applying the Lagrangian similarity hypothesis valid for neutrally stratified flow. This calculation can easily be extended to neutral, heavy-gas flow with a constant Richardson number, and eq. (7.34) can be shown to be still valid. However, it cannot be extended in a straightforward manner to the non-neutral case.

Formulation by Wilson for stratified, passive flow

The along-wind diffusion formulation of Wilson (1981) is based on an equation very similar to eq. (7.30), except that in this equation he evaluates σ_x at x , not at ξ .

Wilson adopts formula (7.31) for the downwind dispersion formula σ_x , which includes both the effects of shear diffusion (σ_{xs}) and turbulent spread (σ_{xt}).

By insertion of the velocity gradient $du/dz = u_*/(kz)$ into Smith's formula (7.33) and subsequent matching of (7.33) with Chatwin's formula (7.34), Wilson derived that du/dz in formula (7.33) needs to be evaluated at the reference height $z_{ref} = 0.483 \sigma_z$. From (7.36) it is seen that the mean convective puff-velocity $U_c = \xi/t_{obs}$ equals the ambient velocity $u = u(z_c) = (u_*/k) \ln[z_c/z_R]$ at the convective height $z_c = 0.207 k u_* t_{obs}$. By thus eliminating t_{obs} and using $du/dz = u_*/kz_{ref}$, eq. (7.33) reduces to

$$\sigma_{xs} = 12^{-\frac{1}{2}} \sigma_z \xi / (z_{ref} \ln(z_c/z_R)) \quad (7.37)$$

Wilson derived an alternative formula by using the wind-speed power-law $u(z) = U_0 (z/Z_0)^n$ in the evaluation of du/dz (at $z = z_{ref}$) in (7.33), and by using $t_{obs} = \xi/U_c = \xi/u(z_c)$ in the evaluation of t_{obs} in (7.33). This formula is as follows,

$$\sigma_{xs} = \sigma_{xs}(\xi) = 12^{-\frac{1}{2}} \sigma_z n \xi / \{z_{ref} (z_c/z_{ref})^n\} \quad (7.38)$$

Wilson assumes that the turbulent spread σ_{xt} is proportional to the vertical dispersion coefficient σ_z with the proportional factor being a constant dependent on the stability class only.

Formulation by Ermak for stratified, passive flow

This formulation was introduced by Ermak (1986) in the finite-release version of the program SLAB. It is an extension of the formulation by Wilson. It can be described as follows.

- Ermak assumes Gaussian decay for the concentration $c(x,y,z,t)$ in the crosswind (y-) and vertical (z-) directions with dispersion coefficients $\sigma_y = \sigma_y(x)$ and $\sigma_z = \sigma_z(x)$. Thus the ratio of the concentration $c(x,y,z,t)$ and the centre-line ground-level concentration $c(x,0,0,t)$ equals

$$\frac{c(x,y,z,t)}{c(x,0,0,t)} = \exp \left\{ -\frac{1}{2} \left(\frac{y^2}{\sigma_y^2} + \frac{z^2}{\sigma_z^2} \right) \right\} \quad (7.39)$$

- Ermak assumes a power-law for the ambient wind speed,

$$u(z) = U_0 (z/Z_0)^n \quad (7.40)$$

with the values for n taken from Irwin (1979); see Table 7.3.

Note that in HEGADAS-T a power-law fit $u(z) = u_0 (z/z_0)^\alpha$ of the logarithmic wind profile is adopted. Thus the HEGADAS-T input data u_0, z_0 and the power-law exponent α calculated in HEGADAS-T should be utilised for U_0, Z_0 and n in the adaptation of this formulation for use in HEGADAS-T.

- Ermak assumes that the vertical dispersion coefficient σ_z equals the vertical turbulent spread σ_{zt} , $\sigma_z = \sigma_{zt}$. The horizontal turbulent spread is assumed to be isotropic so that $\sigma_{xt} = \sigma_{yt}$. The formulas $\sigma_{xt}(x)$ and $\sigma_{yt}(x)$ are taken from formulas recommended by Briggs (1973); see Table 7.3. The formula for $\sigma_z(x) = \sigma_{zt}(x)$ is approximated by Ermak by the power-law $\sigma_{zt} = c x^d$ with c and d given in Table 7.3.
- By utilising eqs. (7.39) and (7.40) for $c(x,y,z,t)$ and $u(z)$, Ermak determines the puff velocity $d\xi/dt$ as a function of σ_z ,

$$\frac{d\xi}{dt} = \frac{\int_{-\infty}^{\infty} \int_0^{\infty} c(\xi,y,z,t) u(z) dy dz}{\int_0^{\infty} \int_0^{\infty} c(\xi,y,z,t) dy dz} = 2^{\frac{1}{2}n} \frac{\Gamma(\frac{1}{2}n + \frac{1}{2})}{\pi^{\frac{1}{2}}} U_0 \left(\frac{\sigma_z}{Z_0} \right)^n \quad (7.41)$$

Integration to the time t while using the above power-law $\sigma_z(\xi) = c \xi^d$ leads to the mean convection velocity $U_c = \xi/t_{obs}$ as a function of σ_z ,

$$U_c = U_0 \left(\gamma \frac{\sigma_z}{Z_0} \right)^n, \quad \text{with} \quad \gamma = 2^{\frac{1}{2}} \left[\frac{(1-nd) \Gamma(\frac{1}{2}n + \frac{1}{2})}{\pi^{1/2}} \right]^{1/n} \quad (7.42)$$

- The power-law (7.40) for $u(z)$ (at $z = z_{ref} = .483\sigma_z$) is now used in eq. (7.33), and the time $t_{obs} = \xi/U_c$ is eliminated in this equation by means of eq. (7.42). This leads to the following formula for $\sigma_{xs}(\xi)$,

$$\sigma_{xs} = \sigma_{xs}(\xi) = (0.60 n [0.48/\gamma]^n) \xi = a_{xs} \xi \quad (7.43)$$

with the stability-class dependent constant $a_{xs} = \sigma_{xs}/\xi$ given in Table 7.3.

Formulation by Wheatley for stratified, passive flow

Wheatley (1988) derived in a more rigorous manner the concentration distribution of a passive puff in a stratified atmosphere from an approximate solution to the diffusion equation. He arrived at an ordinary differential equation for the downwind diffusion coefficient σ_x .

Formulation by Van Ulden for stratified, heavy-gas flow

Currently in development by Van Ulden (1989) is an along-wind diffusion formulation valid for a heavy gas in a non-neutral atmosphere. Van Ulden basically distinguishes three areas of diffusion:

- area very near the source; in this area downwind diffusion is neglected, i.e. $\sigma_x = 0$
- a transition area further downwind
- area downwind of transition area; in this area an extension of Chatwin's formulation to heavy gas in a stratified atmosphere is adopted; unlike

Wheatley's formulation Van Ulden does not adopt a numerical differential equation for σ_x , but he utilises an analytical formula for σ_x

7.4.4. Along-wind-diffusion formulations in new HEGADAS program

7.4.4.1. Description of formulations

As a consequence of the results of the above literature review a number of along-wind-diffusion formulations have been implemented in HEGADAS-T. These formulations are described in this section. In HEGADAS-T the type of along-wind-diffusion formulation is now specified by the input keyword SIGX in the CLOUD data block. This keyword may include the specification of a maximum of three parameters, namely the model type MODSX and two additional model parameters ASIGX, BSIGX; see the HEGADAS user's guide (Chapter 8 in the User's Manual) for further details.

The along-wind-diffusion formulations implemented into HEGADAS-T are as follows.

1. Original HEGADAS-T formulation (MODSX=1)

In this formulation σ_x is directly related via a power-law to the downwind distance ξ and is not altered as a function of stability class; see eq. (7.32). This option is retained in HEGADAS-T for reasons of compatibility with the former HEGADAS-T version. Its use is not recommended.

2. Adaptation of the formulation by Ermak and Wilson (MODSX=2)

In this formulation σ_x is directly related via a stability-class dependent formula to the downwind distance ξ . It is an adaptation of the Ermak/Wilson formulation for stratified, passive flow (see Section 7.4.3). This formulation should not be used in HEGADAS-T for neutral stability. In this formulation, $\sigma_x(\xi)$ is given by

$$\sigma_x(\xi) = \{\sigma_{xs}^2(x=[\max[0, \xi - x_{br}]) + \sigma_{xt}^2(x=[\max[0, \xi - x_{br}])\}^{\frac{1}{2}}$$

$$= [\{a_{xs} \max[0, \xi - x_{br}]\}^2 + \{a_{xt} \sigma_y(x = \max[0, \xi - x_{br}])\}^2]^{\frac{1}{2}} \quad (7.44)$$

In the above equation $\sigma_y(x)$ is defined by equation (7.4), and the model parameters a_{xs} , a_{xt} can be specified by the user. The recommended value (= default value) for a_{xs} is the value defined by eq. (7.43) with the wind-speed exponent n chosen equal to the exponent α adopted in the power-law wind-speed profile $u = u_0(z/z_0)^\alpha$ in HEGADAS and with γ defined by (7.42). The recommended value (=default value) for a_{xt} equals 1 (inclusion of turbulent spread σ_{xt}).

3. Heavy-gas adaptation of the formulation by Chatwin and Wilson (MODSX=3)

This formulation is a heavy-gas extension of the formulation by Chatwin and Wilson for passive, neutrally-stratified flow (see eq. (7.34)). In this formulation σ_x is not directly related to the downwind distance ξ , but it is evaluated as a function of the actual travel time of the cloud. This formulation should be used in HEGADAS-T for neutral stability.

In this formulation downwind diffusion is neglected in the region where the observed bulk Richardson number Ri_*^{obs} is larger than a user-specified value Ri_*^{cr} (default value $Ri_*^{cr} = 10$), say upwind of the point x_{cr}^{obs} . As in (7.32) and (7.44), downwind diffusion is also neglected upwind of the breakpoint $x = x_{br}$. Thus x_{cr}^{obs} is reset to x_{br} if $x_{cr}^{obs} \leq x_{br}$ (with x_{br} taken to be at the middle of the observed pool in the absence of a breakpoint).

The adapted Chatwin/Wilson's formulation is implemented in HEGADAS as follows:

- For each observer, x_{cr}^{obs} is set during its steady-state HEGADAS calculations. The time t_{cr}^{obs} at which the observer is above x_{cr}^{obs} is set from the expression for the position $x^{obs}(t)$ of the observer as a function of the time. The latter expression is derived from the expression for the observer velocity given in eq. (B.11) in Appendix 3,

$$x^{obs}(t) = -R_{max} + CUW (t - t_{st}^{obs})^{1+\alpha} \quad (7.45)$$

with

$$CUW = \left(\frac{u_0 [S_z (x=0.5L_m)/z_0]^\alpha}{(1+\alpha)\Gamma(\frac{1}{1+\alpha})} \right)^{1+\alpha} (0.5L_m + R_{max})^{-\alpha} \quad (7.46)$$

Here it is assumed that the observer is released at time t_{st}^{obs} at $x = -R_{max}$, with R_{max} being the maximum gas-blanket radius (over all times). The value of S_z in the above equation is calculated at the end of a square steady-state source with a length $L_m = \pi^{1/2}R_m$ and a flux Q_m ; here the secondary-pool radius R_m and the flux Q_m correspond to the time at which the take-up rate $\pi R_m^2 Q_m$ is maximum.

- The cloud shape correction is applied as before; see Appendix C included in Appendix 3 contained in this report.
- The actual concentration as a function of time t and downwind distance x is determined from eq. (7.30). Here the downwind dispersion coefficient σ_x is set from eq. (7.34) with the time t_{obs} taken to be the travel time of the observer from x_{cr}^{obs} to ξ , i.e. $t_{obs} = t - t_{cr}^{obs}$. Note that σ_x depends through t_{obs} on the wind-speed parameters u_0 and α .

Note that for given u_* , z_R , z_0 the HEGADAS power-law fit $u = u_0(z/z_0)^\alpha$ depends on the stability class. E.g. for $u_* = 0.125$ m/s, $z_R = 0.007$ m, $z_0 = 10$ m, it can be shown that $u_0 = 1.98, 2.22, 3.00, 4.13$ m/s and $\alpha = 0.144, 0.175, 0.289, 0.423$ for stability classes C, D, E, F, respectively. From the above it follows that the formula for σ_x depends on the stability class, but does not explicitly take into account the change of wind shear. In the end of the next section this is illustrated by means of an example problem.

7.4.4.2. Comparison and validation of formulations (example problem)

In the previous section we have described the several

along-wind-diffusion formulations which have been implemented in the version 5 of HEGADAS-T. In the present section these formulations are compared and tested by means of an example problem involving a finite-duration steady-state gas release.

We consider two cases corresponding to neutral and stable conditions, i.e. neutral stability with wind speed $u_0 = 4$ m/s at 10 m height (D4) and stability class E with $u_0 = 3$ m/s (E3). For both cases the primary source is assumed to have a pool radius $R_p = 3$ m and a release rate $E = 30$ kg/s. The duration of the release is 20 seconds, i.e. gas is released for $0 < t < 20$. Other input parameters are equivalent to the example problem described in Section 7.5. (See Section 7.5 for further details.)

HEGADAS-T simulations have been carried out for the above two sets of meteorological conditions to test the following along-wind-diffusion formulations for σ_x :

1. The original HEGADAS-T power-law (MODSX=1), where σ_x is related to the downwind distance x by $\sigma_x(x) = 0.13x$
2. The adapted Ermak/Wilson formulation (MODSX=2, $\sigma_{xt} > 0$), in which σ_x is a stability-class dependent function of the downwind distance x and in which σ_{xt} is taken into account ($a_{xt} = 1$)
3. As 2, but with the turbulent spread σ_{xt} neglected ($\sigma_x = \sigma_{xs}$; $a_{xt} = 0$). This run is carried out to study the effect of inclusion of turbulent spread.
4. The adapted Chatwin/Wilson formulation (MODSX=3). In this more rigorous formulation σ_x is proportional to the travel time t_{obs} of the puff (observer); t_{obs} equals the present time t minus the time at which the Richardson number (seen by the observer) reduces to $Ri_*^{cr} = 10$. σ_x is taken to be zero in the high-density regions, i.e. if $Ri_* > Ri_*^{cr}$ at the present time t .

5. As 4, but with σ_x not taken to be zero in the high-density near-source region ($Ri_{cr} = 1000$).

The above simulations have been carried out both with (ICSCOR=1) and without (ICSCOR=0) cloud shape correction.

Figures 7.6-11 include predictions by the above HEGADAS-T simulations at time $t = 120$ seconds. The Richardson number Ri_* , downwind dispersion coefficient σ_x and the centre-line ground level concentration c_A are plotted against the downwind distance x . The following observations can be made.

1. For the stable case, E3, entrainment is less than for the neutral case D4. At a given time this results in higher values of the concentration (compare Figures 7.6 and 7.9) and the Richardson number (compare Figures 7.8 and 7.11). Observe that at a given time the cloud has travelled less distance for E3 than for D4.
2. For the original HEGADAS-T formulation (MODSX=1) we have $\sigma_x = \sigma_x(x) = 0.13 x$ (see Figures 7.7 and 7.10).
3. In the adapted Ermak/Wilson formulation (MODSX=2), the shear component varies linearly with x , $\sigma_{xs} = a_{xs} x$. Here a_{xs} is given by eq. (7.43). The value for a_{xs} depends on the stability class and on the fit α of the exponent in the power-law profile for the wind speed. The values calculated by HEGADAS-T were $\alpha = 0.175$, $a_{xs} = 0.115$ and $\alpha = 0.289$, $a_{xs} = 0.192$ for D4 and E3, respectively. These values differ only slightly from the values $\alpha = 0.15$, $a_{xs} = 0.097$ and $\alpha = 0.35$, $a_{xs} = 0.235$ proposed in the original Ermak/Wilson formulation (see Table 7.3).

In the present formulation the power-law formula $\sigma_y(x) = \delta x^\beta$ (MODSY=1) is adopted in the crosswind dispersion calculations. From eq. (7.44) and Table 7.1 it is now inferred that

$$\begin{aligned}\sigma_x &= \sigma_x(x) = \{0.115^2 + (0.128 x^{-0.093})^2\}^{\frac{1}{2}} x, \quad \text{for D4} \\ \sigma_x &= \sigma_x(x) = \{0.192^2 + (0.098 x^{-0.098})^2\}^{\frac{1}{2}} x, \quad \text{for E3}\end{aligned}$$

These equations simplify to $\sigma_x = \sigma_x(x) = 0.115 x$ and $\sigma_x = \sigma_x(x) = 0.192 x$ if the turbulent spread σ_{xt} is neglected.

The following is now concluded for MODSX=2.

- The effect of turbulent spread is much smaller for the stable case E3 than for the neutral case D4 (compare Figures 7.7 and 7.10).
 - For the stable case the stability-class independent, original HEGADAS formulation (MODSX=1) predicts considerably less along-wind diffusion than the adapted Ermak/Wilson formulation (MODSX=2); see Figure 7.10. For the neutral case the difference in prediction is much less (see Figure 7.7).
4. In the adapted Chatwin/Wilson formulation (MODSX=3), σ_x varies according to eq. (7.34) linearly with the friction velocity u_* and the travel time t_{obs} . The friction velocity is calculated by HEGADAS-T in the power-law fit of the logarithmic wind-speed profile. The calculated values are $u_* = 0.226$ m/s and $u_* = 0.126$ m/s for D4 and E3, respectively. This leads to the formulas $\sigma_x = 0.33 t_{obs}$ and $\sigma_x = 0.18 t_{obs}$, respectively.

The following is now noted for MODSX=3 (see Figures 7.7 and 7.10):

- The observers located furthest downwind are released shortly before to the start of the gas release, and the observers located furthest upwind are released shortly before the end of the gas release. All these observers see only a part of the pool. Therefore the concentrations and Richardson numbers seen by these observers are lower. Consequently the downwind position x_{cr}^{obs} at which the Richardson number reduces to $Ri_*^{cr}-10$ is located further upwind. Thus the travel time t_{obs} between x_{cr}^{obs} and the present observer position ξ is larger and therefore the amount of along-wind-diffusion is greater.
- For $Ri_{cr} = 1000$, t_{obs} corresponds to the travel time of the observer from the middle of the pool to the observer position at $t = 120$ s. Note that the observers released shortly before the end of the gas

release see only a upwind part of the pool, and hence the observed middle part of the pool is located upwind of $x = 0$. This explains the positive value for σ_x at $x = 0$ in Figure 7.10.

From Fig. 7.10 and $t_{obs} = \sigma_x / 0.18$, the value of the travel time t_{obs} for the several observers can be determined. For the furthest downwind and upwind observers these times are $t_{obs} = 90$ s and $t_{obs} = 106$ s, respectively. Thus these observers arrive at times $t = 30$ s and $t = 14$ s at the observed middle part of the pool, respectively.

- For the stable case E3 the Richardson number is larger than $Ri_*^{c^x} = 10$ in the middle part of the cloud. Therefore no along-wind-diffusion ($\sigma_x = 0$) is observed in this part of the cloud.
 - The above-mentioned effects are absent if along-wind-diffusion is always taken into account ($Ri_*^{c^x} = 1000$). In this case t_{obs} equals the travel time of the observer from the middle of the observed pool to the present observer position ξ . Because observers located further downwind have been travelling longer, the value of σ_x is larger further downwind in the cloud.
5. For the stable case, because of the lower cloud speed, the cloud has travelled a shorter distance at time $t = 120$ s. For the x -dependent σ_x formulas (MODSX=1,2), the lower x -value causes less along-wind-diffusion (smaller σ_x). For the σ_x -formula dependent on the friction velocity u_* and the travel time t_{obs} (MODSX=3), the lower friction velocity causes less along-wind diffusion. Compare Figures 7.7 and 7.10.
 6. The cloud shape correction for gravitational spreading in the downwind direction is described in detail in Appendix C contained in Appendix 3 to this report. The cloud height, the centre-line ground-level concentration, and the area of each cloud segment (product of length Δx and width $2B_{eff}$) are kept constant. The width $2B_{eff}$ is then reduced and the length Δx increased in such a way that the amount of spreading in the downwind direction x of the cloud as a whole equals the spreading in the crosswind direction.

The cloud shape correction lengthens the gas cloud (see e.g. Figures 7.8 and 7.11), but does not alter the downwind position of the centroid of the cloud. Thus for the x-dependent σ_x formulas (MODSX=1,2) the value of $\sigma_x = \sigma_x(x)$ is on average the same: it is the same at the cloud centroid, somewhat less near the upwind edge of the cloud and somewhat higher near the downwind edge of the cloud. In the travel-time dependent σ_x formula (MODSX=3) the values of σ_x calculated at the observers are independent of the cloud shape correction.

Thus for all along-wind-diffusion formulations, the cloud shape correction induces a lengthening of the cloud and an unchanged average value of $\sigma_x = \sigma_x(x)$. Therefore there is relatively less along-wind-diffusion and less percentage-reduction of peak concentration at the cloud centroid; compare Figures 7.6a, 7.9a against Figures 7.6b, 7.9b.

Results at time $t = 120$ s have been discussed above for the runs D4 and E3. Fig. 7.12 includes additional results for E3 at the much larger times $t = 600$ s and $t = 1200$ s. Note that the two MODSX=3 formulations with $Ri_{cr}=10$ and $Ri_{cr}=1000$ converge to each other for $t \rightarrow \infty$. Thus the effect of zero downwind-diffusion in the high-density region near the source ($Ri_* > Ri_{cr}=10$) dampens out if the cloud moves further downwind.

From Fig. 7.12 it is seen that under stable conditions the downwind diffusion predicted by the adapted Chatwin/Wilson formulation (MODSX=3) is smaller than that predicted by the adapted Ermak/Wilson formulation (MODSX=2). This was expected since the Chatwin/Wilson formulation ignores the effect of increased shear with increased stability.

To study the effect of stability class in the MODSX=3 formulation one needs to keep the value of the friction velocity u_* constant. Fig. 7.13 includes results of runs for stability classes D and F, in which the friction velocity u_* is kept the same as that for the run E3. This was achieved by choosing $u_0 = 2.225$ and $u_0 = 4.13$ m/s, respectively. By comparing Figs. 7.12a, 7.13a and 7.13b it is seen that for the case

$Ri_{cr} = 1000$, the effect of downwind diffusion increases as the flow becomes more stable. the amount of downwind diffusion somewhat increases with stability. However, the sensitivity to stability is considerably smaller than that for the MODSX-2 formulation.

7.4.5. Conclusions and recommendations

In this section the major conclusions for along-wind-diffusion formulations are summarised. Recommendations are made for the HEGADAS-T user in the selection of the appropriate type of along-wind-diffusion formulation.

The following conclusions and recommendations are made.

1. The cloud-shape-correction has been used in the past and seems to improve the predicted cloud shape considerably. It introduces downwind gravitational spreading and reduces the calculated crosswind gravitational spreading, in such a way that the amount of spreading in the downwind direction x of the cloud as a whole equals the spreading in the crosswind direction. This correction should be applied (default option ICSCOR=1 in code).
2. The original HEGADAS-T formulation (MODSX=1) is out-of-date and should not be used any more.
3. The adapted Ermak/Wilson formulation (MODSX=2) is the HEGADAS-T formulation recommended for non-neutral conditions (default option).

This formulation takes into account the effect of increased shear with increased stability. However the formulation has a number of deficiencies. The formulation is partially based on Chatwin's formula (7.33), which is strictly speaking only valid for neutral stability and passive gas dispersion. Moreover in the elimination of the time the (stability-class dependent) ambient wind speed and NOT the cloud speed

is adopted, and downwind diffusion is NOT ignored in regions with high Richardson numbers.

It is noted that diffusion could be ignored in regions with high Richardson number by calculating for each observer the downwind position x_{cr}^{obs} at which the Richardson number reduces to a given critical Richardson number Ri_*^{cr} (x_{cr}^{obs} corresponds to middle of pool, if $Ri_* < Ri_*^{cr}$ always) and replacing in eq. (7.44) the argument $\max[0, \xi - x_{br}]$ by $\max[\xi - x_{cr}^{obs}, \xi - x_{br}]$. However in this manner the σ_x -formula is NOT a direct function of x anymore and the formulation loses its simple nature.

For the above reasons the formulation MODSX=2 may be inaccurate, particularly if high cloud concentrations occur during the dispersion processes.

4. The adapted Chatwin/Wilson formulation (MODSX=3) is the HEGADAS-T formulation recommended for neutral conditions (default option).

This formulation is based on Chatwin's formula (7.33), which is strictly speaking only valid for neutral stability and passive gas dispersion. However, in the elimination of the time the actual true speed of the puffs (observers; cloud speed) as used in HEGADAS-T is adopted, and downwind diffusion is ignored in regions with Richardson number Ri_* larger than a user-specified value Ri_*^{cr} .

Because of the above reasons the adapted Chatwin/Wilson formulation is more compatible with the observer concept adopted in HEGADAS-T and therefore gives more realistic predictions than MODSX=2 in the case of neutral conditions.

In the high-density region $Ri > Ri_{cr}$ downwind diffusion induced by wind shear is assumed not to take place. However, in this region considerable gravitational downwind spreading occurs which is taken into account in HEGADAS-T by the cloud shape correction (see point 1).

It is still questionable what the ideal value is to be selected for $Ri_{*}^{c^r}$. The presently-used default value $Ri_{*}^{c^r} = 10$ seems to be reasonable, but may induce insufficient downwind diffusion. A higher value for $Ri_{*}^{c^r}$ might be more appropriate. An appropriate value for $Ri_{*}^{c^r}$ could be found by means of fitting with experimental data.

5. The adapted Chatwin/Wilson formulation can further be improved for non-neutral stability and heavy-gas-dispersion in the manner as described in Section 7.4.3 (Wheatley's and Van Ulden's formulations). Implementation of (adaptations of) these formulations is a possible further point of investigation.

7.5. GAS-BLANKET FORMULATION FOR TRANSIENT RELEASES

For finite-duration steady-state releases or slowly varying release rates the HEGADAS-T (version 4) formulation lead to erroneous oscillatory behaviour in the predictions of the gas-blanket dimensions. In Section 7.5.1 the original gas-blanket formulation in HEGADAS-T is summarised and the cause of the oscillations is explained. In Section 7.5.2 an improved gas-blanket formulation without oscillatory behaviour is introduced. This formulation has been implemented as an option in HEGADAS-T (version 5). In Section 7.5.3 this formulation is verified by means of an example problem involving a finite-duration steady-state release. The new formulation is chosen as the default option in HEGADAS-T (version 5).

7.5.1. Original formulation in HEGADAS-T (with oscillations)

Description of formulation

The gas-blanket formulation adopted in the transient version HEGADAS-T of the heavy-gas-dispersion program HEGADAS is described in Sections 6.1 and 6.2 of Appendix 3.

In the HEGADAS-T formulation the primary gas source is assumed to be circular with a radius $R_p(t)$, m, with a vapour production rate $E(t)$, kg/s. A 100% vapour blanket forms if the vertical vapour flux $Q_p(t) = E(t)/[\pi R_p^2(t)]$ is larger than the maximum flux $Q_{max}^* = Q_{max}^*(L=\pi^{1/2}R_p)$. This gas blanket is taken to have a flat cylindrical shape of radius $R_g(t)$ and height $H_g(t)$. The blanket dimensions $R_g(t)$ and $H_g(t)$ are determined from the numerical solution of two differential equations,

$$dR_g(t)/dt = C_E \{g [1 - \rho_a(z=0)/\rho_E] H_g(t)\}^{1/2} \quad (7.47)$$

$$dM(t)/dt = E(t) - \pi R_g^2(t) Q_{max}^* [L=\pi^{1/2}R_g(t)] \quad (7.48)$$

In these equations $\rho_a(z=0)$ is the air density at ground level, kg/m³, ρ_E the gas density, kg/m³, $g = 9.81$ m/s² is the acceleration of gravity and $M(t)$ the blanket mass defined by

$$M(t) = \pi \rho_E R_g^2(t) H_g(t) \quad (7.49)$$

Eq. (7.47) is a simple spreading law for the blanket radius, and eq. (7.48) a conservation equation for the blanket mass $M_g(t)$. The reader is referred to Section 6.1 in Appendix 3 for additional details.

At the onset of the formation of the gas blanket, at time $t = t_0$, the blanket radius equals the primary source radius and the blanket mass equals zero. Thus in the numerical solution of eqs. (7.47), (7.48) the initial values $R_g(t_0) = R_p(t_0)$ and $M(t_0) = 0$ are adopted. The differential equations are subsequently solved stepping forward in time.

For $t > t_0$ the blanket radius $R_g(t)$ increases due to gravitational spreading; see eq. (7.47). Mass is added to the gas blanket because of material entering the pool [spill rate $E(t)$] and lost because of evaporation [evaporation rate $\pi R_g^2(t) Q_{\max}^* (L - \pi^{1/2} R_g)$]; see eq. (7.48). Note that the amount of evaporation increases with the blanket radius $R_g(t)$.

For $t > t_0$ the blanket radius $R_g(t)$ is initially small and therefore the evaporation rate is less than the spill rate. Hence the mass of gas in the blanket initially increases. Because of this accumulation of gas, the blanket continues to spread beyond the radius at which the evaporation rate would equal the spill rate, and thereafter the evaporation exceeds the source rate. The mass of gas in the blanket therefore decreases, eventually reaching zero.

Let $t = t_1$ be the time at which the blanket height reduces to zero, i.e. the time at which the entire gas blanket is taken up into the air. If the primary vapour flux $Q_p(t_1)$ is smaller than the maximum flux $Q_{\max}^* = Q_{\max}^* [L - \pi^{1/2} R_p]$, the gas blanket disappears at time $t = t_1$ and the secondary pool is set equal to the primary pool. If the primary vapour flux $Q_p(t_1)$ is larger than $Q_{\max}^*$, a new gas blanket forms at $t = t_1$. This is assumed to happen in the same manner as described above, but now with the associated initial values $R_g(t_1) = R_p(t_1)$ and $M(t_1) = 0$.

Cause of oscillations in formulation

The original formulation yields a well-defined gas blanket for problems in which the spill rate $E(t)$ first "sufficiently" fast increases and subsequently decays to zero. For this type of problem the following subsequent phases usually occur:

- a. the secondary pool equals the primary pool, and the vapour concentration of the pool increases from 0 to 100%
- b. formation of a 100% vapour blanket; spreading of vapour blanket in the radial direction; initial increase of the blanket height and subsequent decrease to 0
- c. the secondary pool equals the primary pool, and the vapour concentration of the pool reduces to 0%

The original formulation gives rise to oscillations in the predicted gas-blanket dimensions for problems in which the spill rate $E(t)$ is constant or slowly varies for a sufficiently long time. At the start of each oscillatory cycle a 100% vapour blanket forms, which spreads out in the radial direction (initial radius = primary-pool radius). The blanket height initially increases and subsequently decrease to 0 at the end of the cycle.

From the above it follows that for steady-state sources the former gas-blanket formulation in HEGADAS-T does NOT properly reproduce the steady-state solution.

7.5.2. Improved gas-blanket formulation in HEGADAS-T (no oscillations)

The above oscillations are caused by resetting the blanket dimensions to the primary-pool dimensions if the blanket height reduces to zero. The much smaller primary-pool dimensions then lead immediately to the formation of another blanket etc.

In HEGADAS-T (version 5) a new gas-blanket formulation is implemented, which eliminates the oscillatory behaviour for slowly-varying or constant

spillage rates $E(t)$. In this formulation the following is carried out if the blanket height reduces to zero, say at $t = t_1$:

- If the primary vapour flux $Q_p(t_1)$ is smaller than the maximum flux $Q_{\max}^* = Q_{\max}^* [L - \pi^{1/2} R_p(t_1)]$, the gas blanket disappears and the secondary pool equals the primary pool
- If the primary vapour flux $Q_p(t_1)$ is larger than the maximum flux $Q_{\max}^* = Q_{\max}^* [L - \pi^{1/2} R_p(t_1)]$, a zero-height gas blanket forms. This gas blanket is assumed to equal the steady-state blanket corresponding to the present spillage rate $E(t_1)$. Thus according to eq. (7.48) the pool radius $R_g(t_1)$ of this blanket is determined from inversion of the formula $E(t_1) = \pi R_g^2(t_1) Q_{\max}^* [L - \pi^{1/2} R_g(t_1)]$.

For $t > t_1$ a gas blanket with zero height is assumed to remain in existence as long as the gas-release rate does not increase [$dE(t)/dt \leq 0$] and the blanket radius exceeds the primary radius [$R_g(t) > R_p(t)$]. Let the end of this period be at time $t = t_2$. During the period $t_1 < t < t_2$ the blanket radius $R_g(t)$ is determined from $E(t) = \pi R_g^2(t) Q_{\max}^* [L - \pi^{1/2} R_g(t)]$. At the end $t = t_2$ of the period the following two cases can be distinguished:

- The blanket radius $R_g(t)$ reduces to the primary radius $R_p(t)$ at $t = t_2$. In this case the zero-height gas blanket disappears and the secondary pool becomes equals to the primary pool.
- The release rate $E(t)$ starts to increase at time $t = t_2$. In this case a finite-thickness gas blanket forms and eqs. (7.47), (7.48) are solved with the initial values $R_g(t_2)$ (unchanged blanket radius) and $M(t_2) = 0$.

7.5.3. Example: finite-duration steady-state gas release

The above formulation will now be tested for a primary pool with a

radius of $R_p = 3$ m, a constant release rate $E = 30.0$ kg/s, and a release duration of 200 seconds. Figures 7.14 and 7.15 depict results for the following HEGADAS-S and HEGADAS-T simulations:

1. STEADY-STATE HEGADAS-S SIMULATIONS

- Simulation with release rate $E = 30$ kg/s, length $L_p = \pi^{1/2} R_p = 3 \pi^{1/2}$ and half-width $B_p = L_p/2$. This simulation corresponds to the square primary source adopted by HEGADAS-T to calculate the gas-blanket dimensions. The gas-blanket dimensions calculated by HEGADAS-S were $L = 25.9$ m and $B = L/2$ corresponding to a blanket radius $R_g = L / \pi^{1/2} = 14.6$ m. The latter value is used as the steady-state radius in Fig. 7.14a.
- Simulation with release rate $E = 30$ kg/s, length $L_p = 2 * R_p = 6$ and half-width $B_p = (\pi R_p^2)/(2L_p)$. This simulation corresponds to the sources seen by the observers in the HEGADAS-T formulation (see Section 6.2 in Appendix 3). The concentration calculated by this simulation is depicted in Fig. 7.15.

2. TRANSIENT HEGADAS-T SIMULATIONS

- Former HEGADAS-T formulation (BLMODEL = 0). In this formulation the gas-blanket radius is reset to the primary-pool radius, every time if the blanket height $H_g(t)$ reduces to zero. It is seen from Figure 7.14 that this gives rise to oscillations in the predicted blanket dimensions with an average cycle length of about 23 seconds. Fig. 7.15 illustrates that the blanket oscillations cause oscillations in the predicted observer concentrations which are not sufficiently damped out by the downwind diffusion. In the present simulation the Chatwin/Wilson downwind spreading formulation without a cloud shape correction is chosen.
- New non-oscillatory HEGADAS-T formulation (BLMODEL = 1). See the listing of HEGADAS-T report file included in Table 7.4 for full details of the calculations. In this formulation the gas-blanket

radius is reset to the steady-state blanket radius if the blanket height $H_g(t)$ reduces to zero. From Table 7.4 it is seen that this happens at $t = 24.8$ seconds. The result for the non-oscillatory formulation depicted in Fig. 7.15 can be explained as follows.

- a. It is seen from Table 7.4 that observers are released at the times -12, -8, ..., 192 seconds at the downwind position $x = -RGMAX = -20.608$ m ($RGMAX$ = maximum blanket radius). All observers released between 24 seconds and 176 seconds observe a gas blanket with the steady-state blanket radius $R_g = 14.6$ m (see Table 7.4). At time $t = 100$ seconds the observer released at 24 seconds arrives at the downwind position of $x = 137$ m. This explains the convergence of the observer concentration for $0 < x < 137$ m to the steady-state HEGADAS-S limit (see Fig. 7.15).
- b. The blanket radius overshoots the steady-state radius for $13 < t < 28$ seconds; see Fig. 7.14a. This results in the observers released between 0 and 20 seconds (see Table 7.4) observing an evaporation rate which is higher than the steady-state rate $E = 30$ kg/s. At time $t = 100$ seconds these observers occupy the downwind distance region $147 < x < 198$. This explains the over-prediction of the observer concentrations for this region (see Fig. 7.15).
- c. The observers released at the times -12, -8, -4 did only see a part of the source. At time $t = 100$ seconds these observers occupy the downwind distance region $208 < x < 229$ m. This explains the lower observer concentration for this region (see Fig. 7.15).

7.6. BREAKPOINT FACILITY

7.6.1. Introduction

The breakpoint facility in HEGADAS allows the user to start a HEGADAS run at a specified distance downwind of the source (breakpoint). The gas-blanket calculations do not need to be performed, but the properties of the cloud at the breakpoint (centre-line ground-level concentration, cloud width, etc.) must be input to HEGADAS. These data are typically provided by near-source programs such as PLUME or HFPLUME (see Chapter 5) or in some cases experimental data.

The steady-state HEGADAS-S model (version 5) allows for multiple breakpoints (at several distances downwind of the source). By specifying changes of surface roughness at breakpoints, the user can perform a simulation of heavy-gas dispersion over terrain with a surface roughness varying in the downwind direction. Section 7.6.2 gives a description of the breakpoint facilities in HEGADAS-S.

Sections 7.6.3 and 7.6.4 discuss the breakpoint facilities available in the time-dependent HEGADAS-T model (version 5). Multiple breakpoints in a single HEGADAS-T run are not allowed. At present the following two major types of breakpoints are implemented

- A "full" breakpoint. In this formulation all required dispersion parameters are specified at the breakpoint as a function of the time, and gas-blanket calculations are not performed. Observers are released at this breakpoint at constant time intervals, and HEGADAS-S dispersion calculations are carried out downwind of this breakpoint for each observer. Section 7.6.3 gives a description of this type of breakpoint.
- A "partial" breakpoint (former HEGADAS formulation). This type of breakpoint is out-of-date and is not advocated to be used. In this formulation data defining the primary pool are specified and gas-blanket calculations are carried out as usual. Dispersion calculations are performed upwind of the breakpoint and at the breakpoint only a subset

of the dispersion parameters is reset. The specified breakpoint data are constant, i.e. they do not depend on the time. Section 7.6.4 gives a description of this simple type of breakpoint.

7.6.2. Steady-state version

The HEGADAS equations are described in detail in Appendix 3 and have been outlined in Section 7.1. Typically HEGADAS calculates six basic variables by solving a set of ordinary differential equations stepping forward in the downwind direction. These variables are as follows.

- c_A , ground-level concentration at centre-line of cloud (kg dry gas / m^3); c_A is related to the wet-gas fraction y_{wg} by

$$c_A = y_{wg} M_g / \{(1+\omega'_2) V_m\} \quad (7.50)$$

with M_g the molecular weight of the gas (kg/kmole), V_m the mixture volume (m^3 /kmole) and ω'_2 the molar fraction of water (initially) in the gas. [Note that for HF, the gas must be always dry ($\omega'_2=0$) and y_{wg} is the equivalent HF monomer molar fraction.]

- S_z , vertical dispersion coefficient (m)
- S_y , cross-wind dispersion coefficient (m)
- b , half-width of middle part of cloud, along which the ground-level concentration is taken to be equal to c_A (m)
- H_e , heat transfer from the surface (Joule / mole of mixture)
- y_{w3} , water-vapour transfer from the surface (moles of water / mole of mixture)

In a HEGADAS-S simulation the above data are first determined above the pool. Data further downwind are found by solving the set of differential

equations downwind of the pool. This type of simulation may be applied if HEGADAS can accurately be applied near the source and all source data (pool dimensions, temperature of released gas, etc.) are known.

In many cases the near-source region involves high plume speeds (jets), two-phase behaviour and possible other physical phenomena which are not (properly) taken into account in the HEGADAS model. For these situations HEGADAS can be accurately applied downwind of this region provided sufficient data (experimental data or data obtained from a near-source program) are available at the transition point (downwind edge of the near-source region).

In HEGADAS it is possible to specify one or more breakpoints (transition points), at which the above-mentioned solution variables may be entirely or partly specified. In addition, to enable the user to simulate heavy-gas-dispersion over terrain with a varying surface roughness, the surface roughness parameter may be changed at a breakpoint. If all breakpoint data are specified for the first breakpoint (i.e. breakpoint most close to the source) HEGADAS calculations upwind of the breakpoint need not to be performed (user-specified option). In this case the pool dimensions do not need to be specified, HEGADAS gas-blanket calculations are not performed, and the HEGADAS calculations are started from the first breakpoint, i.e. at that downwind distance.

The following types of breakpoints are allowed in the new HEGADAS program.

1. A "FULL" BREAKPOINT.

In this case all 6 solution variables are specified at the breakpoint, and the dispersion calculations downwind of the breakpoint are fully independent of the (optional) calculations upwind of the breakpoint. The solution variables at the breakpoint are set as follows.

- The cross-wind concentration profile is taken to be uniform with a user-specified half-width WS, i.e. $b = WS$, $S_y = 0$
- The amount of water-vapour added from the surface is taken to be zero, $y_{w3} = 0$
- The centre-line ground-level concentration y_{wg} is specified by the user, $y_{wg} = CONCS$
- One of the following two options is used to set the added heat from the surface H_g :
 - o H_g is calculated from the user-specified mixture temperature $T = TMPS$ at the breakpoint and the user-specified ground-level concentration $y_{wg} = CONCS$. This is done by solving iteratively the equation $TMPS = T(y_g, H_g)$, with the mixture temperature T as a function of y_g, H_g determined from the thermodynamics subroutine THERMO. Note that this option can be chosen only if CONCS is also prescribed
 - o H_g is taken to be zero, $H_g = 0$, if no mixture temperature TMPS is prescribed
- The vertical dispersion coefficient S_z is set from the gas-mass conservation equation [see eq. (4.14) in Appendix 3],

$$c_A = \frac{E(1+\alpha)z_0^\alpha}{2(b+\pi^{1/2}S_y/2) u_0 S_z^{1+\alpha}} \quad (7.51)$$

in which E is the dry-gas source strength, u_0 the ambient wind speed at the reference height z_0 , and c_A is given by eq. (7.50).

2. A "PARTIAL" BREAKPOINT

For this case some of the breakpoint data are not specified, but they are calculated from the results of the dispersion calculations upwind of

the breakpoint. Thus for this type of breakpoint calculations upwind of the breakpoint need always to be performed. The user may choose one or more of the following options.

- o The half-width WS of the cross-wind profile is not specified. In this case the cross-wind profile is not changed at the breakpoint. Thus the "old" values for $b = b^{\text{old}}$, $S_y = S_y^{\text{old}}$ are used as the "new" values at the breakpoint, i.e. the values derived from the calculations upwind of the breakpoint are used as starting values for the calculations downwind of the breakpoint.
- o The concentration CONCS is not specified, but instead the effective cloud height H_{eff} is specified. For this case S_z is set from eq. (3.6) in Appendix 3 for H_{eff} . Subsequently new values $y_{\text{wg}}^{\text{new}}$, H_e^{new} , $y_{\text{w3}}^{\text{new}}$ are calculated iteratively from the old values $y_{\text{wg}}^{\text{old}}$, H_e^{old} , $y_{\text{w3}}^{\text{old}}$ until convergence is obtained:
 - $y_{\text{wg}}^{\text{new}}$ is set from from eqs. (7.50) and (7.51)
 - the new values H_e^{new} , $y_{\text{w3}}^{\text{new}}$ are derived from the old values $y_{\text{wg}}^{\text{old}}$, H_e^{old} , $y_{\text{w3}}^{\text{old}}$ by setting $y_{\text{wg}}^{\text{new}} / y_{\text{wg}}^{\text{old}} = H_e^{\text{new}} / H_e^{\text{old}} = y_{\text{w3}}^{\text{new}} / y_{\text{w3}}^{\text{old}}$; the mixture volume V_m and the mixture temperature T are set from the thermodynamic subroutine THERMO

3. CHANGE OF SURFACE ROUGHNESS AT BREAKPOINT

In addition to the data specified at the "full" breakpoint and the "partial" breakpoint, the user may also specify the value of the surface roughness z_R downwind of the breakpoint. It is also allowed to specify only z_R at a breakpoint.

For a given (fixed, user-specified) value of the speed u_0 at a reference height z_0 , the modified value for z_R induces a modified value for the ambient friction velocity u_* and a modified logarithmic profile for the ambient wind-speed. This also induces a change of the exponent α in the power-law fit of this profile. Therefore, in order to satisfy gas-mass

conservation at the breakpoint, the vertical dispersion coefficient is re-calculated from eq. (7.51).

It is not expected that the provision of this facility will give a simple means of performing accurate simulations of dispersion over a change in surface roughness. The effect of a sudden change in surface roughness in the atmosphere is that an internal boundary layer develops, which slowly increases in height downwind of the roughness change (Wood, 1982, Raabe, 1983). The effects of the upstream roughness can be felt typically for many hundreds of metres downwind of the change (see also Puttock, 1987).

The provision of the formal capability of making a sudden roughness change in the model allows investigation of the possible effects of roughness changes on dispersion. Multiple breakpoints do allow the change to be spread over some distance.

Two further points can be made: we expect that making a rough-to-smooth transition suddenly should at least give conservative concentration predictions in general (although the interaction of the effects of vertical mixing and gravity spreading in dense-gas dispersion make it difficult to make any such general comments with certainty). Secondly, if the cloud is dense and low, it may be contained completely within the internal boundary layer much sooner than a passive release would be.

7.6.3. Transient version - full breakpoint (vertical time-dependent source)

In the HEGADAS-T formulation without a breakpoint, gas-blanket calculations are carried out based on user-specified time-dependent pool data (pool strength, pool dimensions) and dispersion calculations are performed downwind of the blanket.

As in HEGADAS-S (version 5), dispersion calculations in HEGADAS-T (version 5) are started at a specified distance downwind of the source when a "full" breakpoint is used. The gas-blanket calculations are not carried out, and the user needs to specify time-dependent properties of the cloud at the breakpoint.

The breakpoint data are specified with a user-specified time interval Δt . Let n_{td} be the number of specified times, then the breakpoint data are specified at the times $t = \Delta t, 2\Delta t, \dots, n_{td}\Delta t$. Zero concentrations are assumed at x_{br} for $t \leq 0$ and $t \geq (n_{td}+1)\Delta t$.

At each of the times $t = \Delta t, 2\Delta t, \dots, n_{td}\Delta t$ an observer is released at the breakpoint. Steady-state HEGADAS-S dispersion calculations downwind of the breakpoint are carried out for each observer.

This section first discusses the specification of the time-dependent breakpoint data by the user and the conversion of these data into values of basic dispersion variables. The latter values are required as starting values for the dispersion calculations carried out for the observer released at time t . These calculations provide values of the observer-dispersion data, while the observer travels in the downwind direction.

In the second part of this section a formula for the observer position as a function of time is derived. This formula enables the observer-dispersion data to be expressed as a function of position and time.

The actual concentration data are derived from the observer-dispersion data by inclusion of a cloud shape correction and downwind diffusion effects. This is discussed in the third part of this section.

In the final part of this section the new breakpoint formulation is tested by means of a number of test problems.

Specification of data at breakpoint; effective cloud data

At each time $t = \Delta t, 2\Delta t, \dots, n_{td}\Delta t$ the user needs to specify three data at the breakpoint x_{br} . These are the effective cloud half-width $B_{eff}^{br}(t)$ and any two of the following breakpoint data: the ground-level centre-line wet-gas fraction $y_{wg}^{br}(t)$, the effective cloud height $H_{eff}^{br}(t)$ or the gas-mass flow $E^{br}(t)$ through the plane $x = x_{br}$ (dry gas; kg/s).

At each downwind position, the gas cloud in HEGADAS may be replaced by an "effective" gas cloud with an effective cloud half-width B_{eff} , an effective cloud height H_{eff} , an effective cloud speed u_{eff} , and a uniform concentration chosen to be equal to c_A . The centre-line ground-level concentration c_A is related to y_{wg} by eq. (7.50). The effective cloud data B_{eff} , H_{eff} , and u_{eff} are defined by the expressions (3.14), (3.6) and (3.10) in Appendix 3 as functions of S_z , b and S_y ,

$$B_{eff} = b + \frac{1}{2}\pi^{\frac{1}{2}} S_y \quad (7.53)$$

$$H_{eff} = \frac{1}{(1+\alpha)} \Gamma\left(\frac{1}{1+\alpha}\right) S_z \quad (7.54)$$

$$u_{eff} = \frac{u_0}{\Gamma[1/(1+\alpha)]} \left(\frac{S_z}{z_0}\right)^\alpha \quad (7.55)$$

By using the above expressions it follows from eq. (7.51) that the flow E of dry gas (kg/s) through a plane $x = \text{constant}$ can be expressed as

$$E = 2 B_{eff} H_{eff} u_{eff} c_A \quad (7.56)$$

Calculation of dispersion variables at breakpoint

Analogous to the "full" steady-state breakpoint discussed in Section 7.6.2, the observer calculations are started at the breakpoint, after the required start values of the six dispersion variables y_{wg} (or c_A), S_z , b , S_y , H_e , y_{w3} have been set. These values are derived from the breakpoint data specified at the observer release time t . This derivation is similar to that for the steady-state breakpoint (cf. Section 7.6.2):

1. The cross-wind concentration profile is taken to be uniform with a user-specified half-width $B_{eff}^{br}(t)$, i.e. $b = B_{eff}^{br}(t)$, $S_y = 0$
2. The amount of water vapour added from the surface is taken to be zero, $y_{w3} = 0$
3. The added heat from the surface H_e is taken to be zero, $H_e = 0$
4. From the specified breakpoint data described above, the dispersion variables y_{wg} and S_z at the breakpoint at time t are set as follows:

A. y_{wg} is specified; either H_{eff} or E is specified

A.1. First the thermodynamic calculations are carried out to calculate from y_{wg} the mixture volume V_m , the mixture density ρ_m , the ground-level centre-line concentration c_A , and the mixture temperature T_m . See eq. (7.50), Section 7.2 (for HF gas), and Appendix A contained in Appendix 3 (for non-reactive gases) for further details.

A.2. Secondly the vertical dispersion coefficient S_z is calculated. It is set by means of eqs. (7.53-7.56), the calculated value of c_A , and the specified value for H_{eff} or E .

B. y_{wg} is not specified; both H_{eff} and E are specified

B.1. First S_z is set from eq. (7.54)

B.2. c_A is set from (7.56) and $c_A = c_A(y_{wg})$ is solved iteratively for y_{wg} by means of the thermodynamic subroutine THERMO.

Observer velocities and positions

The calculation of the observer velocity and observer position in the original HEGADAS-T formulation without a full breakpoint is described in Appendix B contained in Appendix 3 to this report. In this formulation observers are released upwind of this pool, and the adopted formula for the observer velocity is based on pool data at which the take-up rate is maximum.

The above formula is clearly not applicable for the present breakpoint formulation, in which time-dependent breakpoint data are specified instead of pool data. Therefore new formulas for the observer velocity and position are proposed. It has been attempted in the derivation of these formulas to follow the concepts adopted in the original HEGADAS-T formulation (without a full breakpoint) as closely as possible. Compare the derivation of the new formulas given below with that for the old formulas given in Appendix B contained in Appendix 3 to this report.

Ideally the observers should move with the average transport velocity u_{eff} of the vapour molecules (effective cloud speed) defined by eq. (7.55). At a given location x the value of S_z and accordingly u_{eff} differ from observer to observer and consequently some observers may overtake others. Therefore a simplified formula will be introduced which is a function of x only.

The simplified formula is assumed to be based on the two-dimensional case (no cross-wind spreading effects) with a certain constant Richardson number Ri_0 . For this case the entrainment equation presented in eq. (3.8) in Appendix 3 can be solved for S_z ,

$$S_z = S_z(x) = z_0 \left(\frac{k}{z_0} \frac{u_*}{u_0} \frac{(1+\alpha)^2}{\Phi(Ri_0)} (x - x_0) \right)^{1/(1+\alpha)} \quad (7.57)$$

with x_0 an integration constant. Insertion of eq. (7.57) into (7.55) yields the following formula for the observer speed as a function of x ,

$$u_{obs} = u_{obs}(x) = C_0 (x - x_0)^{\alpha/(1+\alpha)} \quad (7.58)$$

with

$$C_0 = C_0[Ri_0] = \frac{u_0}{\Gamma[1/(1+\alpha)]} \left\{ \frac{k}{z_0} \frac{u_*}{u_0} \frac{(1+\alpha)^2}{\Phi(Ri_0)} \right\}^{\alpha/(1+\alpha)} \quad (7.59)$$

By integrating the above equation to time the following formula for the observer position can be derived

$$x(t) = x_0 + \left\{ (x_{br} - x_0)^{1/(1+\alpha)} + \frac{C_0}{1+\alpha} (t - t_{st}^{obs}) \right\}^{1+\alpha} \quad (7.60)$$

with t_{st}^{obs} being the time at which the observer is released at the breakpoint $x = x_{br}$.

It now remains to evaluate the constants C_0 and x_0 in the above equations. The constant x_0 is first determined by matching at $x = x_{br}$ eq. (7.58) for the effective cloud speed against a typical value of u_{eff} derived from the breakpoint data. Subsequently the constant C_0 is determined. In two different approaches it is set either from a typical Richardson number (derived from the breakpoint data), or by assuming that the vapour molecules originate from a low-momentum source.

The effective cloud speed u_{eff} can be set from eq. (7.55) and the value of S_z calculated at the breakpoint $x = x_{br}$. However the latter value for S_z varies from observer to observer. Therefore to arrive at a fixed value, the value of S_z is chosen to correspond to the value $S_z^{br}(t_m)$ at the time t_m when the gas-flow rate $E^{br}(t)$ is maximum. The value for u_{eff} thus obtained from eq. (7.55) is now assumed to be the value of the observer speed at x_{br} ,

$$u_{obs}(x_{br}) = \frac{u_0}{\Gamma[1/(1+\alpha)]} \left(\frac{S_z^{br}(t_m)}{z_0} \right)^\alpha \quad (7.61)$$

Thus by inserting eq. (7.61) into (7.58) it follows that

$$x_0 = x_{br} - \left(\frac{u_0}{C_0 \Gamma[1/(1+\alpha)]} \right)^{(1+\alpha)/\alpha} \left(\frac{S_z^{br}(t_m)}{z_0} \right)^{1+\alpha} \quad (7.62)$$

For the determination of the second constant C_0 the following two different approaches can be selected in HEGADAS-T (IOBSXT=1 or IOBSXT=2).

1. The effective cloud speed at the breakpoint is chosen above to correspond with the typical time t_m . Likewise it can be assumed that the Richardson number Ri_0 introduced above corresponds to t_m , i.e. $Ri_0 = Ri_*^{br}(t_m)$. Thus the formula for the observer position adopted in the first approach (IOBSXT=1) is defined by eq. (7.60) with the constant $C_0 = C_0[Ri_*^{br}(t_m)]$ given by eq. (7.59) and the constant x_0 by eq. (7.62).
2. In the HEGADAS-T formulation without a full breakpoint an unpressurised gas release is assumed. The vapour molecules are released at (the upwind edge of the) pool with a zero velocity and are subsequently convected downwind by the ambient air. Thus the observer velocity (speed of vapour molecules) is taken to be zero at $x = -R_{max}$, with R_{max} being the maximum gas-blanket radius.

Likewise, in the HEGADAS-T formulation with a full breakpoint, the breakpoint data may be assumed to be associated with an unpressurised gas release at a source located at $x = 0$. Thus in this case x_{br} should be an estimate of the downwind distance from (the upwind edge of) the pool. The observers may assumed to have actually been released from a pool located at $x = 0$, and the observer speed (speed of vapour molecules) at the point of release $x = 0$ should be zero.

By using $u_{obs}(0) = 0$ and eq. (7.61) into (7.58) the constants C_0 and x_0 can be determined,

$$x_0 = 0, \quad C_0 = \frac{u_0}{\Gamma[1/(1+\alpha)]} \left(\frac{S_z^{br}(t_m)}{z_0} \right)^\alpha x_{br}^{-\alpha/(1+\alpha)} \quad (7.63)$$

Thus the formula adopted for the observer position in the second approach (IOBSXT-2) is defined by eq. (7.60) with the constants C_0 , x_0 given by the above equation. This formula may be compared with the expression (7.45) adopted for a HEGADAS-T analysis without a full breakpoint. Note that the approach IOBSXT-2 should be used only in the case of low-momentum unpressurised gas releases if the distance between the breakpoint and the source is known.

..... Calculation of observer-dispersion data

When the observer-dispersion data at the breakpoint have been established, the steady-state observer calculations downwind of the breakpoint are performed. Thus the observer-dispersion data are calculated as a function of the downwind distance x . By use of the formula (7.60) for the observer position, the observer data are stored at those downwind positions, which correspond to a number of user-specified output times.

..... Cloud shape correction for gravitational spreading

The cloud shape correction for gravitational spreading in the downwind direction is carried out following an approach which is similar to that for the HEGADAS-T formulation without a breakpoint; see Appendix C contained in Appendix 3 to this report for full details of the latter formulation.

Before describing the cloud shape correction we introduce the following notation. Let t_k be the k^{th} output time specified by the user. Let observer i be the observer released at time $i\Delta t$ ($1 \leq i \leq n_{td}$), and let x_i^k be the downwind position of observer i at time t_k . Let the observers i_L^k , i_R^k ($i_L^k \geq i_R^k$) be the observers which at time t_k see some gas ($c_{A,i}^k > 0$) and which are located most upwind ("left") and downwind ("right"), respectively. The corrected downwind positions and crosswind dispersion data at time k for observer i are denoted by $x_i^{cor,k}$, $b_i^{cor,k}$ and $S_{y,i}^{cor,k}$.

The major differences between the cloud shape correction with and without a breakpoint are now as follows:

- In the absence of a breakpoint the cloud shape correction is started at the observer at which the maximum concentration c_A is found. In case of a partial breakpoint, it is started at the closest upwind observer to the breakpoint. In case of a full breakpoint, it is started at the downwind observer i_L^k which is closest to the breakpoint, i.e. at the observer which has been most recently released (at time $t \leq t_k$).
- In the absence of a full breakpoint, the "initial" cloud width W_0 is taken to be the maximum diameter $2 R_{\max}$ of the gas blanket above the source. In case of a full breakpoint, it is set equal to the maximum cloud width specified at the breakpoint. Thus $W_0 = 2 B_{\text{eff}}^{\text{br}}(M\Delta t)$, if this maximum is assumed at time $t = M\Delta t$.

Using these modifications the algorithm for cloud shape correction is as follows in the case of a full breakpoint (see Appendix C contained in Appendix 3 to this report for omitted details)

1. Set "initial" cloud width $W_0 = 2 B_{\text{eff}}^{\text{br}}(M\Delta t)$
2. Loop over the specified output times t_k ($k = 1, 2, \dots$):
 - 2.1. Determine observers $IL = i_L^k$, $IR = i_R^k$ ($IL \geq IR$). Set cloud length $L_c = (x_{IR}^k - x_{IL}^k)$. Set $L_c^* = L_c / W_0$
 - 2.2. Loop over the observers $i = IL, IL-1, \dots, IR+1, IR$:
 - 2.2.1. If $b_i^k > 0$, set $B_{\text{eff},i}^* = B_{\text{eff},i}^k / B_{\text{eff}}^{\text{br}}(i\Delta t)$. If $b_i^k = 0$, set $B_{\text{eff},i}^* = 1$. Set S_i^* from eq. (C.7) in Appendix 3
 - 2.2.2. Correct crosswind dispersion parameters for observer i :

$$b_i^{\text{cor},k} / b_i = S_{y,i}^{\text{cor},k} / S_{y,i} = (1+S_i^*) / B_{\text{eff},i}^*$$
 - 2.2.3. If $i < i_L$, correct downwind position of observer i : $x_i^{\text{cor},k} = x_{i+1}^{\text{cor},k} + (x_i^k - x_{i+1}^k)(L_c^* + S_i^*) / L_c^*$

Note that the conditions at the breakpoint x_{br} remain satisfied during the cloud shape correction. If the output time t_k equals the time $i\Delta t$ at which the present observer i is released at the breakpoint, it follows from the above that $B_{eff,i}^* = 1$, $S_i^* = 0$, $IL = i$. Thus the crosswind dispersion parameters b , S_y and the downwind position x remain unchanged.

Calculation of dispersion data (inclusion of downwind diffusion)

After the cloud shape correction, downwind diffusion effects are taken into account in the same way as for the HEGADAS-T formulation without a (full) breakpoint. It must be noted that in these calculations the observer position is now NOT given by (7.45) but by (7.60).

Note that the conditions at the breakpoint x_{br} remain satisfied during the inclusion of downwind diffusion. This is because zero diffusion ($\sigma_x=0$) is assumed at $x = x_{br}$ in all currently implemented along-wind-diffusion formulations (see Section 7.4).

Testing of "full" breakpoint formulation

The breakpoint formulation has been verified using the following test problems.

1. A HEGADAS-T simulation with breakpoint data at $x = 30$ m corresponding to a constant gas release with a long duration T , i.e. with constant breakpoint data $B_{eff}^{br}(t) = B = 13.6$ m, $E^{br}(t) = E = 32$ kg/s, $y_{wg}^{br}(t) = Y = 0.73$ ($0 < t < T$) and $T = 100$ seconds so large such that steady-state has been closely achieved at time T for a considerable downwind distance.

The results of this simulation have been compared with a corresponding steady-state simulation. Note that the observer-dispersion data prior to the cloud shape correction should match exactly with the steady-state predictions. This is confirmed by the centre-line ground-level concentration plot depicted in Fig. 7.16.

2. In Section 7.4.4.2 HEGADAS-T simulations were carried out for neutral stability and a constant gas release with a duration of 20 seconds ($E = 30 \text{ kg/s}$, $0 < t < 20$). The simulation included a cloud shape correction and downwind diffusion according to the adapted Chatwin/Wilson formulation ($\text{MODSX}=3, \text{Ri}_{cr}=10$). In order to test the HEGADAS-T breakpoint, this simulation was repeated with a larger number of observers, i.e. with a time interval of 1 second in between their release times. In this manner accurate predictions were obtained of the observer dispersion data (prior to the cloud shape correction) at the downwind distance $x = 20 \text{ m}$ (just downwind of the maximum-size gas blanket).

The observer dispersion data deduced in the above manner at the times $t = 2.5, 5, \dots, 45$ were used as breakpoint data in two HEGADAS-T simulations WITH a breakpoint at $x_{br} = 20 \text{ m}$. In the two simulations the two different formulas IOBSXT=1,2 for the observer position were adopted. See the listing of the report file for IOBSXT=1 included in Table 7.5 for further details.

Predictions of the observer concentrations (prior to the cloud shape correction) for the above three simulations at the time $t = 40$ and $t = 600$ are presented in Figures 7.17a and 7.18a. Note that the concentrations differ for $x > x_{br}$, because the formulas for the observer positions are different for the three formulations. The formulae used in HEGADAS-T were found to be

$$\begin{aligned} x^{obs}(t) &= -20.6 + 0.974(t - t_{st}^{obs})^{1.175} && \text{(no breakpoint; IOBSXT=0)} \\ x^{obs}(t) &= -6.27 + 0.998(16.2 + t - t_{st}^{obs})^{1.175} && \text{(IOBSXT=1)} \\ x^{obs}(t) &= 1.05(12.3 + t - t_{st}^{obs})^{1.175} && \text{(IOBSXT=2)} \end{aligned}$$

Note that in the simulation without a breakpoint t_{st}^{obs} is the time at which the observer is released at $x = -20.6$ ($20.6 = \text{maximum gas-blanket radius}$). In the simulations with the breakpoint $x_{br} = 20$, t_{st}^{obs} is the time at which the observer is released at x_{br} . From the above formulae it follows that for very large times the observer position prior to the

cloud shape correction will be further downwind for a larger value of IOBSXT (larger observer velocities); see Fig. 7.18a.

Figure 7.17b and 7.18b include predictions of the cloud concentrations, after the effects of cloud cloud shape correction and downwind diffusion are taken into account. When a breakpoint is used the cloud shape correction starts at the most upwind observer, otherwise it starts at the observer with the highest concentration. It is seen from Figures 7.17b and 7.18b that when a breakpoint is used the cloud shape correction induces a larger movement of the downwind edge of the cloud in the downwind direction and a smaller movement of the upwind edge of the cloud in the upwind direction.

3. The reader is referred to the time-dependent simulation of the first Goldfish experiment in Section 9.4 for an example of a HEGADAS-T simulation where the breakpoint data are derived from the near-source jet/plume program HFPLUME. The predicted time-dependent variation of both the center-line ground-level concentrations and the cloud shape are found to be in reasonable agreement with the experimental data.

7.6.4. Transient version - partial breakpoint

In this section the former HEGADAS-4 "partial" breakpoint formulation is discussed. This formulation is retained as an option in HEGADAS-5 for reasons of compatibility. However this formulation is out-of-date and is not advocated to be used. The description of this formulation is included in this section for reasons of completeness.

In the "partial" breakpoint formulation first the steady-state HEGADAS dispersion calculations upwind to the breakpoint $x = x_{br}$ are performed for each observer. Then the breakpoint data are transformed, whereby the user may presently choose between the following two options.

1. Specification of the effective cloud height $H_{eff} = HS$ only.

In this case the cross-wind concentration profile is not changed at the breakpoint. Thus the "old" values for $b = b^{old}$, S_y^{old} are used as the "new" values at the breakpoint, i.e. the values derived from the calculations upwind of the breakpoint are used as starting values for the calculations downwind of the breakpoint. Furthermore S_z is set from eq. (3.7) in Appendix 3 for H_{eff} . Subsequently the new values y_{wg}^{new} , H_e^{new} , y_{w3}^{new} are derived iteratively from the old values y_{wg}^{old} , H_e^{old} , y_{w3}^{old} as follows:

- y_{wg} is set from from eqs. (7.50) and (7.51)
- the new values H_e^{new} , y_{w3}^{new} are derived from the old values y_{wg}^{old} , H_e^{old} , y_{w3}^{old} by setting $y_{wg}^{new} / y_{wg}^{old} = H_e^{new} / H_e^{old} = y_{w3}^{new} / y_{w3}^{old}$; the mixture volume V_m and the mixture temperature T are set from the thermodynamic subroutine THERMO

2. Specification of the scaling factor CONCRS for y_{wg} , and optional specification of a maximum value FRAMAX (default = 1) for y_{wg} and a maximum value WSMAX for the effective cloud half-width B_{eff} (default = ∞). The breakpoint data are set as follows:

- added molar heat from surface $H_e = 0$
- molar water vapour surface flux $y_{w3} = 0$

- molar wet-gas fraction $y_{wg} = \min(y_{wg}^{old} * CONCRS, FRAMAX)$
- for effective cloud-width $B_{eff}^{old} > WSMAX$, set cross-wind dispersion coefficient $S_y = 0$ and $b = B_{eff} = WSMAX$; else use old values S_y^{old} , b^{old} .

7.7. IMPROVED EFFICIENCY AND USER-FRIENDLINESS; NEW POST-PROCESSORS

Extensions and modifications to the theoretical formulation in the extended version HEGADAS-5 of the program HEGADAS have been discussed in the previous sections. In addition, the HEGADAS-5 program has been enhanced to make it more user-friendly. The following provides an overview of these enhancements. See the User's manual for detailed information.

1. MORE USER-FRIENDLY INPUT

- The calculation of the Monin-Obukhov length λ and the cross-wind dispersion parameters δ, β has been automated. Instead of specifying λ, δ, β the user can now specify values for the atmospheric stability class PQSTAB (A,B,C,D,E or F) and the averaging time AVTIMC for the predicted concentrations.

The Monin-Obukhov length λ is calculated as a function of the stability class PQSTAB and the surface roughness parameter z_R from Table I in Irwin (1979). The power-law expression $\lambda = a z_R^b$ is adopted, with (in SI-units) $a = -11.43, -25.97, -123.5, \infty, 123.5, 25.97$ and $b = 0.1028, 0.1715, 0.3044, 0, 0.3044, 0.1715$ for stability classes A, B, C, D, E, F, respectively. See Figure 7.6 for λ as a function of z_R and PQSTAB. See Section 7.3.1.1. and Tables 7.1 and 7.2 for the calculation of δ, β as a function of PQSTAB and AVTIMC.

- The program input has been improved an additional error-checking facilities have been incorporated.
- Many other minor improvements have been implemented, e.g. option to allow specification of source flow (kg/s) instead of source flux (kg/m²/s), specification of molar fraction of gas at source and specification of ambient air temperature at any height.

2. OPTION OF USER-SPECIFIED FIXED OR VARIABLE OUTPUT STEPS IN HEGADAS-S.

In HEGADAS-5 the downwind direction step-size, controlling the

dispersion data output in the HEGADAS report file, is not necessarily fixed and can be fully controlled by the user. By selecting larger output steps further downwind, the user may reduce the CPU-time considerably.

3. IMPROVED OUTPUT FILES; NEW POST-PROCESSORS HSPOST AND HTPOST.

The layout of the HEGADAS report file has been improved. Furthermore new programs HSPOST and HTPOST are developed. These programs are post-processors to the steady-state version (HEGADAS-S) and the transient version (HEGADAS-T) of HEGADAS, respectively. They are interactive and allow the user to create a printout or data files for a wide range of concentration variables. In addition, the user can use the data files as input to most commercial plotting software for plotting such variables as concentration versus distance, cloud dimensions, concentration contour plots, time-history plots, etc.

The post-processor HSPOST includes an option to include an error-function correction for finite-duration releases to the steady-state HEGADAS-S concentrations; see Section 8.6.1 in the User's Manual for full details. However, to obtain more accurate concentration predictions, the user is advised to apply HEGADAS-T in case of finite-duration releases.

The post-processor HTPOST allows the time-dependent concentrations to be averaged over any user-specified averaging time; see Section 7.3.1.3 in the Technical Report and Section 8.6.2 in the User's Manual for full details.

7.8. LINKS WITH NEAR-SOURCE PROGRAMS

7.8.1. Introduction

Both the steady-state and transient version of HEGADAS-5 can be interfaced to the pool evaporation program EVAP, the HF-flash calculation program HFFLASH, and the near-source plume/jet programs PLUME and HFPLUME.

The program EVAP outputs the (steady-state or time-dependent) pool data which are required by (the steady-state or transient version of) HEGADAS. See Chapter 4 for details on EVAP and the EVAP user's guide in the User's Manual for details on the interface of HEGADAS with the pool evaporation program EVAP.

Section 7.8.2 describes the program HFFLASH. This program calculates the conditions immediately after the flash and outputs the post-flash data required by HEGADAS.

Section 7.8.3 describes the interface between HEGADAS and the near-source models HFPLUME and PLUME. The latter models have been described in Chapter 5. HFPLUME has been designed to simulate the release of pressurised, anhydrous, liquid hydrogen-fluoride to a co-flowing atmosphere. PLUME is an equivalent model to HFPLUME which treats non-HF ideal-gas releases.

The models HFPLUME and PLUME comprise the following parts:

- a simple reservoir model,
- a model of the external "flashing" assumed to occur upon first release of superheated liquid or saturated two-phase mixture to atmosphere (HFPLUME only)
- an isobaric jet entrainment model in which are conserved mass, momentum and energy excesses above ambient values and gas mass-flux

- a plume touch-down model.

The thermodynamic model for HF adopted in HFPLUME corresponds to that used in the heavy gas dispersion program HEGADAS (see Chapter 2, Section 7.2 and Appendix 5).

7.8.2. Link with HF-flash calculation program HFFLASH

Flashing of HF may occur for the case of an pressurised release of liquid HF. In this case the flash program HFFLASH can be used to calculate the conditions immediately after the flash. These data are the post-flash gas temperature and the post-flash liquid mass fraction of the HF.

The program HFFLASH requires as input the reservoir pressure, the reservoir temperature, the HF-release rate and the effective pipe exit-plane diameter. The program HFFLASH produces a HFFLASH/HEGADAS link file, which contains the calculated flash data and HFFLASH input data common to the HEGADAS input data. See Chapter 7 in the User's manual for further details.

7.8.3. Link with near-source program HFPLUME or PLUME (steady release)

The near-source programs HFPLUME and PLUME simulate the release and the near-field dispersion of HF and ideal gas, respectively. HFPLUME/PLUME is based on a top-hat model which consists of ordinary differential equations describing conservation of total mass, gas mass, momentum and energy. These equations are solved by numerical integration in the downwind direction. HFPLUME/PLUME simulates cloud behaviour in a near-source region. In order to provide a transition between HFPLUME/PLUME and HEGADAS we need to answer two questions:

- Which termination criteria must be chosen to determine when HFPLUME/PLUME calculations are stopped and HEGADAS calculations are started?

- At this transition point how do we match or transfer cloud characteristics from HFPLUME/PLUME into HEGADAS variables?

TERMINATION CRITERION

The transition of HFPLUME/PLUME with HEGADAS should be chosen at the point where the cloud conditions become more appropriate with the physical assumptions in HEGADAS. The following criteria should be satisfied simultaneously:

- The HFPLUME/PLUME jet speed u^{p1} is sufficiently close to the ambient wind speed u_a at the centroid height. The ambient wind speed is adopted in the HEGADAS program to approximate the velocity.
- The total HFPLUME/PLUME entrainment is sufficiently close to the heavy-gas entrainment $\text{Entr}_{\text{gas}}^{\text{heavy}}$, which is taken to be the entrainment in HEGADAS; see Chapter 5 for details about the different types of entrainment taken into account by HFPLUME/PLUME.

These criteria are included in HFPLUME/PLUME by adding the following conditions

$$|u^{p1}/u_a - 1| < \text{RULST} \quad \text{and} \quad 1 - \text{Entr}_{\text{gas}}^{\text{heavy}}/\text{Entr}_{\text{total}} < \text{RELST} \quad (7.64)$$

The HFPLUME/PLUME input parameters RULST and RELST have the recommended and default values RULST = 0.1 and RELST = 0.3. See Section 10.3 for further details on the choice of the values of these parameters.

In addition to the two criteria described by (7.64), an "advection" criterion also needs to be satisfied. This criterion stops the transition to HEGADAS, if the cloud is too buoyant; see Chapter 5 for further details.

Section 5.6 discussed the subsequent phases of the jet/plume flow in HFPLUME/PLUME, i.e. the "airborne" region (elevated jet-flow/dispersion; circular plume cross section), the "touchdown" region (transitional region)

and "slumped" region (ground-level dispersion; semi-elliptic plume cross section). The transition from HFPLUME/PLUME to the ground-level dispersion program HEGADAS is only allowed to be made in the "slumped" region.

HFPLUME/PLUME VARIABLES AND HEGADAS VARIABLES

The HFPLUME/PLUME equations are described in detail in Chapter 5. HFPLUME/PLUME assumes a "top-hat" model that assumes uniform, averaged data within the jet/plume. These data are a function of the downwind distance only. The basic unknowns in HFPLUME/PLUME are the concentration of the gas (plume concentration), c^{p1} , the total mixture density (plume density), ρ^{p1} , the plume speed, u^{p1} and the plume enthalpy, h^{p1} . These four unknowns are determined from four conservation equations (excess of ambient quantities), i.e. conservation of gas-mass flow, total-mass flow, extra momentum and extra energy.

At the transition point the plume will be in the "slumped" region and the axis inclination of the plume will be nearly horizontal. Thus (see Section 5.6) the area A^{p1} of the semi-elliptic cross-section of the plume is related to the plume diameter D^{p1} and the plume centroid z_c^{p1} by

$$A^{p1} = 3 \pi^2 z_c^{p1} D^{p1} / 16 \quad (7.65)$$

The HEGADAS equations are described in detail in Appendix 3. For the most general problem it calculates six basic variables by solving a set of ordinary differential equations stepping forward in the downwind direction. These variables are:

- c_A , ground-level concentration at centre-line of cloud, or alternatively, the equivalent HF monomer molar fraction y_g
- S_z , vertical dispersion coefficient
- S_y , cross-wind dispersion coefficient
- b , half-width of middle part of cloud, along which the ground-level concentration is taken to be equal to c_A
- H_e , heat added from the surface

- y_{w3} , water vapour added from the surface

MATCHING OF HFPLUME/PLUME VARIABLES WITH HEGADAS VARIABLES

The HEGADAS variables c_A , S_z , S_y , b , H_e , y_{w3} are set at the transition point from the HFPLUME variables by means of appropriate matching criteria. These criteria transfer cloud characteristics and are described below.

The HFPLUME/PLUME formulation does not take into account heat transfer and water-vapour transfer from the ground. Thus it is consistent with the HEGADAS formulation to take $H_e = y_{w3} = 0$ at the transition point.

HFPLUME/PLUME assumes a uniform, averaged concentration within the jet. Thus it is consistent with the HEGADAS formulation to take $S_y = 0$ corresponding to a uniform concentration for $|y| < b$ and a zero concentration for $|y| > b$. Thus the concentration c and the wind speed u adopted in HEGADAS are given at the breakpoint by (see Section 7.1.2)

$$c(x,y,z) = c_A(x) \exp \left[- \left[\frac{z}{S_z(x)} \right]^\beta \right], \quad |y| < b, \quad u = u_0 \left[\frac{z}{z_0} \right]^\alpha \quad (7.66)$$

with $\beta = 1 + \alpha$.

It remains to determine the variables c_A , S_z and b in equation (7.66). One might consider to determine these variables by imposing the conservation equations adopted in HFPLUME. Conservation of extra momentum is not applicable, because HEGADAS assumes the velocity to be the ambient wind speed (zero extra momentum). Conservation of extra energy seems not to be appropriate because by setting $H_e = 0$ in HEGADAS we actually have ignored heat effects at the transition point. Instead the following three conditions are imposed to determine the variables c_A , S_z and b :

- o Conservation of gas-mass flow.

This means that the total flow of gas (kg/s), E , flowing through the transition plane $x = x_{br}$ is preserved. E is given by the following integral as a 'first' moment M_1 in concentration:

$$E = M_1 = \int_{-\infty}^{\infty} \int_0^{\infty} c u \, dy \, dz \quad (7.67)$$

o Conservation of total mass.

This means that the flow of total plume mass (kg/s) is conserved. For small concentrations, the total density ρ can be written as a function $\rho(c)$ of $c(z)$. Thus it can be shown that up to leading order (for $c \rightarrow 0$) conservation of total mass is implied by eq. (7.67) and conservation of the 'second' moment M_2 in concentration:

$$M_2 = \int_{-\infty}^{\infty} \int_0^{\infty} c^2 u \, dy \, dz \quad (7.68)$$

o Plume centroid height

The centroid height z_c is given by

$$z_c = \frac{1}{M_1} \int_{-\infty}^{\infty} \int_0^{\infty} c u z \, dy \, dz \quad (7.69)$$

Both the HEGADAS similarity profile (eq. (7.66)) and the HFPLUME top-hat profile for c and u are now inserted into the above conditions (7.67), (7.68) and (7.69). Subsequent matching leads to the following three matching conditions:

$$M_1 = A^{p1} c^{p1} u^{p1} = \frac{2}{\beta} \Gamma\left(\frac{1+\alpha}{\beta}\right) z_0^{-\alpha} S_z^{1+\alpha} b c_A u_0 \quad (7.70)$$

$$M_2 = A^{p1} (c^{p1})^2 u^{p1} = 2^{-(1+\alpha)/\beta} \frac{2}{\beta} \Gamma\left(\frac{1+\alpha}{\beta}\right) z_0^{-\alpha} S_z^{1+\alpha} b (c_A)^2 u_0 \quad (7.71)$$

$$z_c = z^{p1} = S_z \Gamma\left(\frac{2+\alpha}{\beta}\right) / \Gamma\left(\frac{1+\alpha}{\beta}\right) \quad (7.72)$$

In HEGADAS the exponent β in the vertical concentration profile is related to the wind-speed exponent α by $\beta = 1+\alpha$ (see eq. (7.66)). From HEGADAS simulations of experiments it is known that HEGADAS accurately predicts ground-level concentrations, but often badly predicts vertical variations of the concentration. Thus in the matching process it is not appropriate to adopt $\beta=1+\alpha$ to obtain from the HFPLUME (uniform) data accurate estimates of the parameters c_A and b that determine the ground-level concentration (see eq. (7.68)). Instead, in particular in the far-field, a Gaussian concentration profile defined by $\beta=2$ will be more appropriate. Moreover the windspeed $u(z)$ is approximated by the (uniform) centroid plume speed. Thus $u(z) = u^{p1} = u_0 (z/z_0)^\alpha$, $\alpha=0$, $\beta=2$ are inserted in the above matching conditions (7.70), (7.71) and (7.72). By eliminating z^{p1} and using eq. (7.65), the following conditions are then derived:

$$c_A = 2^{\frac{1}{2}} c^{p1} \quad (7.73)$$

$$b = \frac{3 \pi}{16 2^{\frac{1}{2}}} D^{p1} \quad (7.74)$$

Finally the HEGADAS variable S_z is set from the gas-mass conservation equation with the value of β taken to be consistent with the HEGADAS assumption $\beta=1+\alpha$ (see eq. (7.51)).

IMPLEMENTATION OF TRANSITION INTO CODE

The program HFPLUME/PLUME enables the user to apply the termination criteria described above. HFPLUME/PLUME produces a link file from HFPLUME/PLUME to HEGADAS. This file contains the input data common to the HEGADAS input data, the calculated post-flash data and the transition data. The latter transition data are the HEGADAS variables c_A and b , which are calculated from the HFPLUME/PLUME variables c^{p1} , D^{p1} by means of equations (7.73) and (7.74). See Sections 6.4, A2.4, 8.5, 10.4.2 and 10.5.2 in the User's Manual for further details and examples.

7.8.3. Link with near-source program HFPLUME or PLUME (finite-duration release)

In the previous section the transition of HFPLUME/PLUME with the steady-state HEGADAS-S model is discussed. For the same reasons as for HEGADAS-S the time-dependent model HEGADAS-T may not be applied in case of pressurised releases in the high-momentum near-source region. Thus HEGADAS-T should be only applied downwind of an appropriately chosen transition point or breakpoint $x = x_{br}$. The time-dependent data at the breakpoint should be obtained from a near-source dispersion program or from experimental data.

For finite-duration releases the program HEGADAS-T can automatically be interfaced with the near-source model HFPLUME/PLUME. To this purpose the (steady-state) transition data are applied at the breakpoint x_{br} for a period corresponding to the release duration T_{dur} . Thus at the breakpoint x_{br} , the total gas flow E (kg/s), the center-line ground-level concentration c_A (kg/m³; from eq. (7.73)) and the cloud half-width b (m; from eq. (7.74)) are applied for a period of T_{dur} (s).

Gas is being released at the release point $x = 0$ during the period $0 < \text{time } t < T_{dur}$. In applying the above transition data at $x = x_{br}$ one must take into account the travel time T_{br} of the plume between the release point $x = 0$ and the transition point $x = x_{br}$. Thus the transition data should be applied for $T_{br} < \text{time } t < T_{br} + T_{dur}$. The travel time T_{br} can be expressed in terms of the plume speed $u = u(x)$ by the following formula,

$$T_{br} = \int_0^{x_{br}} \frac{dx}{u_x(x)} \quad (7.75)$$

where $u_x(x)$ is the horizontal component of the HFPLUME/PLUME plume speed u^{pl} .

The link from HFPLUME/PLUME to HEGADAS-T should be used for finite-duration release problems in which steady conditions are not reached at the further downwind distances of interest. Note that it cannot be

applied for time-varying gas releases. See Sections 10.4.3 and 10.5.1 in the User's Manual for further details and examples.

7.9. AUTOMATION OF RELEASE OF OBSERVERS FOR TIME-DEPENDENT SOURCES

7.9.1. Introduction

In HEGADAS-4 the user needed to provide the time interval Δt_{obs} with which observers were released. This procedure required know-how by the user of the observer concept (see Section 7.1.2), since selection of a too large time step lead to inaccurate concentration predictions at the specified output times.

In HEGADAS-5 Δt_{obs} is determined internally in the program to ensure accurate predictions. This Section discusses in detail the automated release of observers in HEGADAS-T.

For ground-level gas sources, the theoretical basis of the time-dependent version HEGADAS-T of the heavy-gas-dispersion program HEGADAS is outlined in Section 7.1.2 and described in detail in Section 6 of Appendix 3. See Section 7.6.3 for the HEGADAS-T model for a vertical source (full breakpoint).

For the case of a horizontal ground-level source, observers are released with a constant time interval Δt_{obs} at the upwind edge of the source. The observers travel with the wind in the downwind direction. While travelling over the time-varying source, each observer i ($i=1,2,\dots,M$) 'sees' a source length L^i (m; in downwind direction), a (averaged) source half-width B^i (m; in crosswind direction), a source strength E^i (kg/s) and a downwind edge of the source x_{dw}^i (m). Steady-state dispersion calculations based on these data yield the observer-dispersion data: ground-level center-line wet-gas volume fraction $c_{AV}^i(x) = c_{AV}(x - x_{dw}^i + L^i/2; E^i, B^i, L^i)$, vertical dispersion coefficient $S_z^i(x) = S_z(x - x_{dw}^i + L^i/2; E^i, B^i, L^i)$, etc. Here e.g. $c_{AV}(x;E,B,L)$ corresponds to a steady-state ground-level source with strength E , half-width B , length L and source centroid at $x=y=0$.

For the case of a vertical source (breakpoint), observers $i=1,2,\dots,M$ are released with a constant time interval Δt_{obs} at the breakpoint. For

each observer i , steady-state dispersion calculations are carried out based on the breakpoint data valid at the release time of the observer.

Let x_j^1 be the position of observer i at the output time t_j ($j = 1, 2, \dots, N$; $t_1 < t_2 < \dots < t_N$). Then $x_j^1 > x_j^2 > \dots > x_j^M$, i.e. observers released earlier are located further downwind. For both types of sources, the concentration data $c_{AV}(x, t_j)$ as a function of the downwind distance x at the output time t_j , is derived from the observer-dispersion data $c_j^i = c_{AV}^i(x_j^i)$, $i=1, 2, \dots, N$ by the inclusion of a cloud-shape correction for gravitational spreading and the inclusion of downwind diffusion effects. Thus for an accurate evaluation of $c_{AV}(x, t)$, the release interval Δt_{obs} (determining the observer spacing) must be smaller if larger gradients of $c_{AV}(x, t)$ do occur.

The observer concept in HEGADAS-T is a quasi-steady-state solution method for determining the concentration $c_{AV}(x, t)$ as a function of the downwind distance x and the time t . This method may be seen as a first-order inclusion of time-dependent effects. It produces accurate predictions for slowly varying time-dependent sources, but it may lead to more inaccurate predictions for highly time-dependent sources.

In Section 7.9.2 criteria for the appropriate choice of the number of observers and output times are discussed, and in Section 7.9.3 automation of the release of observers in HEGADAS-5 is discussed.

7.9.2. Criteria for choice of number of observers and output times

In a HEGADAS-T run the following two conditions must be satisfied:

A. The concentrations calculated at each output time t_j are accurate

This condition requires a sufficiently small spacing of the observers, i.e. a sufficiently small value of the observer-release interval Δt_{obs} such that the concentration curve $c_A(x, t_j)$ can be evaluated accurately from the observer-dispersion data. A too large observer spacing leads to too smooth concentration curves (peaks are eroded away).

Consider the positions $x_j^{i+1}, x_j^i, x_j^{i-1}$ ($x_j^{i+1} < x_j^i < x_j^{i-1}$) and the concentrations $c_j^{i+1}, c_j^i, c_j^{i-1}$ seen by three adjacent observers $i+1, i, i-1$ ($i=2, \dots, M-1$). Let C_j^i be the estimate of the concentration at x_j^i based on linear interpolation of the data for observers $i+1$ and $i-1$ (prior to the inclusion of the cloud shape correction and downwind-diffusion effects); C_j^i equals

$$C_j^i = c_j^{i+1} + (x_j^i - x_j^{i+1}) \left[\frac{c_j^{i-1} - c_j^{i+1}}{x_j^{i-1} - x_j^{i+1}} \right] \quad (7.76)$$

This would have been the HEGADAS estimate of the concentration at x_j^i , if observer i would not have been released. Thus the estimates of the absolute error $\epsilon_j^{abs,i}$ and relative error $\epsilon_j^{rel,i}$ at x_j^i are

$$\epsilon_j^{abs,i} = |C_j^i - c_j^i|, \quad \epsilon_j^{rel,i} = |C_j^i - c_j^i|/c_j^i \quad (7.77)$$

A convergence criterion for the observer concentrations must be chosen carefully. For smaller output times, the gas cloud may have very 'sharp' edges. The relative and absolute concentration errors near these edges will only be small for a very large number of observers and an excessive amount of CPU-time. Hence, instead of demanding that the maximum value of the concentration error is small, it is more appropriate to demand that the mean concentration error is small. Effectively this means that the predicted cloud volume or cloud shape is accurately modelled.

The peak concentrations must be accurately predicted. Thus at each output time, error estimates for observers with larger concentrations should contribute more than those with minute concentrations. Hence it is more appropriate to demand small mean absolute concentration errors than small mean relative concentration errors.

The relative error in the predicted cloud volume or cloud shape must be small for every output time. Hence it is appropriate to scale the mean absolute concentration error at a given output time with the peak concentration at that time. Thus the following convergence criterion for the observer concentrations is adopted in HEGADAS-5,

$$\max_{1 \leq j \leq N} \left[\frac{\frac{1}{M-2} \sum_{i=2}^{M-1} \epsilon_j^{abs,i}}{\max_{1 \leq i \leq M} c_j^i} \right] < \epsilon_{obs} \quad (7.78)$$

The above criterion implies that for all times t_j ($j = 1, 2, \dots, N$) the ratio of the mean error in absolute concentration and the peak concentration is smaller than the convergence tolerance ϵ_{obs} . The default value of ϵ_{obs} adopted in HEGADAS-T equals $\epsilon_{obs} = 0.05$. This value was found to lead to accurate concentration predictions without an excessive number of observers for most types of source conditions. [It is noted that the averaging of the concentration in the numerator of eq. (7.78) is only applied to those observers which actually have seen (some part of) the source at time t_j .]

B. The maximum concentration over all times, $c_{max}(x)$, can be determined

This condition requires a sufficiently close spacing between the output times $t_1, t_2, \dots, t_N$, such that the envelope $c_{max}(x)$ of the curves $c(x, t_1), c(x, t_2), \dots, c(x, t_N)$ is well defined.

The user can verify that this condition is satisfied by plotting a series of these curves in one graph. The plot file corresponding to each curve $c(x, t_j)$ can be generated by the interactive HEGADAS-T post-processor HTPOST.

7.9.3. HEGADAS-T algorithm with automated release of observers

In HEGADAS the time-dependent pool data are specified in the TIMEDATA data block. Zero pool data are assumed for time $t \leq t_{st}$, where $t_{st} =$ TSTPOOL is the time at which the pool becomes active. Pool data at subsequent times are given with a fixed timestep $\Delta t =$ TSTEPR in either the SOURCE records (case of a ground-level pool) or BRKDATA records (case of vertical pool or breakpoint). Let n_{td} be the number of records, than the pool data are specified at the input times $t_{st} + \Delta t, t_{st} + 2\Delta t, \dots, t_{st} + n_{td} \Delta t$

records). Zero pool data are assumed for time $t \geq (n_{td}+1)*\Delta t$. Data are linearly interpolated between the input times.

In HEGADAS-4 zero source data were assumed for time $t < 0$, i.e. $t_{st} = 0$ always. The user determined the time interval Δt_{obs} with which observers were released by selecting the timestep $\Delta t = TSTEPR$, i.e. $\Delta t_{obs} = \Delta t$. This procedure required know-how by the user of the observer concept, since selection of a too big time step lead to inaccurate concentration predictions at the specified output times.

In HEGADAS-5 zero pool data are assumed for time $t \leq t_{st}$, where the start time t_{st} is specified by the user. To ensure accurate predictions by HEGADAS-T, Δt_{obs} is determined internally in the program and is set independent from $\Delta t = TSTEPR$.

The automation of the release of observers in HEGADAS-T is carried out by means of the following consecutive algorithmic steps:

1. a In case of a ground-level source, the primary-pool data and secondary-pool (gas-blanket) data are set as a function of time with a minimum of 40 and a maximum of 100 time steps. The maximum blanket radius R_{max} is determined.

The observers are released at $x = - R_{max}$. The minimum and maximum observer-start times for which an observer may see a pool (t_{min}^{st} , t_{max}^{st}) are determined. Observer-source data (secondary source data seen by the observer while travelling over the pool) are set for the maximum number of 161 observers. Observers 1, 2, ..., 160, 161 are released at the times t_{min}^{st} , $t_{min}^{st} + \Delta t_{obs}$, ..., $t_{max}^{st} - \Delta t_{obs}$, t_{max}^{st} , with the observer-release interval given by $\Delta t_{obs} = (t_{max}^{st} - t_{min}^{st})/160$.

- b In case of a breakpoint (vertical pool), breakpoint data are set at the times $t_{st} + \Delta t_{obs}$, $t_{st} + 2*\Delta t_{obs}$, ..., $t_{st} + 161*\Delta t_{obs}$, where $\Delta t_{obs} = (n_{td}+1)*\Delta t/162$.

Observers 1, 2, ..., 160, 161 are released at the breakpoint at the above times.

2.
 - a The initial observer release interval is chosen to be equal to $IFREQ = 32$, and dispersion data are set for observers 1, 33, ..., 129, 161 (6 observers, 5 observer intervals).
 - b If the convergence criterion (7.78) is satisfied for the current observers 1, $1+IFREQ$, ..., $161-IFREQ$, 161 go to step 3.
 - c If $IFREQ=1$, printout message that convergence cannot be obtained with the maximum number of 161 observers and terminate program.
 - d Double the number of observer intervals, i.e. set dispersion data for the additional, intermediate observers $1+IFREQ/2$, $1+3*IFREQ/2$, ..., $161-3*IFREQ/2$, $161-IFREQ/2$, and half observer frequency ($IFREQ = IFREQ/2$). Go to step 2b.
3. Carry out cloud shape correction of dispersion data for observers 1, $1+IFREQ$, ..., $161-IFREQ$, 161 and include downwind-diffusion effects.

The reader is referred to the time-dependent simulation of the first Goldfish experiment in Section 9.4 for an example of a HEGADAS-T simulation adopting the above algorithm. See also the examples included in the HEGADAS User's Guide (Section 8.7.2 of the User's Manual).

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Table 7.1. Constants in formula $\sigma_y = \delta x^\beta$ for crosswind dispersion coefficient. δ_{600} are the values of δ for an averaging time for the concentration measurement of 600 seconds; δ can be calculated as a function of the averaging time t (in seconds) using the formula $\delta = \delta_{600} (t/600)^{0.2}$. The values of δ_{ins} apply to instantaneous sources. These values are found by using an averaging time of 18.75 seconds in the above formula, and are recommended for use in dispersion calculations for flammable gases. The values for δ_{600} , δ_{ins} and β given in this table are derived from non-dense dispersion experiments for a point source. Source: "Methods for calculations of the physical effects of the escape of dangerous materials", Part II, Report of the committee for the prevention of disasters, Netherlands Organisation for Applied Scientific Research (TNO), 1979.

Pasquill stability class	δ_{600}	δ_{ins}	β
A	0.527	0.264	0.865
B	0.371	0.186	0.866
C	0.209	0.105	0.897
D	0.128	0.064	0.907
E	0.098	0.049	0.902
F	0.065	0.033	0.902

Table 7.2. Constants in formula $\sigma_y = \delta x(1+\beta x)^{-1/2}$ for crosswind dispersion coefficient. δ_{600} are the values of δ for an averaging time for the concentration measurement of 600 seconds; δ can be calculated as a function of the averaging time t (in seconds) using the formula $\delta = \delta_{600}(t/600)^{0.2}$. The values for δ_{600} and β given in this table are recommended by Briggs (1973) for open-country conditions and $100 < x < 10000$ m, and are based on McElroy and Pooler's (1968) diffusion experiment in St. Louis. It is noted that the values of δ, β quoted by Briggs for urban conditions are not much different.

Pasquill stability class	δ_{600}	β

A	0.22	0.0001
B	0.16	0.0001
C	0.11	0.0001
D	0.08	0.0001
E	0.06	0.0001
F	0.04	0.0001

Table 7.3. Stability-class dependent constants adopted in along-wind diffusion formulation by Ermak: exponent n in power-law $u(z) = (U_0/Z_0)^n$ for ambient wind speed (from Irwin (1979)), parameters a_y , b_y , formula for crosswind dispersion coefficient $\sigma_{yt} = a_y x / (1 + b_y x)^{1/2}$ (= turbulent-spread component σ_{xt} of downwind dispersion coefficient) and vertical dispersion coefficient $\sigma_z = a_z x / (1 + b_z x)^{1/2}$ (values taken from Table 4.5 in Hanna, Briggs and Hosker (1982)), and approximate power-law formula $\sigma_z = c x^d$ (from Ermak (1986)).

Stability class	n	a_y	b_y	a_z	b_z	c	d	γ	σ_{xs}/x
A	0.07	0.22	0.0001	0.20	0.0	0.20	1.0	0.11	0.047
B	0.07	0.16	0.0001	0.12	0.0	0.12	1.0	0.16	0.045
C	0.1	0.11	0.0001	0.08	0.0002	0.25	0.82	0.24	0.064
D	0.15	0.08	0.0001	0.06	0.0015	0.38	0.66	0.29	0.097
E	0.35	0.06	0.0001	0.03	0.003	0.52	0.55	0.35	0.235
F	0.55	0.04	0.0001	0.016	0.003	0.28	0.55	0.38	0.375

Table 7.4. Listing of HEGADAS-T report file [ad example in Section 7.5.3 - new non-oscillatory gas-blanket formulation]
 ===== [release rate = 30 kg/s, primary source radius = 3m for 200 seconds]

```

HTMAIN                                HEGADAS-T PROGRAM ( VERSION JUL90      )                                PAGE      0
DATE 09/08/90                        STANDARD REPORT FILE                                TIME 09:01
-----
<<<<  Modified gas-blanket formulation; MODSX=3, ICSCOR=0  >>>>
-----

=====
HEGADAS-T INPUT DATA
=====

-----> CONTROL data block: control parameters
OUTPUT CODE                          ICNT =      0      (no output of cumulative cloud data)
SURFACE-TRANSFER CODE                ISURF =      3      (only heat transfer, no water vapour)
GAS-BLANKET FORMULATION              BLMODEL =      1      (new, non-oscillatory formulation)
CLOUD-SHAPE CORRECTION CODE          ICSCOR =      0      (correction not included)

-----> AMBIENT data block: ambient data
AIR TEMP. AT HEIGHT ZAIRTEMP AIRTEMP = 20.000      CELSIUS
REF. HEIGHT FOR AIR TEMP. ZAIRTEMP = 0.00000E-01 M
RELATIVE HUMIDITY                    RHPERC = 70.000      %
WIND VELOCITY AT HEIGHT Z0           UO = 4.0000      M/S
REFERENCE HEIGHT FOR WIND VEL. Z0 = 10.000      M
EARTH-S SURFACE TEMPERATURE TGROUND = 20.000      CELSIUS

-----> DISP data block: dispersion data
SURFACE ROUGHNESS PARAMETER          ZR = 7.00000E-03 M
PASQUILL STABILITY CLASS              POSTAB =      0
AVERAG. TIME FOR CONC. MEAS. AVTIMC = 600.00      SECONDS
MONIN - OBUKHOV LENGTH               OBUKL = 1.00000E+05 M
TYPE OF FORMULA FOR SIGMA_Y           MODSY =      1      (power-law)
with parameters: DELTA = 0.12800      M**(1-BETA)
BETA = 0.90500
CONST. IN GRAV. SPREADING LAW         CE = 1.1500
CONST. IN GRAV. SPREADING LAW         CD = 5.0000
TYPE OF FORMULA FOR SIGMA_X           MODSX =      3      (Chatwin/Wilson)
with parameters: ASIGX = 10.000
BSIGX = 0.10000

-----> GASDATA data block: gas data
TEMPERATURE OF EMITTED GAS TEMPGAS = -42.000      CELSIUS
SPECIFIC HEAT OF EMITTED GAS CPGAS = 68.000      J/MOLE/CELSIUS
MOLECULAR WEIGHT OF EM. GAS MWGAS = 44.100      KG/KMOLE
PICKED-UP WATER BY EM. GAS WATGAS = 0.00000E-01 (MOLAR FRACTION)
HEAT GROUP IN HEAT FLUX QH HEATGR = 29.000
THERMODYNAMIC MODEL THERMOD =      1      (normal, non-reactive gas)

-----> TIMEDATA data block: source/breakpoint data
TIME-DEPENDENT RECORD DATA: ITPBR =      0      (primary pool data: radius, strength)
- skip increment for reading INCRT =      0
- time step between read records DT = 4.0000      S
- number of records read NTYD = 50      (see list of pool data below for record data read)

-----> CLOUD data block: control of cloud output
OUTPUT STEP LENGTH XSTEP = 30.000      M
CA AT WHICH CALC. IS STOPPED CAMIN = 1.75000E-02 KG/M3
UPPER CONCENTRATION LIMIT CU = 3.60000E-02 KG/M3
LOWER CONCENTRATION LIMIT CL = 1.80000E-02 KG/M3

-----> CALC data block: control of output times
PNTS. OF TIME FOR CLOUD CALC. TSTAR = 50.000      SEC
                                      100.00      SEC
                                      150.00      SEC
                                      200.00      SEC

=====

WIND PROFILE EXPONENT ALPHA = 0.17547
FRICTION VELOCITY USTAR = 0.22571      M/S
AIR TEMP. AT GROUND LEVEL TAP = 20.000      CELSIUS

```

Table 7.4. Listing of HEGADAS-T report file [continued]
=====

HTMAIN HEGADAS-T PROGRAM (VERSION JUL90) PAGE 1
DATE 09/08/90 STANDARD REPORT FILE TIME 09:01

<<<< Modified gas-blanket formulation; MODSX=3, ICSCOR=0 >>>>

=====

DATA FOR PRIMARY POOL AND SECONDARY VAPOUR BLANKET

=====

TIME (S)	POOL RADIUS (M)	POOL STRENGTH (KG/S)	BLANKET RADIUS (M)	BLANKET HEIGHT (M)	BLANKET EV.RATE (KG/S)	BLANKET MASS (KG)
4.00	3.00	30.0	5.23	0.262	5.16	52.5
8.00	3.00	30.0	9.97	0.181	15.6	132.
12.0	3.00	30.0	13.8	0.119	27.3	166.
16.0	3.00	30.0	16.9	7.356E-02	38.5	154.
20.0	3.00	30.0	19.2	3.682E-02	48.0	99.5
24.0	3.00	30.0	20.6	4.382E-03	54.0	13.6
blanket height reduces to zero; time, blanket mass, blanket radius = 24.8 -5.79 20.7						
28.0	3.00	30.0	14.6	0.000E-01	30.0	0.000E-01
32.0	3.00	30.0	14.6	0.000E-01	30.0	0.000E-01
36.0	3.00	30.0	14.6	0.000E-01	30.0	0.000E-01
40.0	3.00	30.0	14.6	0.000E-01	30.0	0.000E-01
44.0	3.00	30.0	14.6	0.000E-01	30.0	0.000E-01
48.0	3.00	30.0	14.6	0.000E-01	30.0	0.000E-01
52.0	3.00	30.0	14.6	0.000E-01	30.0	0.000E-01
56.0	3.00	30.0	14.6	0.000E-01	30.0	0.000E-01
60.0	3.00	30.0	14.6	0.000E-01	30.0	0.000E-01
64.0	3.00	30.0	14.6	0.000E-01	30.0	0.000E-01
68.0	3.00	30.0	14.6	0.000E-01	30.0	0.000E-01
72.0	3.00	30.0	14.6	0.000E-01	30.0	0.000E-01
76.0	3.00	30.0	14.6	0.000E-01	30.0	0.000E-01
80.0	3.00	30.0	14.6	0.000E-01	30.0	0.000E-01
84.0	3.00	30.0	14.6	0.000E-01	30.0	0.000E-01
88.0	3.00	30.0	14.6	0.000E-01	30.0	0.000E-01
92.0	3.00	30.0	14.6	0.000E-01	30.0	0.000E-01
96.0	3.00	30.0	14.6	0.000E-01	30.0	0.000E-01
100.	3.00	30.0	14.6	0.000E-01	30.0	0.000E-01
104.	3.00	30.0	14.6	0.000E-01	30.0	0.000E-01
108.	3.00	30.0	14.6	0.000E-01	30.0	0.000E-01
112.	3.00	30.0	14.6	0.000E-01	30.0	0.000E-01
116.	3.00	30.0	14.6	0.000E-01	30.0	0.000E-01
120.	3.00	30.0	14.6	0.000E-01	30.0	0.000E-01
124.	3.00	30.0	14.6	0.000E-01	30.0	0.000E-01
128.	3.00	30.0	14.6	0.000E-01	30.0	0.000E-01
132.	3.00	30.0	14.6	0.000E-01	30.0	0.000E-01
136.	3.00	30.0	14.6	0.000E-01	30.0	0.000E-01
140.	3.00	30.0	14.6	0.000E-01	30.0	0.000E-01
144.	3.00	30.0	14.6	0.000E-01	30.0	0.000E-01
148.	3.00	30.0	14.6	0.000E-01	30.0	0.000E-01
152.	3.00	30.0	14.6	0.000E-01	30.0	0.000E-01
156.	3.00	30.0	14.6	0.000E-01	30.0	0.000E-01
160.	3.00	30.0	14.6	0.000E-01	30.0	0.000E-01
164.	3.00	30.0	14.6	0.000E-01	30.0	0.000E-01
168.	3.00	30.0	14.6	0.000E-01	30.0	0.000E-01
172.	3.00	30.0	14.6	0.000E-01	30.0	0.000E-01
176.	3.00	30.0	14.6	0.000E-01	30.0	0.000E-01
180.	3.00	30.0	14.6	0.000E-01	30.0	0.000E-01
184.	3.00	30.0	14.6	0.000E-01	30.0	0.000E-01
188.	3.00	30.0	14.6	0.000E-01	30.0	0.000E-01
192.	3.00	30.0	14.6	0.000E-01	30.0	0.000E-01
196.	3.00	30.0	14.6	0.000E-01	30.0	0.000E-01
200.	3.00	30.0	14.6	0.000E-01	30.0	0.000E-01
204.	0.000E-01	0.000E-01	-	-	-	-

Maximum source radius RGMAX = 20.608 M

Source/blanket data set; total CPU = 4 seconds

Table 7.4. Listing of HEGADAS-T report file [continued]

SOURCE DATA SEEN BY OBSERVERS						
OBSERVER	START TIME (S)	PLACE OF DOWNWIND EDGE (M)	LENGTH (M)	HALF- WIDTH (M)	TAKE-UP FLUX (KG/M2/S)	TAKE-UP RATE (KG/S)
1	-12.00	6.400	7.529	2.292	6.6399E-02	2.292
2	-8.000	14.81	18.93	7.012	5.0267E-02	13.34
3	-4.000	18.76	25.79	10.33	4.5595E-02	24.28
4	0.0000E-01	20.25	30.05	12.89	4.3253E-02	33.51
5	4.000	16.77	29.00	14.92	4.2200E-02	36.52
6	8.000	14.56	28.92	15.00	4.1951E-02	36.40
7	12.00	14.56	30.95	14.15	4.2404E-02	37.16
8	16.00	14.56	32.52	13.26	4.3143E-02	37.19
9	20.00	14.56	34.11	11.91	4.3959E-02	35.71
10	24.00	14.56	29.11	11.52	4.4714E-02	29.98
11	28.00	14.56	29.11	11.52	4.4714E-02	29.98
12	32.00	14.56	29.11	11.52	4.4714E-02	29.98
13	36.00	14.56	29.11	11.52	4.4714E-02	29.98
14	40.00	14.56	29.11	11.52	4.4714E-02	29.98
15	44.00	14.56	29.11	11.52	4.4714E-02	29.98
16	48.00	14.56	29.11	11.52	4.4714E-02	29.98
17	52.00	14.56	29.11	11.52	4.4714E-02	29.98
18	56.00	14.56	29.11	11.52	4.4714E-02	29.98
19	60.00	14.56	29.11	11.52	4.4714E-02	29.98
20	64.00	14.56	29.11	11.52	4.4714E-02	29.98
21	68.00	14.56	29.11	11.52	4.4714E-02	29.98
22	72.00	14.56	29.11	11.52	4.4714E-02	29.98
23	76.00	14.56	29.11	11.52	4.4714E-02	29.98
24	80.00	14.56	29.11	11.52	4.4714E-02	29.98
25	84.00	14.56	29.11	11.52	4.4714E-02	29.98
26	88.00	14.56	29.11	11.52	4.4714E-02	29.98
27	92.00	14.56	29.11	11.52	4.4714E-02	29.98
28	96.00	14.56	29.11	11.52	4.4714E-02	29.98
29	100.0	14.56	29.11	11.52	4.4714E-02	29.98
30	104.0	14.56	29.11	11.52	4.4714E-02	29.98
31	108.0	14.56	29.11	11.52	4.4714E-02	29.98
32	112.0	14.56	29.11	11.52	4.4714E-02	29.98
33	116.0	14.56	29.11	11.52	4.4714E-02	29.98
34	120.0	14.56	29.11	11.52	4.4714E-02	29.98
35	124.0	14.56	29.11	11.52	4.4714E-02	29.98
36	128.0	14.56	29.11	11.52	4.4714E-02	29.98
37	132.0	14.56	29.11	11.52	4.4714E-02	29.98
38	136.0	14.56	29.11	11.52	4.4714E-02	29.98
39	140.0	14.56	29.11	11.52	4.4714E-02	29.98
40	144.0	14.56	29.11	11.52	4.4714E-02	29.98
41	148.0	14.56	29.11	11.52	4.4714E-02	29.98
42	152.0	14.56	29.11	11.52	4.4714E-02	29.98
43	156.0	14.56	29.11	11.52	4.4714E-02	29.98
44	160.0	14.56	29.11	11.52	4.4714E-02	29.98
45	164.0	14.56	29.11	11.52	4.4714E-02	29.98
46	168.0	14.56	29.11	11.52	4.4714E-02	29.98
47	172.0	14.56	29.11	11.52	4.4714E-02	29.98
48	176.0	14.56	29.11	11.52	4.4714E-02	29.98
49	180.0	12.13	26.68	12.06	4.4714E-02	28.76
50	184.0	4.528	19.07	12.20	4.4714E-02	20.81
51	188.0	-2.743	11.80	10.83	4.4714E-02	11.43
52	192.0	-9.594	4.952	7.731	4.4714E-02	3.424

Observer-source data set; total CPU = 10 seconds

Table 7.4. Listing of HEGADAS-T report file [continued]

DISPERSION DATA AT TIME = 200. SEC									
DISTANCE (M)	CONC (% VOL.)	SZ (M)	SY (M)	MIDP (M)	YCU (M)	ZCU (M)	YCL (M)	ZCL (M)	CA (KG/M3)
0.000E-01	100.	0.168	0.000E-01	11.3	11.3	0.565	11.3	0.644	2.33
30.0	61.2	0.313	7.58	14.3	28.6	0.918	29.9	1.07	1.25
60.0	21.8	0.511	15.6	21.9	46.2	1.09	49.4	1.35	0.412
90.0	10.6	0.877	22.0	19.6	48.2	1.38	53.6	1.84	0.197
120.	6.74	1.27	27.0	15.5	45.5	1.52	53.0	2.22	0.124
150.	5.07	1.64	31.2	12.2	42.6	1.58	52.2	2.51	9.339E-02
180.	3.94	2.01	35.0	9.28	38.5	1.49	50.6	2.67	7.250E-02
210.	3.20	2.37	38.4	6.73	33.6	1.30	48.5	2.74	5.881E-02
240.	2.68	2.73	41.6	4.41	27.6	1.01	46.1	2.74	4.919E-02
270.	2.29	3.07	44.6	2.29	19.9	0.633	43.4	2.67	4.209E-02
300.	1.97	3.41	47.4	0.319	3.48	3.417E-02	39.9	2.51	3.616E-02
330.	1.67	3.79	50.1	0.000E-01	0.000E-01	0.000E-01	36.5	2.21	3.057E-02
360.	1.40	4.18	52.8	0.000E-01	0.000E-01	0.000E-01	31.6	1.74	2.574E-02
390.	1.25	4.59	55.6	0.000E-01	0.000E-01	0.000E-01	27.5	1.39	2.299E-02
420.	1.19	4.73	60.6	0.000E-01	0.000E-01	0.000E-01	26.8	1.18	2.189E-02
450.	0.978	5.14	63.1	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	1.795E-02
480.	0.588	5.99	62.2	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	1.079E-02
510.	0.262	13.6	53.3	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	4.802E-03

Cloud data set; total CPU = 64 seconds

Table 7.5. Listing of HEGADAS-T report file [ad example in Section 7.6.3 - 'full' time-dependent breakpoint formulation]
[breakpoint at 20 m; non-reactive gas; IOBSXT=1]

```

HTMAIN                      HEGADAS-T PROGRAM ( VERSION JUL90      )          PAGE    0
DATE 09/08/90              STANDARD REPORT FILE                      TIME 09:58
=====
<<<<  STNOBR. Breakpoint at 20m; ideal gas; IOBSXT=1  >>>>
=====

=====
HEGADAS-T INPUT DATA
=====

-----> CONTROL data block: control parameters
OUTPUT CODE                  ICNT =      0      (no output of cumulative cloud data)
SURFACE-TRANSFER CODE        ISURF =      3      (only heat transfer, no water vapour)
GAS-BLANKET FORMULATION      BLMODEL =      1      (new, non-oscillatory formulation)
CLOUD-SHAPE CORRECTION CODE  ICSCOR =      1      (correction included)

-----> AMBIENT data block: ambient data
AIR TEMP. AT HEIGHT ZAIRTEMP AIRTEMP = 20.000    CELSIUS
REF. HEIGHT FOR AIR TEMP.    ZAIRTEMP = 0.00000E-01 M
RELATIVE HUMIDITY            RHPERC = 70.000    %
WIND VELOCITY AT HEIGHT Z0    U0 = 4.0000    M/S
REFERENCE HEIGHT FOR WIND VEL. Z0 = 10.000    M
EARTH-S SURFACE TEMPERATURE TGROUND = 20.000    CELSIUS

-----> DISP data block: dispersion data
SURFACE ROUGHNESS PARAMETER  ZR = 7.00000E-03 M
PASQUILL STABILITY CLASS     POSTAB =      D
AVERAG. TIME FOR CONC. MEAS. AVTIMC = 600.00    SECONDS
MONIN - OBUKHOV LENGTH       OBUKL = 1.00000E+05 M
TYPE OF FORMULA FOR SIGMA_Y   MODSY =      1      (power-law)
    with parameters:          DELTA = 0.12800    M**(1-BETA)
                                BETA = 0.90500
CONST. IN GRAV. SPREADING LAW  CE = 1.1500
CONST. IN GRAV. SPREADING LAW  CD = 0.00000E-01
TYPE OF FORMULA FOR SIGMA_X   MODSX =      3      (Chatwin/Wilson)
    with parameters:          ASIGX = 10.000
                                BSIGX = 0.10000

-----> GASDATA data block: gas data
TEMPERATURE OF EMITTED GAS    TEMPGAS = -42.000    CELSIUS
SPECIFIC HEAT OF EMITTED GAS  CPGAS = 68.000    J/MOLE/CELSIUS
MOLECULAR WEIGHT OF EM. GAS    MWGAS = 44.100    KG/KMOLE
PICKED-UP WATER BY EM. GAS     WATGAS = 0.00000E-01 (MOLAR FRACTION)
HEAT GROUP IN HEAT FLUX QH     HEATGR = 29.000
THERMODYNAMIC MODEL           THERMOD =      1      (normal, non-reactive gas)

-----> TIMEDATA data block: source/breakpoint data
TIME-DEPENDENT RECORD DATA:  ITPBR =      1      (breakpoint data: B_eff, CONC, H_eff)
- skip increment for reading  INCRT =      0
- time step between read records DT = 2.5000    S
- number of records read      NTYD = 18      (see list of breakpoint data below for record data read)

-----> CLOUD data block: control of cloud output
OUTPUT STEP LENGTH            XSTEP = 10.000    M
CA AT WHICH CALC. IS STOPPED  CAMIN = 1.00000E-02 KG/M3
UPPER CONCENTRATION LIMIT      CU = 3.60000E-02 KG/M3
LOWER CONCENTRATION LIMIT      CL = 1.80000E-02 KG/M3

-----> CALC data block: control of output times
PNTS. OF TIME FOR CLOUD CALC. TSTAR = 10.000    SEC
                                   40.000    SEC
                                   600.00    SEC

-----> TRANSIT data block(s): breakpoint data
FULL BREAKPOINT AT            DISTS = 20.000    M

=====

WIND PROFILE EXPONENT         ALPHA = 0.17547
FRICTION VELOCITY             USTAR = 0.22571    M/S
AIR TEMP. AT GROUND LEVEL     TAP = 20.000    CELSIUS

```


Table 7.5. Listing of HEGADAS-T report file [continued]

HTMAIN		HEGADAS-T PROGRAM (VERSION JUL90)						PAGE 1
DATE 09/08/90		STANDARD REPORT FILE						TIME 09:58

<<<< STNOBR. Breakpoint at 20m; ideal gas; IOBSXT=1 >>>>								

=====								
TIME-DEPENDENT DATA AT FULL BREAKPOINT X = 20.0 M								
=====								
TIME (S)	CONC (% VOL.)	CLOUD HALF-WIDTH (M)	CLOUD HEIGHT (M)	GAS FLOW (KG/S)	SZ (M)	RIB	TMP (C)	CA (KG/M3)
2.50	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	20.0	0.000E-01
5.00	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	20.0	0.000E-01
7.50	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	20.0	0.000E-01
10.0	2.75	2.96	0.669	0.456	0.707	3.58	16.2	5.104E-02
12.5	54.1	8.94	0.194	7.28	0.205	18.1	-19.1	1.15
15.0	82.2	10.1	0.214	14.8	0.226	30.8	-34.6	1.86
17.5	94.2	10.7	0.247	21.8	0.261	40.7	-39.8	2.17
20.0	98.9	11.7	0.270	27.9	0.285	46.7	-41.6	2.30
22.5	91.4	15.6	0.257	32.0	0.272	41.1	-38.6	2.10
25.0	74.2	19.8	0.253	31.6	0.267	32.7	-30.6	1.65
27.5	56.1	22.8	0.267	28.2	0.282	25.8	-20.3	1.20
30.0	39.6	24.7	0.295	23.2	0.312	19.7	-9.45	0.813
32.5	25.8	25.6	0.338	17.7	0.357	14.6	-5.874E-02	0.511
35.0	15.6	25.1	0.400	12.5	0.423	10.6	6.50	0.302
37.5	8.30	23.2	0.493	7.72	0.521	7.27	11.3	0.157
40.0	3.55	19.7	0.644	3.78	0.681	4.45	15.1	6.633E-02
42.5	0.949	13.1	0.913	1.00	0.965	1.70	18.6	1.749E-02
45.0	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	20.0	0.000E-01

Observer-dispersion data set at breakpoint; total CPU = 2 seconds

Table 7.5. Listing of HEGADAS-T report file (continued)

HTMAIN HEGADAS-T PROGRAM (VERSION JUL90) PAGE 2
DATE 09/08/90 STANDARD REPORT FILE TIME 09:58
-----<<<< STNOBR. Breakpoint at 20m; ideal gas; IOBSXT=1 >>>>-----

Cloud shape correction performed

Observer-dispersion data set; total CPU = 20 seconds

No cloud data are output at time = 10.0 seconds, since less than 2 observers see cloud (observer concentration > 0)

DISPERSION DATA AT TIME = 40. SEC									
DISTANCE (M)	CONC (% VOL.)	SZ (M)	SY (M)	MIDP (M)	YCU (M)	ZCU (M)	YCL (M)	ZCL (M)	CA (KG/M3)
20.0	3.55	0.681	2.095E-03	19.7	19.7	0.448	19.7	0.854	6.633E-02
30.0	9.21	0.527	7.01	20.7	29.5	0.777	31.2	1.06	0.175
40.0	17.6	0.482	9.44	20.9	35.0	0.956	37.0	1.20	0.337
50.0	23.1	0.467	10.4	19.4	35.8	1.02	38.0	1.26	0.443
60.0	25.7	0.464	10.0	16.4	32.7	1.05	34.7	1.28	0.491
70.0	23.3	0.481	9.16	13.3	27.8	1.05	29.7	1.29	0.442
80.0	16.1	0.546	9.14	11.9	25.2	1.04	27.2	1.32	0.304
90.0	8.85	0.661	9.42	10.6	22.2	0.944	24.6	1.30	0.165
100.	3.03	0.878	9.50	8.12	14.4	0.439	18.2	0.979	5.605E-02
110.	0.891	1.56	6.15	1.06	0.000E-01	0.000E-01	0.000E-01	0.000E-01	1.645E-02
120.	0.160	1.71	7.05	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	2.958E-03

DISPERSION DATA AT TIME = 600. SEC									
DISTANCE (M)	CONC (% VOL.)	SZ (M)	SY (M)	MIDP (M)	YCU (M)	ZCU (M)	YCL (M)	ZCL (M)	CA (KG/M3)
1.730E+03	1.167E-02	39.5	161.	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	2.141E-04
1.740E+03	1.209E-02	38.7	163.	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	2.218E-04
1.750E+03	1.247E-02	33.0	176.	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	2.288E-04
1.760E+03	1.288E-02	27.8	189.	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	2.362E-04
1.770E+03	1.324E-02	24.9	172.	1.28	0.000E-01	0.000E-01	0.000E-01	0.000E-01	2.428E-04
1.780E+03	1.357E-02	24.4	120.	4.01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	2.490E-04
1.790E+03	1.385E-02	23.9	96.9	6.43	0.000E-01	0.000E-01	0.000E-01	0.000E-01	2.540E-04
1.800E+03	1.411E-02	23.5	96.3	8.58	0.000E-01	0.000E-01	0.000E-01	0.000E-01	2.589E-04
1.810E+03	1.435E-02	23.2	95.2	10.3	0.000E-01	0.000E-01	0.000E-01	0.000E-01	2.633E-04
1.820E+03	1.453E-02	22.9	93.8	11.6	0.000E-01	0.000E-01	0.000E-01	0.000E-01	2.665E-04
1.830E+03	1.470E-02	22.7	91.9	12.5	0.000E-01	0.000E-01	0.000E-01	0.000E-01	2.696E-04
1.840E+03	1.481E-02	22.6	89.5	12.9	0.000E-01	0.000E-01	0.000E-01	0.000E-01	2.717E-04
1.850E+03	1.488E-02	22.5	87.0	13.1	0.000E-01	0.000E-01	0.000E-01	0.000E-01	2.730E-04
1.860E+03	1.492E-02	22.4	83.6	12.6	0.000E-01	0.000E-01	0.000E-01	0.000E-01	2.736E-04
1.870E+03	1.491E-02	22.4	80.1	12.0	0.000E-01	0.000E-01	0.000E-01	0.000E-01	2.735E-04
1.880E+03	1.485E-02	22.5	76.7	11.1	0.000E-01	0.000E-01	0.000E-01	0.000E-01	2.725E-04
1.890E+03	1.475E-02	22.7	73.5	9.91	0.000E-01	0.000E-01	0.000E-01	0.000E-01	2.707E-04
1.900E+03	1.462E-02	22.9	70.2	8.69	0.000E-01	0.000E-01	0.000E-01	0.000E-01	2.682E-04
1.910E+03	1.445E-02	23.2	68.6	7.46	0.000E-01	0.000E-01	0.000E-01	0.000E-01	2.651E-04
1.920E+03	1.424E-02	23.5	67.7	6.22	0.000E-01	0.000E-01	0.000E-01	0.000E-01	2.612E-04
1.930E+03	1.400E-02	23.8	66.9	4.99	0.000E-01	0.000E-01	0.000E-01	0.000E-01	2.567E-04
1.940E+03	1.370E-02	24.3	66.3	3.38	0.000E-01	0.000E-01	0.000E-01	0.000E-01	2.514E-04
1.950E+03	1.338E-02	24.7	65.7	1.69	0.000E-01	0.000E-01	0.000E-01	0.000E-01	2.454E-04
1.960E+03	1.306E-02	25.6	72.9	0.102	0.000E-01	0.000E-01	0.000E-01	0.000E-01	2.396E-04
1.970E+03	1.269E-02	34.3	181.	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	2.328E-04
1.980E+03	1.230E-02	43.7	165.	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	2.256E-04

Cloud data set; total CPU = 23 seconds

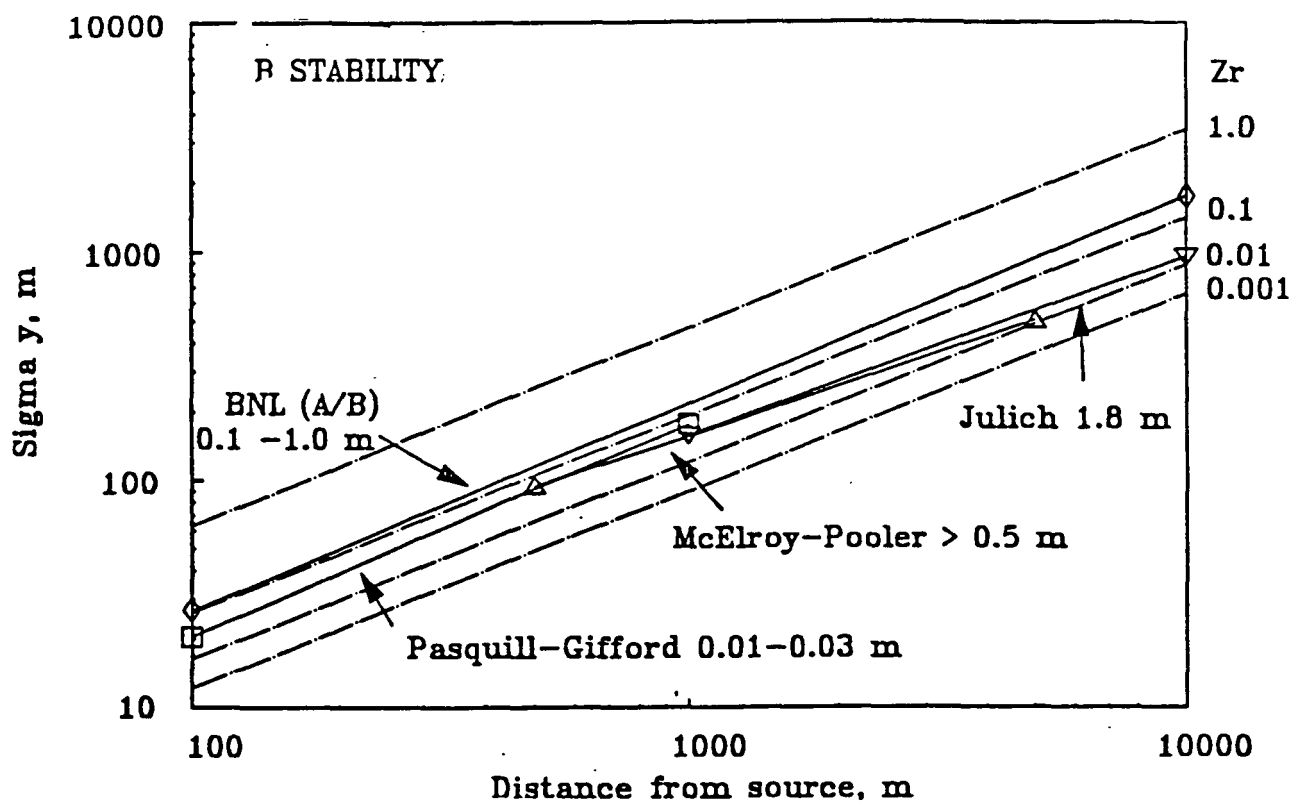


Fig. 7.1. Correlations for the crosswind dispersion coefficient σ_y (σ_y) measured over different roughness lengths z_r compared with the assumption that σ_y is proportional to the friction velocity u_* ; B stability

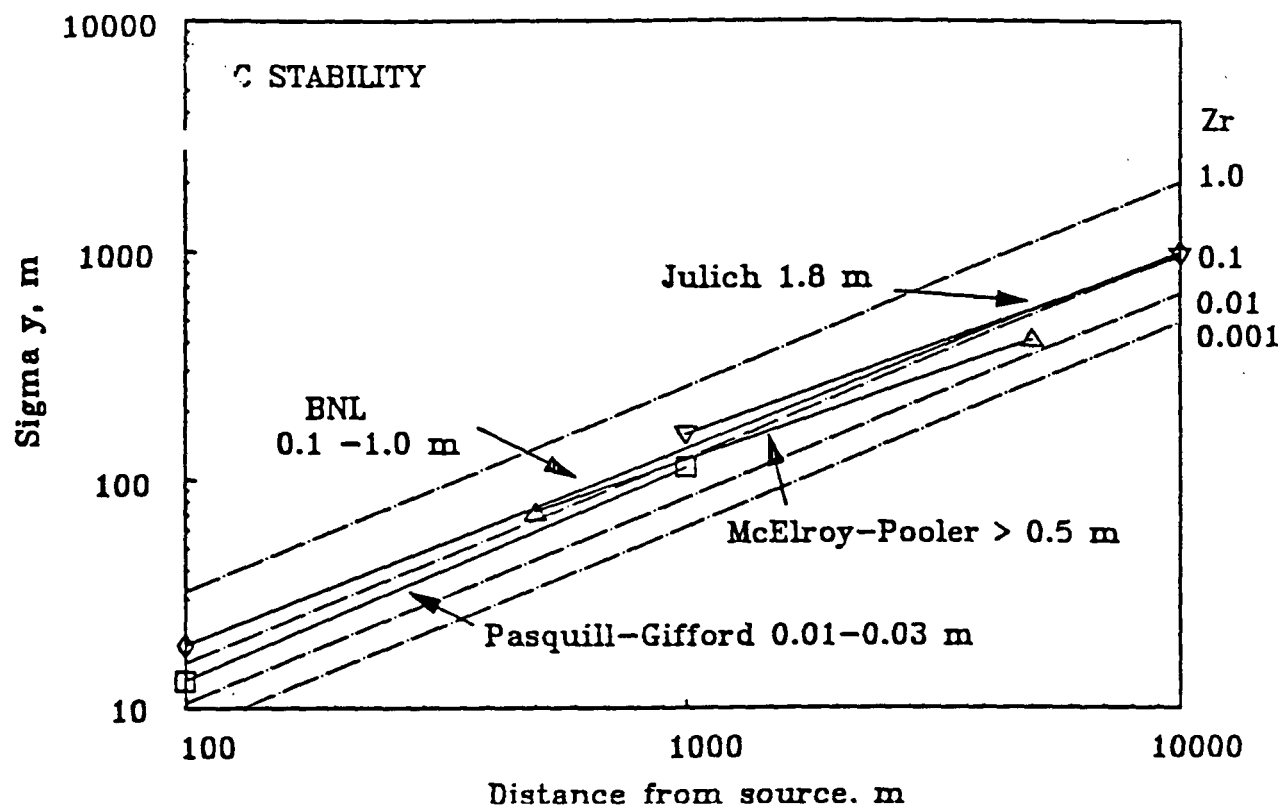


Fig. 7.2. Correlations for the crosswind dispersion coefficient σ_y (Sigma y) measured over different roughness lengths z_r compared with the assumption that σ_y is proportional to the friction velocity u_* ; C stability

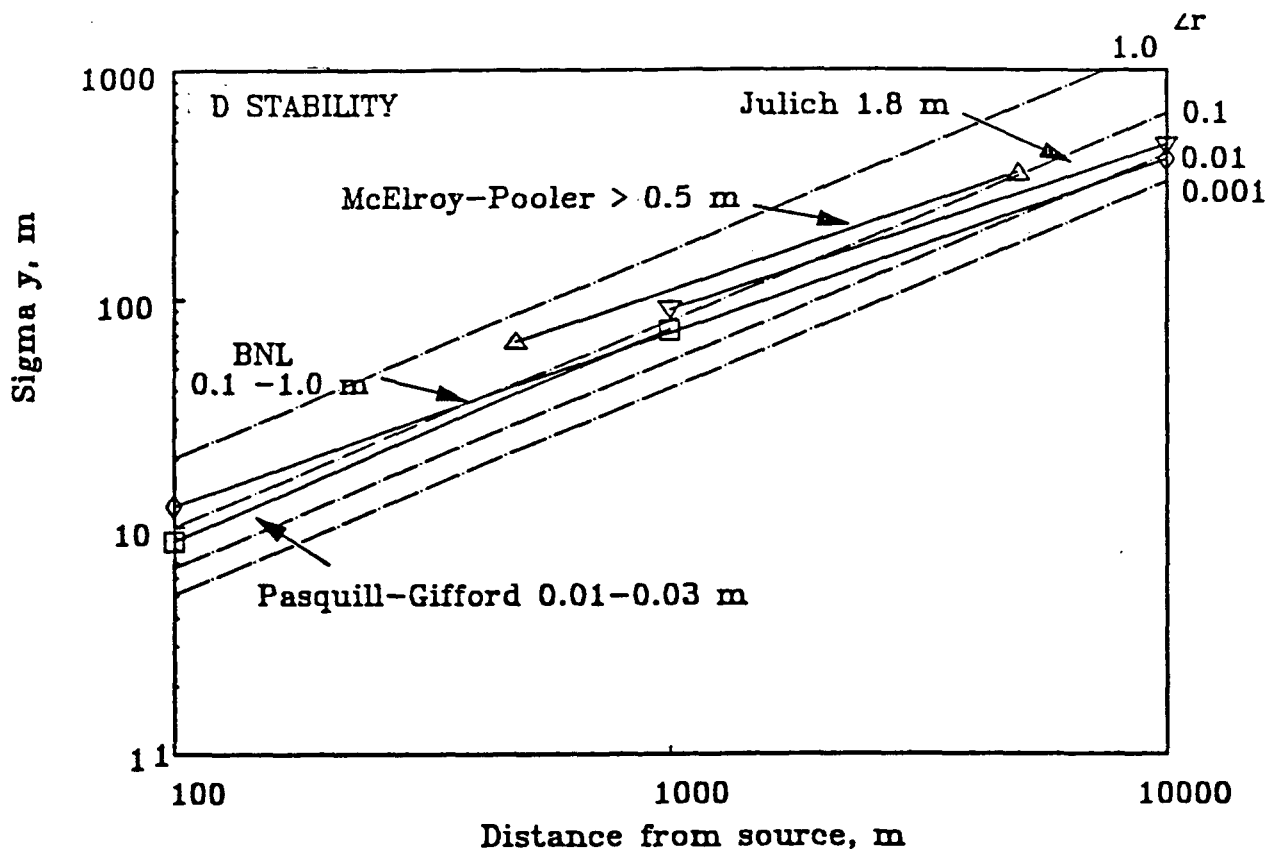


Fig. 7.3. Correlations for the crosswind dispersion coefficient σ_y (Sigma y) measured over different roughness lengths z_R compared with the assumption that σ_y is proportional to the friction velocity u_* ; D stability

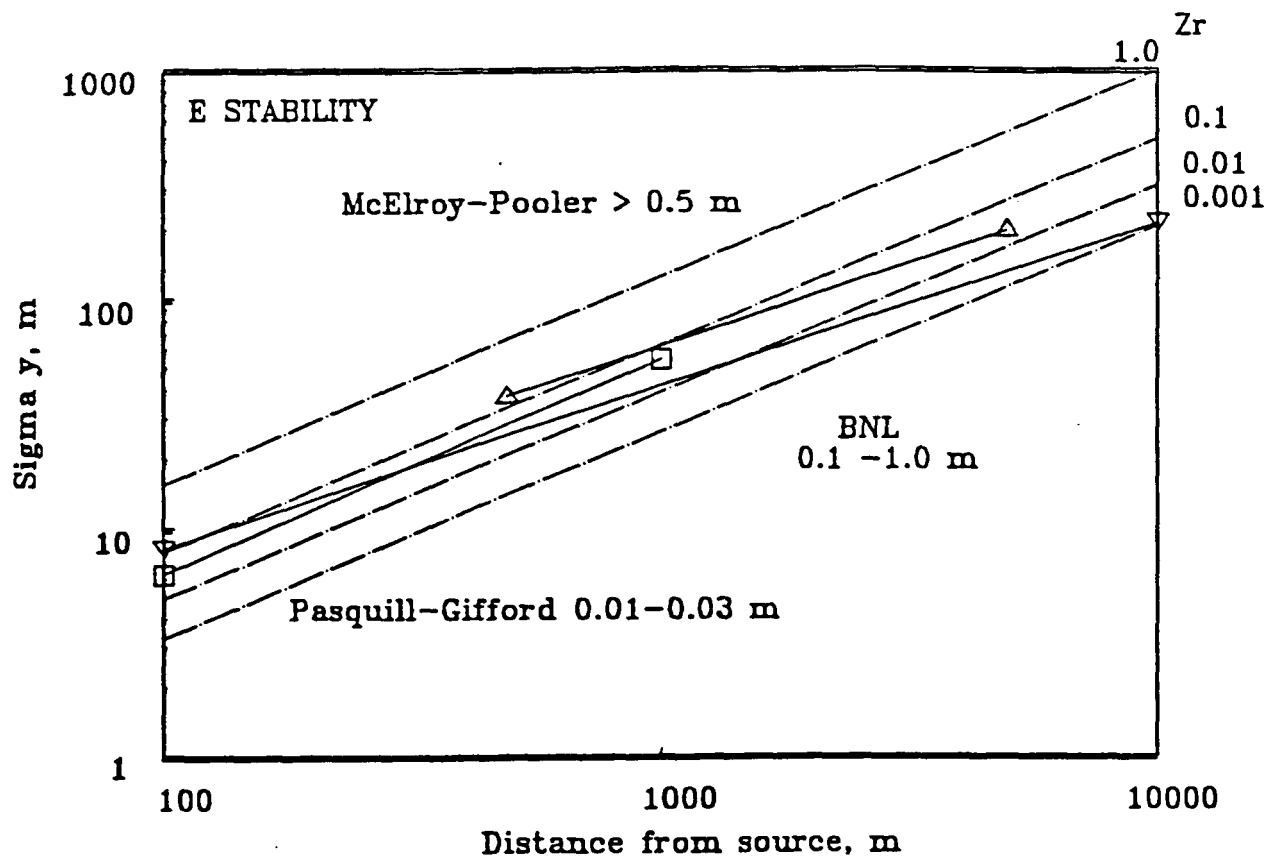


Fig. 7.4. Correlations for the crosswind dispersion coefficient σ_y (Sigma y) measured over different roughness lengths z_r compared with the assumption that σ_y is proportional to the friction velocity u_* ; E stability

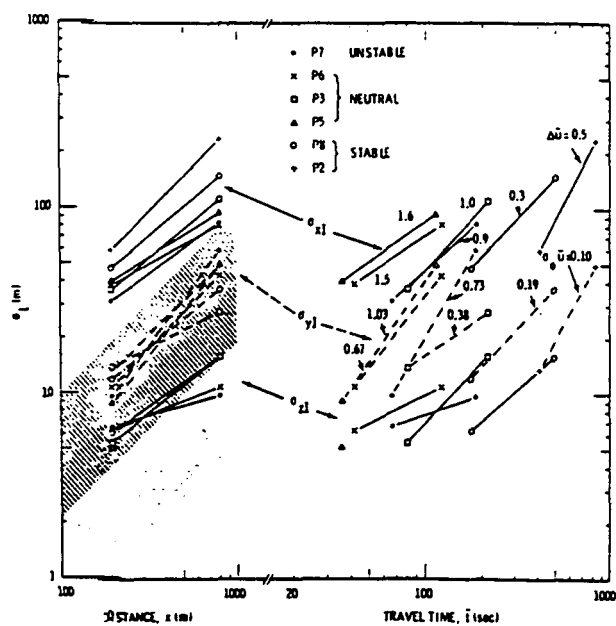


Fig. 7.5. Standard deviations of puff tracer distributions versus distance and travel time [from Nickola, 1971]

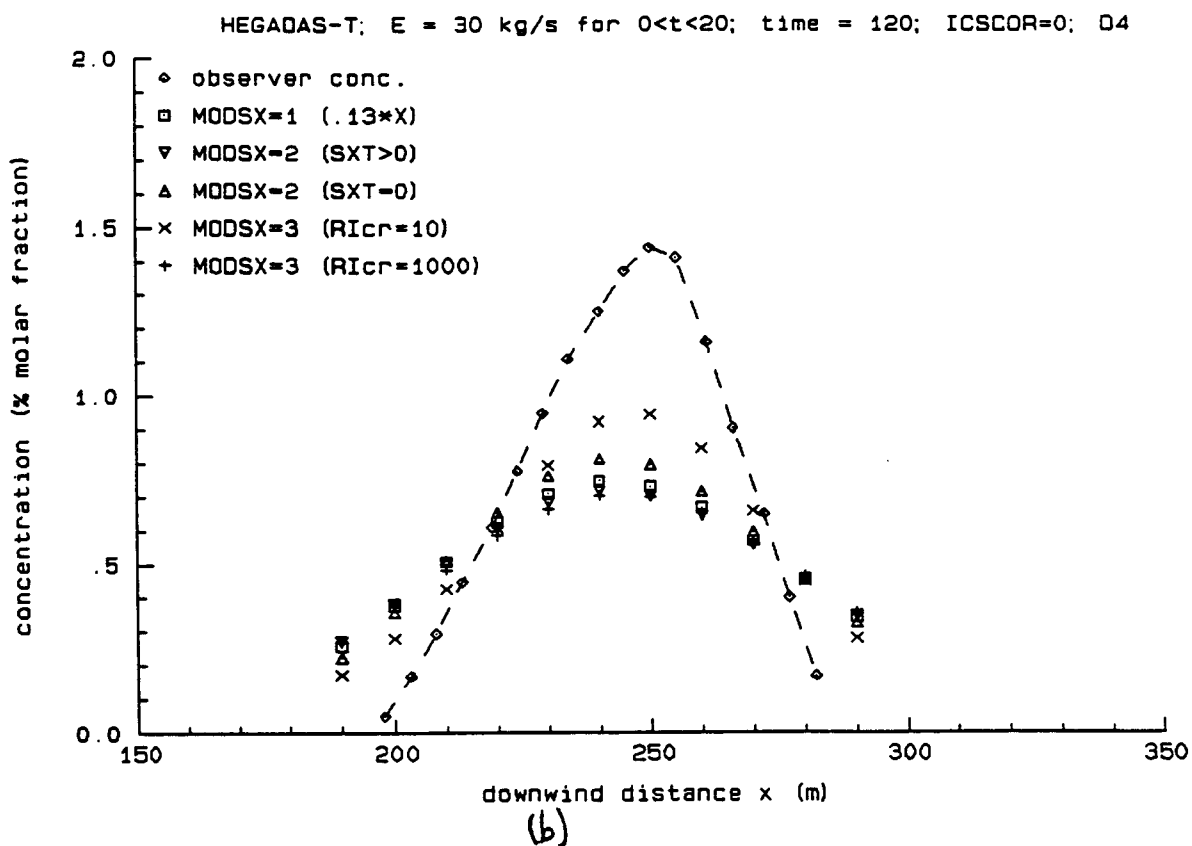
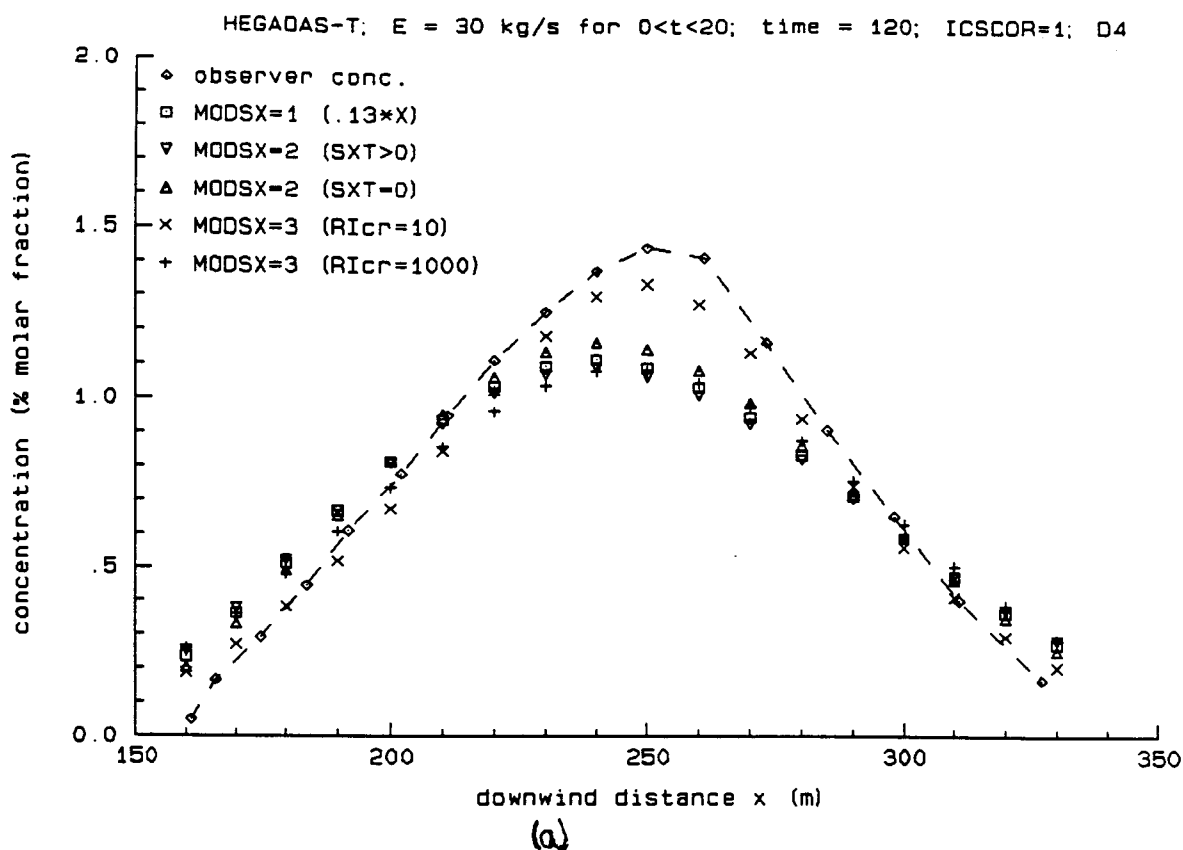


Fig. 7.6. Finite-duration steady-state gas release; source strength $E(t) = 30 \text{ kg/s}$, $0 < t < 20$ seconds; HEGADAS-T predictions at time $t = 120$ of center-line groundlevel concentration c_A (% molar fraction) for several along-wind-diffusion formulations
 (a) stability class D4 with cloud-shape correction (ICSCOR=1)
 (b) stability class D4 without cloud-shape correction (ICSCOR=0)

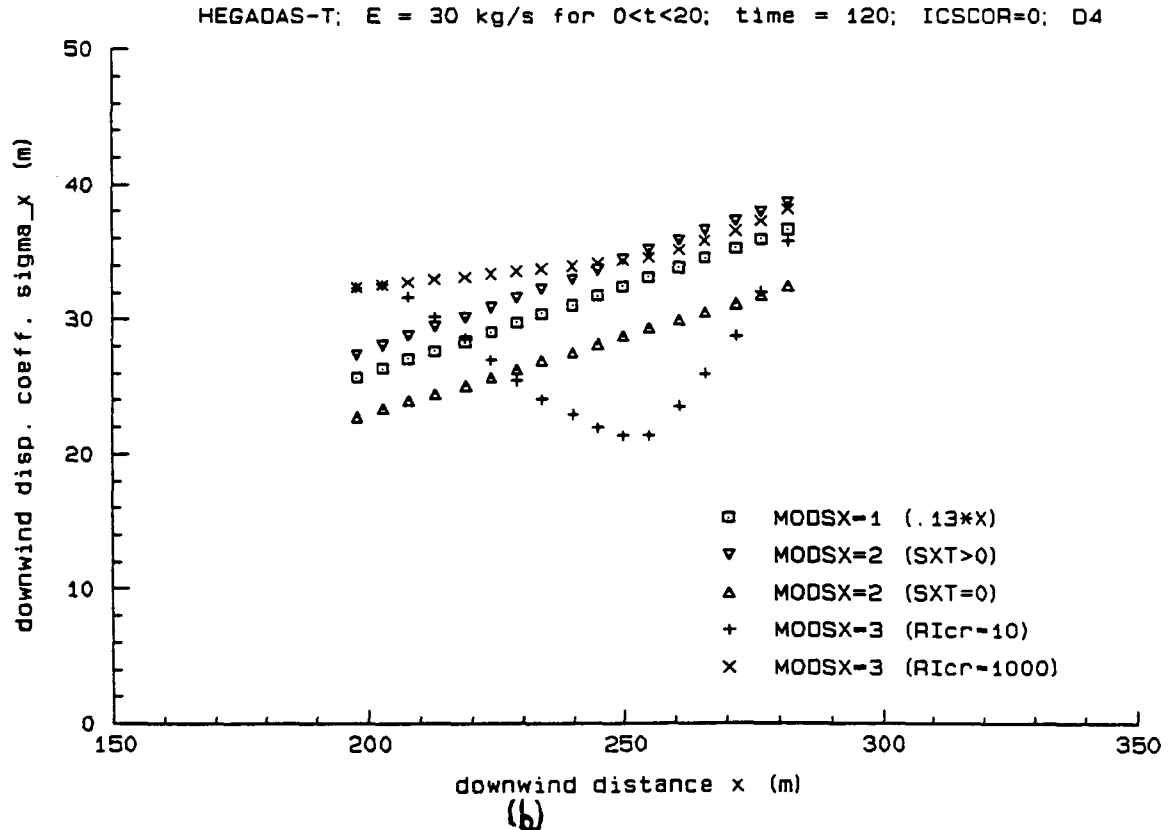
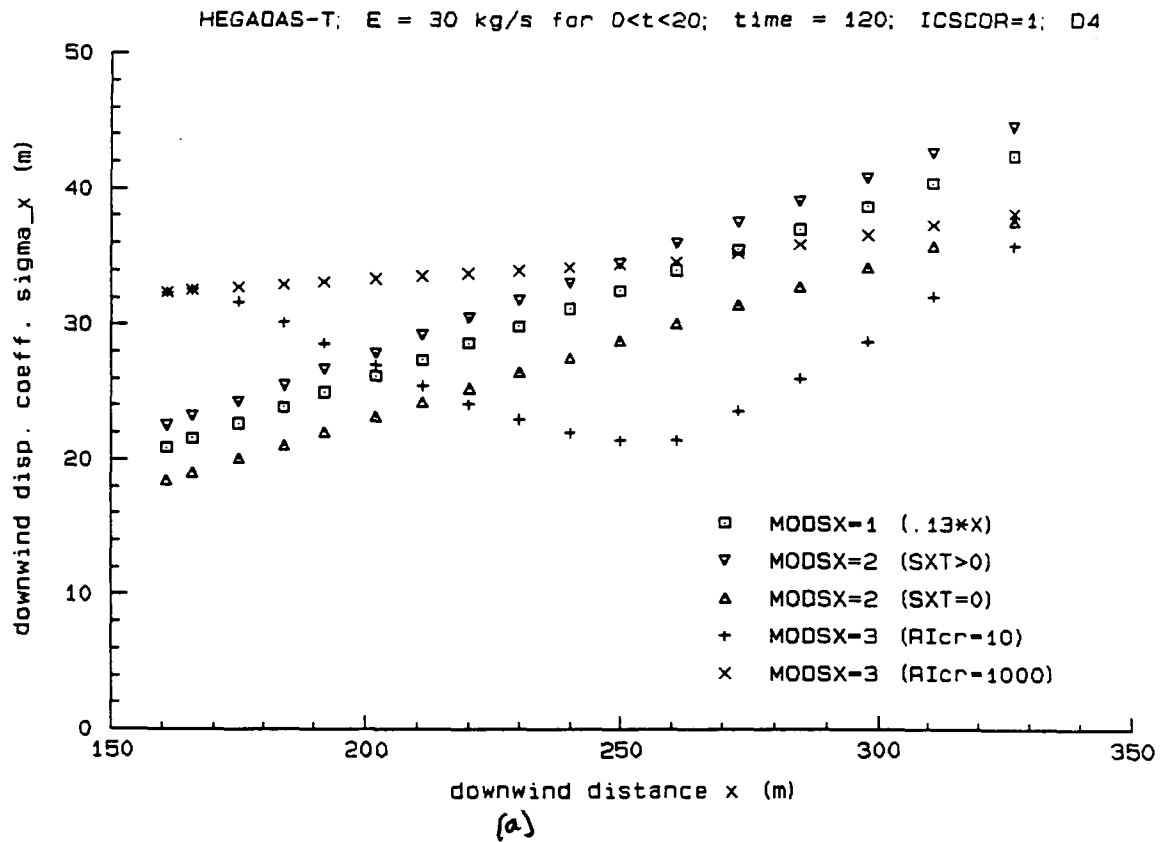


Fig. 7.7. Finite-duration steady-state gas release; source strength $E(t) = 30 \text{ kg/s}$, $0 < t < 20$ seconds; HEGADAS-T predictions at time $t = 120$ of downwind dispersion coefficient σ_x (observer data) for several along-wind-diffusion formulations
 (a) stability class D4 with cloud-shape correction (ICSCOR=1)
 (b) stability class D4 without cloud-shape correction (ICSCOR=0)

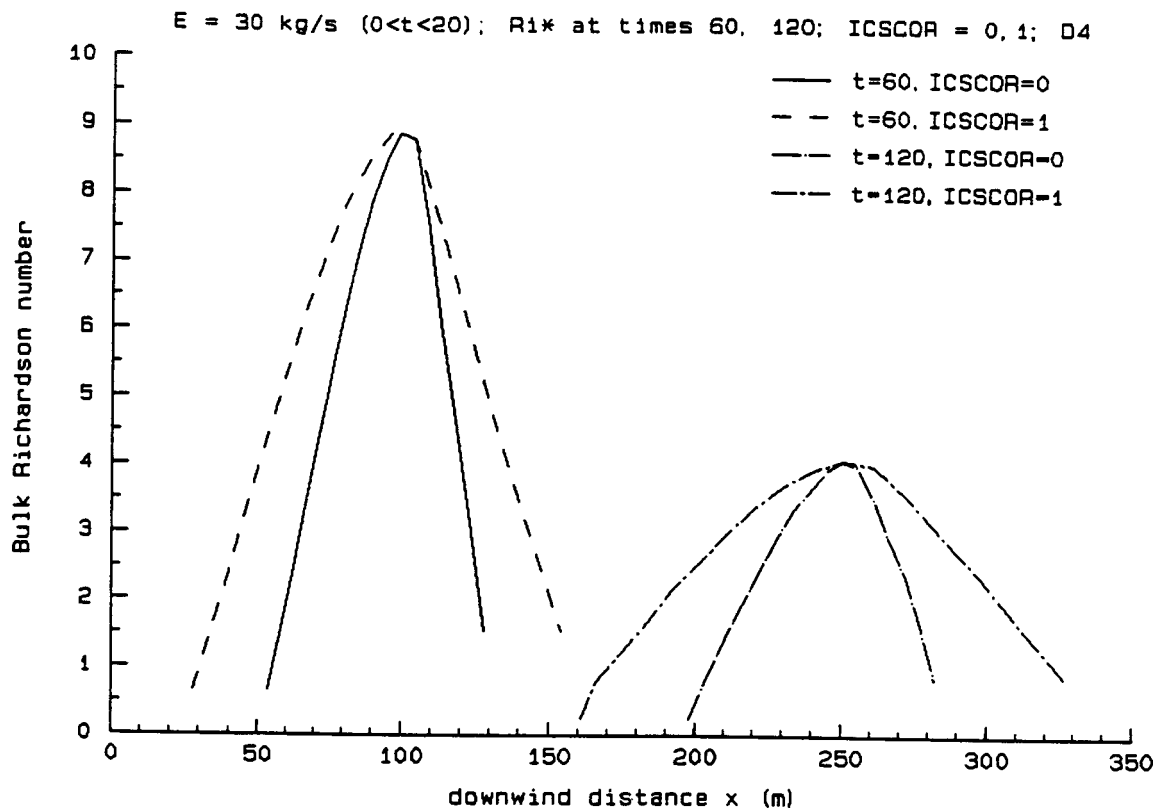


Fig. 7.8. Finite-duration steady-state gas release; source strength $E(t) = 30 \text{ kg/s}$, $0 < t < 20$ seconds; HEGADAS-T predictions at time $t = 120$ of bulk Richardson number Ri_* (observer data); stability class D4 with (ICSCOR=1) or without (ICSCOR=0) cloud-shape correction

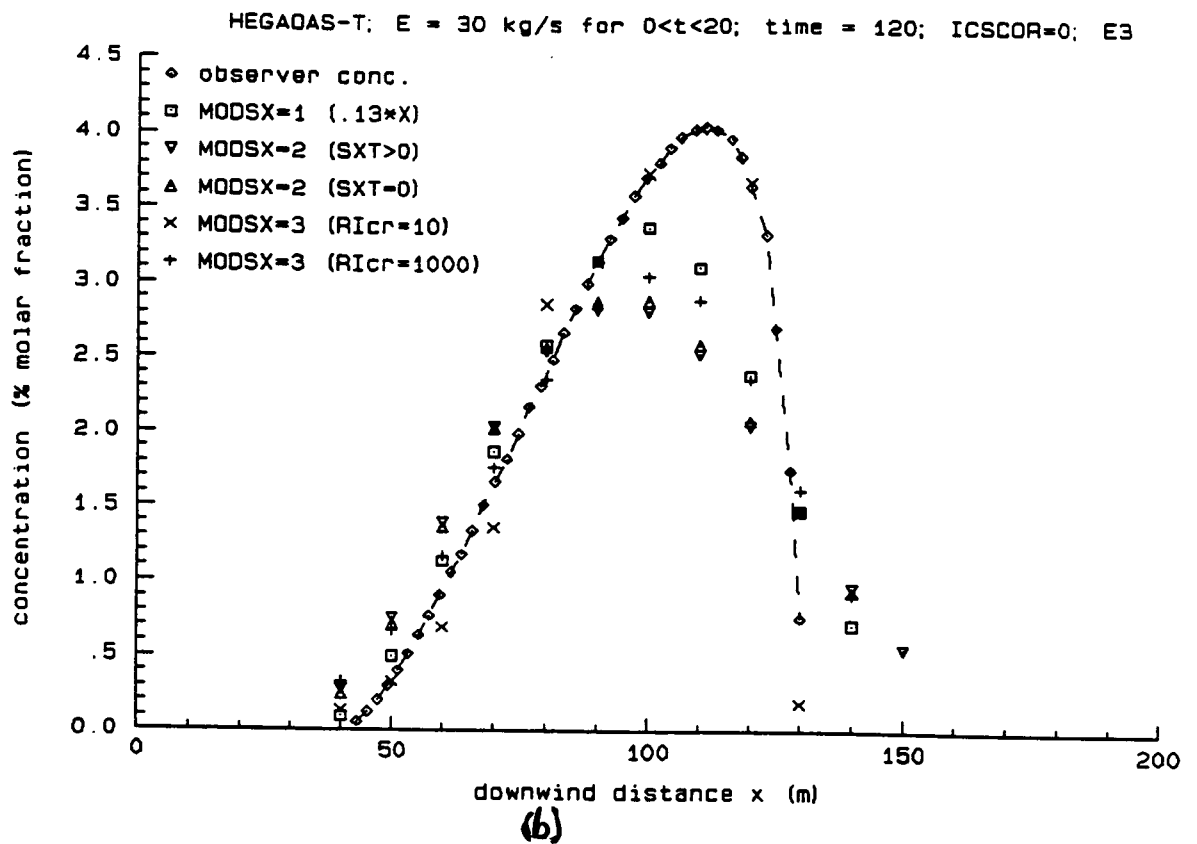
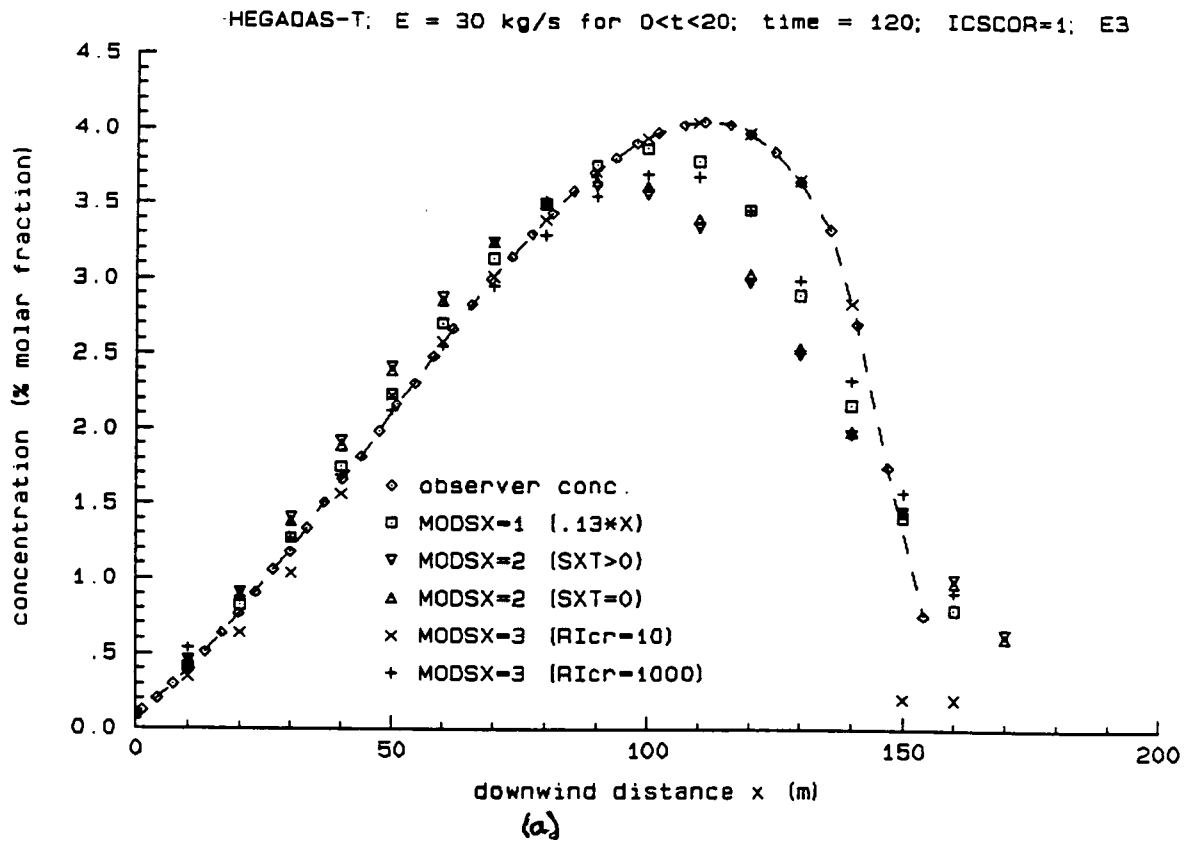


Fig. 7.9. Finite-duration steady-state gas release; source strength $E(t) = 30 \text{ kg/s}$, $0 < t < 20$ seconds; HEGADAS-T predictions at time $t = 120$ of center-line groundlevel concentration c_A (% molar fraction) for several along-wind-diffusion formulations

(a) stability class E3 with cloud-shape correction (ICSCOR=1)

(b) stability class E3 without cloud-shape correction

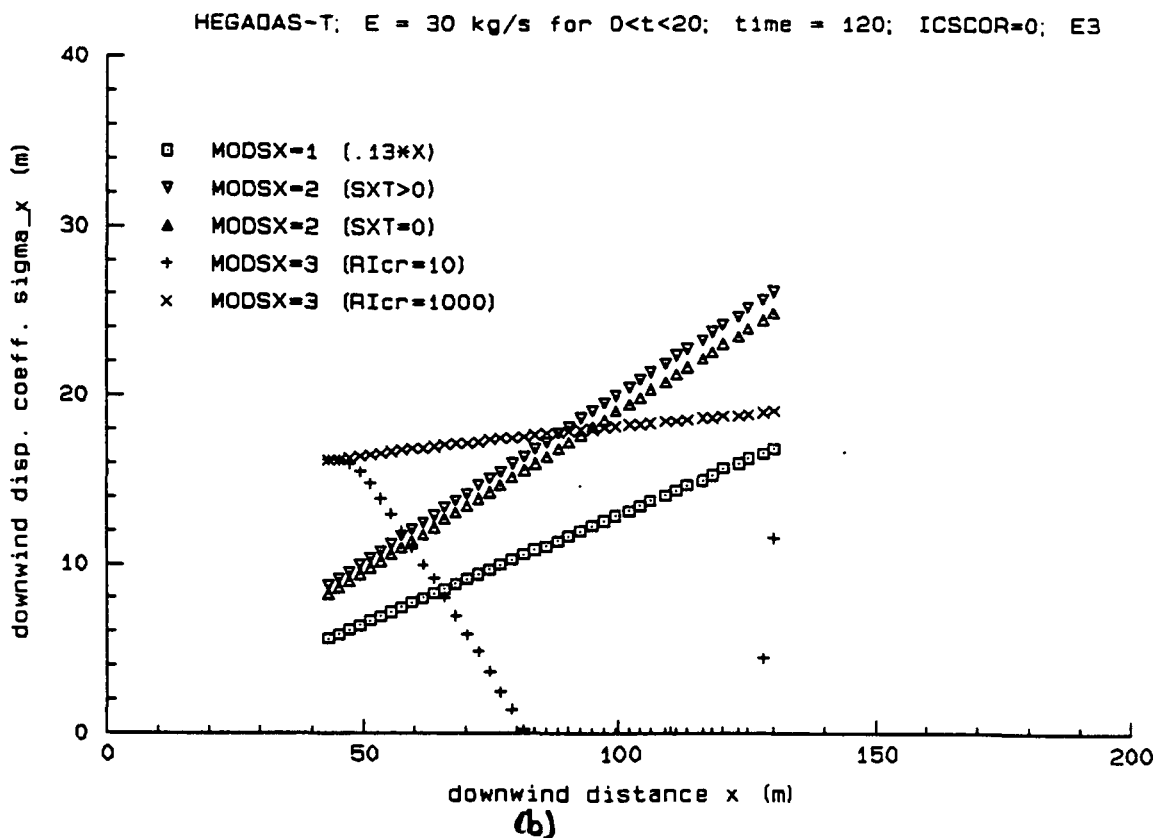
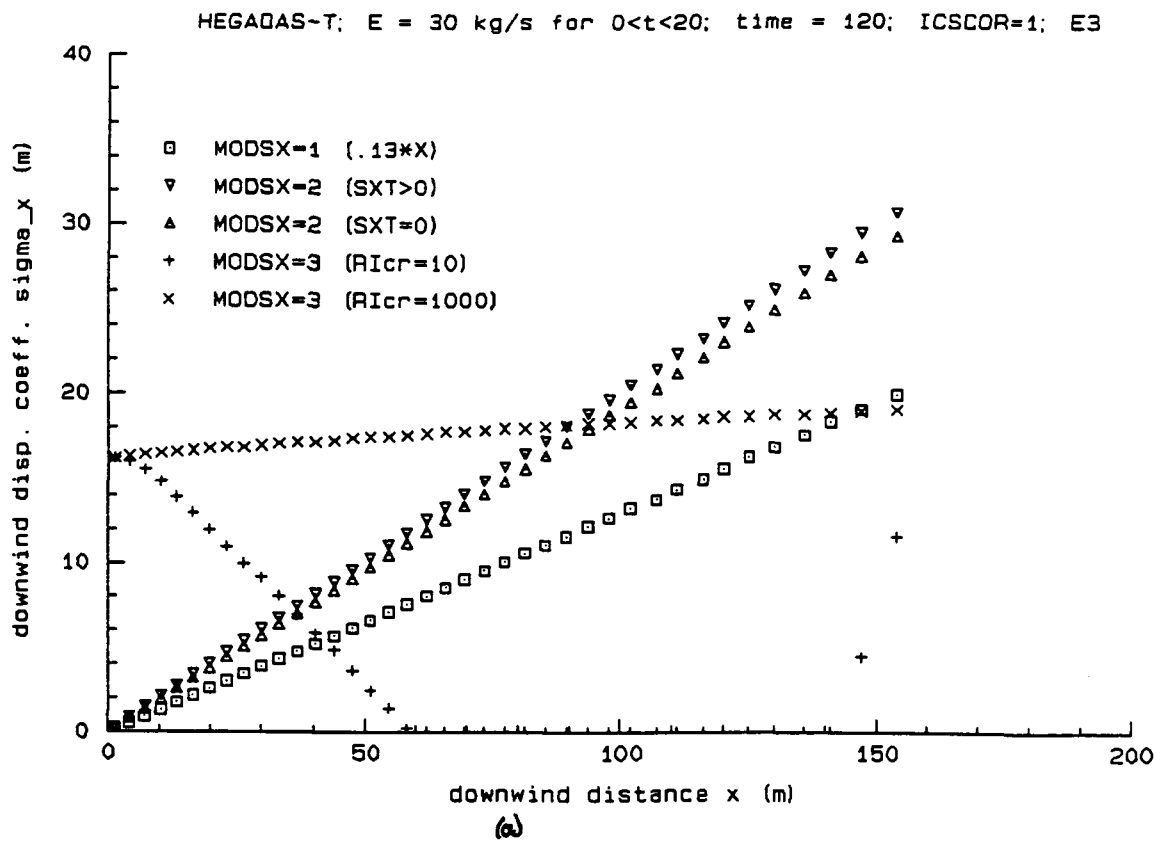


Fig. 7.10. Finite-duration steady-state gas release; source strength $E(t) = 30$ kg/s, $0 < t < 20$ seconds; HEGADAS-T predictions at time $t = 120$ of downwind dispersion coefficient σ_x (observer data) for several along-wind-diffusion formulations
 (a) stability class E3 with cloud-shape correction (ICSCOR=1)
 (b) stability class E3 without cloud-shape correction (ICSCOR=0)

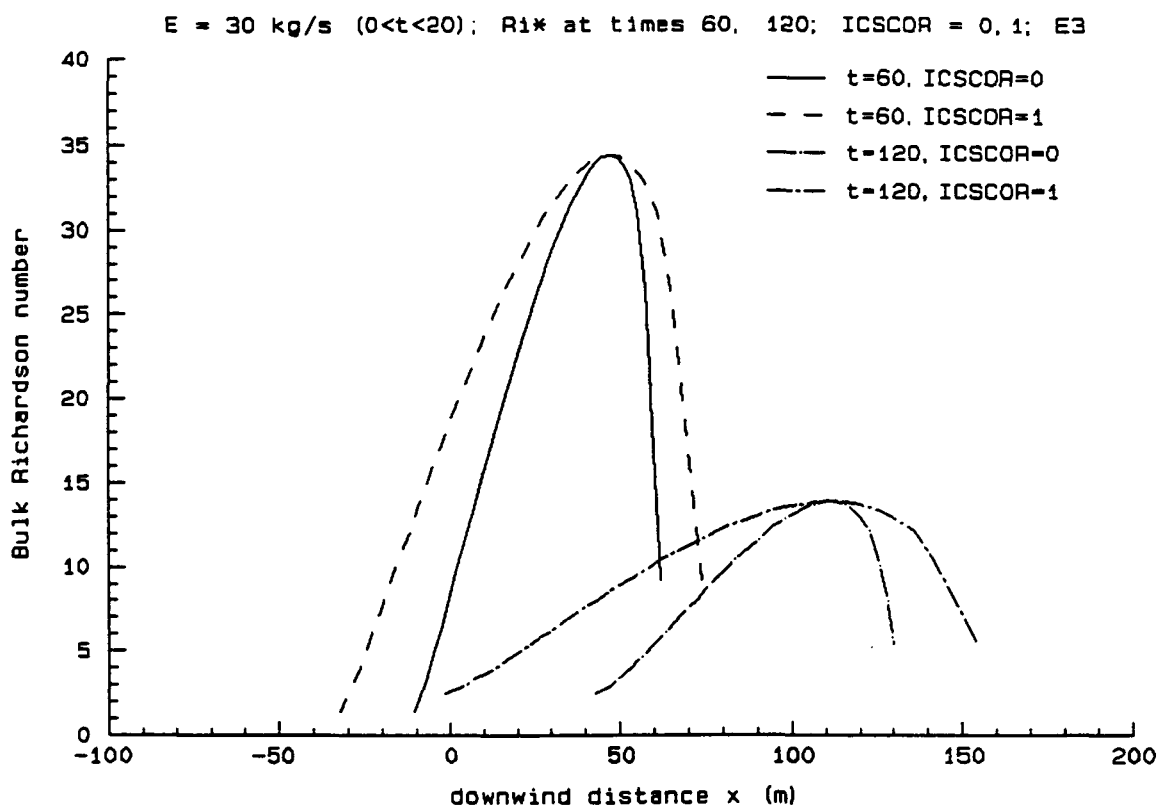
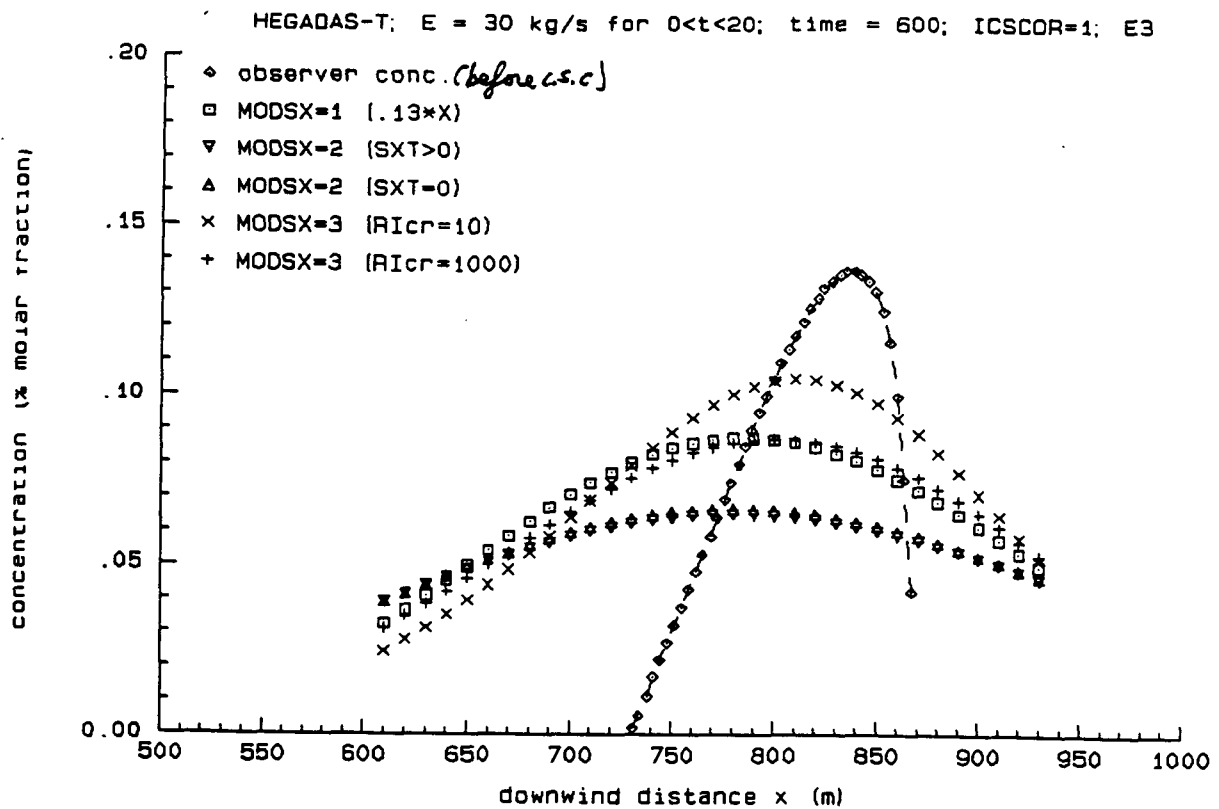
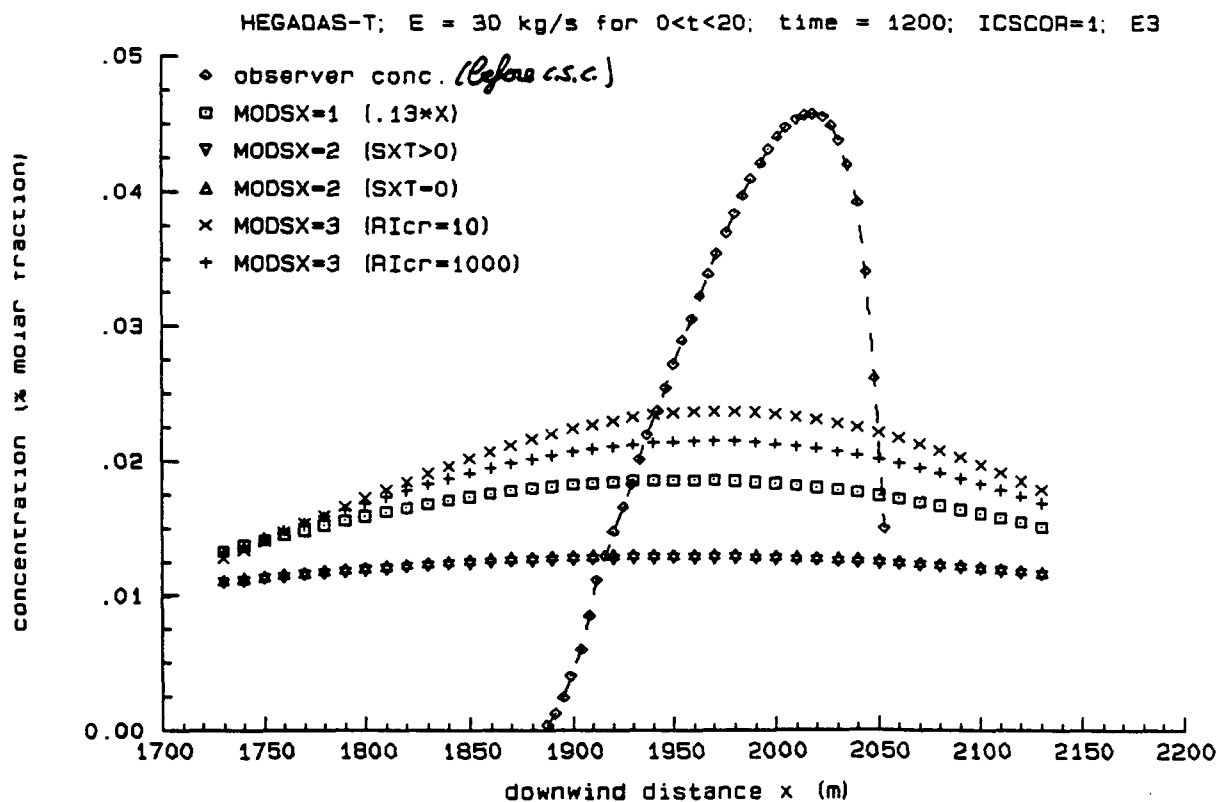


Fig. 7.11. Finite-duration steady-state gas release; source strength $E(t) = 30 \text{ kg/s}$, $0 < t < 20$ seconds; HEGADAS-T predictions at time $t = 120$ of bulk Richardson number Ri^* (observer data); stability class E3 with (ICSCOR=1) or without (ICSCOR=0) cloud-shape correction



(a)



(b)

Fig. 7.12. Finite-duration steady-state gas release; source strength $E(t) = 30 \text{ kg/s}$, $0 < t < 20$ seconds; HEGADAS-T predictions of center-line groundlevel concentration c_A (% molar fraction) for several along-wind-diffusion formulations; stability class E3 with cloud-shape correction

(a) time $t = 600$ seconds

(b) time $t = 1200$ seconds

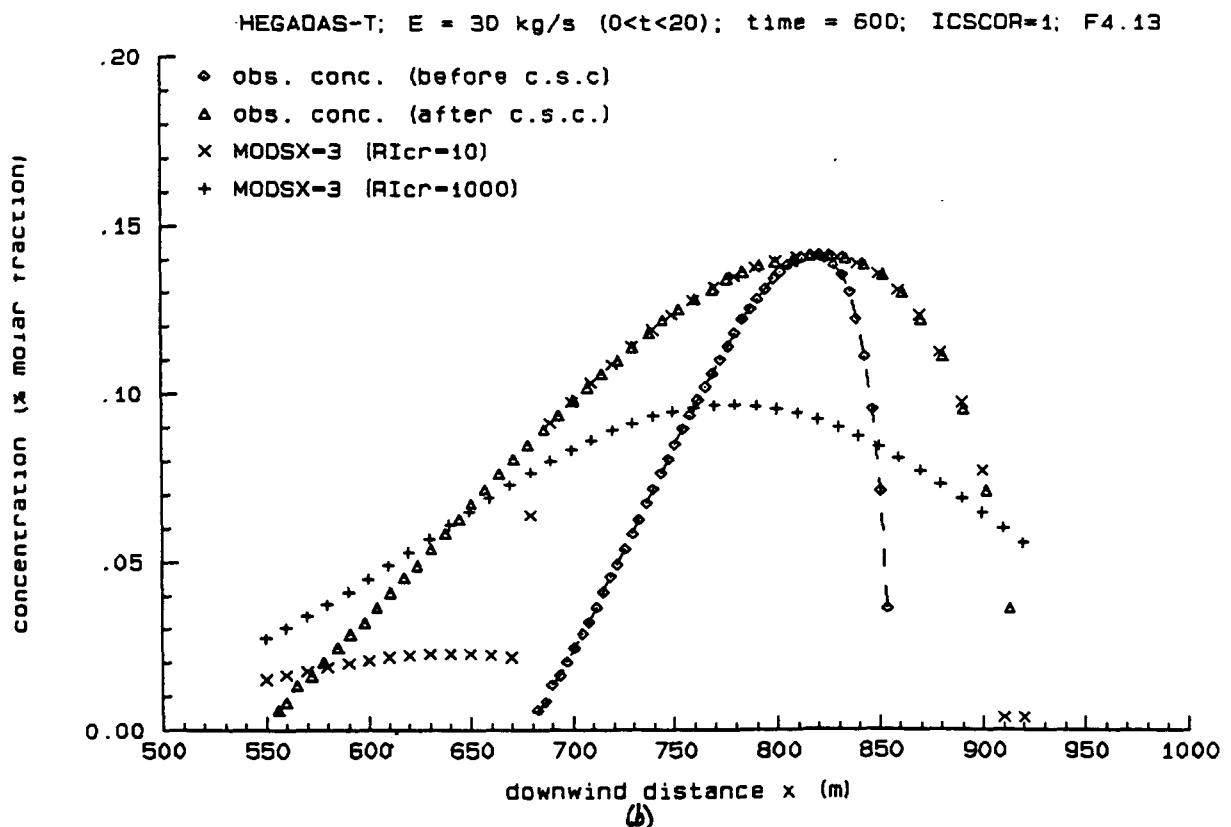
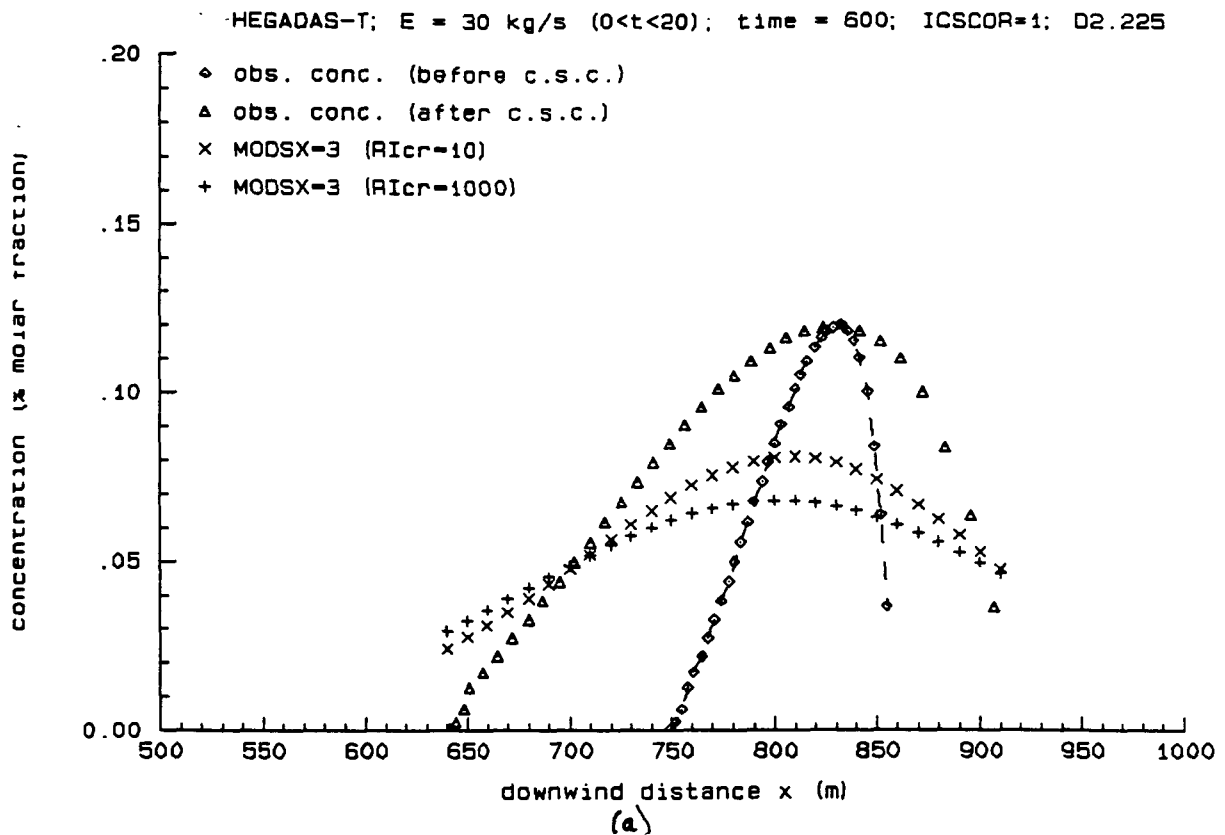


Fig. 7.13. Finite-duration steady-state gas release; source strength $E(t) = 30 \text{ kg/s}$, $0 < t < 20$ seconds; HEGADAS-T predictions at time $t = 600$ of center-line groundlevel concentration c_A (% molar fraction) for several along-wind-diffusion formulations; runs with cloud-shape correction

(a) stability class D, $u_0 = 2.22 \text{ m/s}$

(b) stability class F, $u_0 = 4.13 \text{ m/s}$

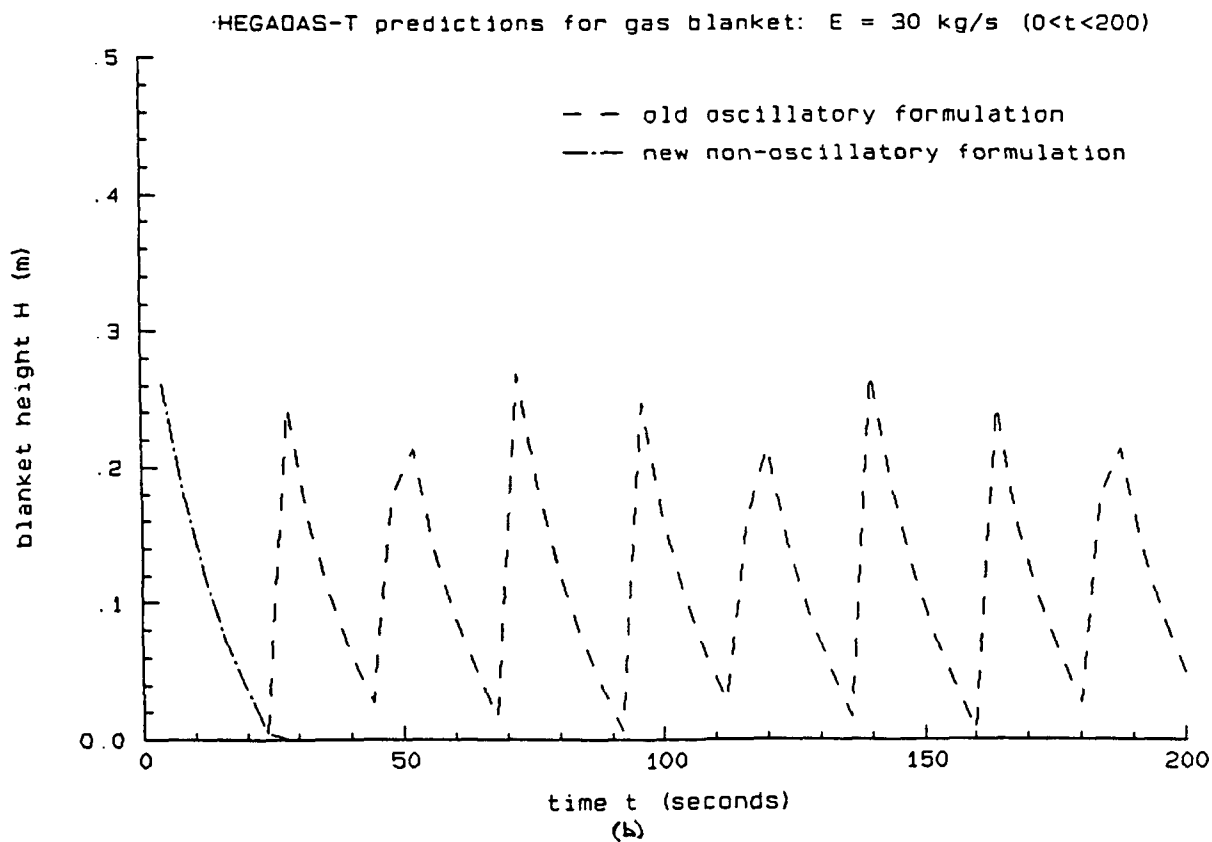
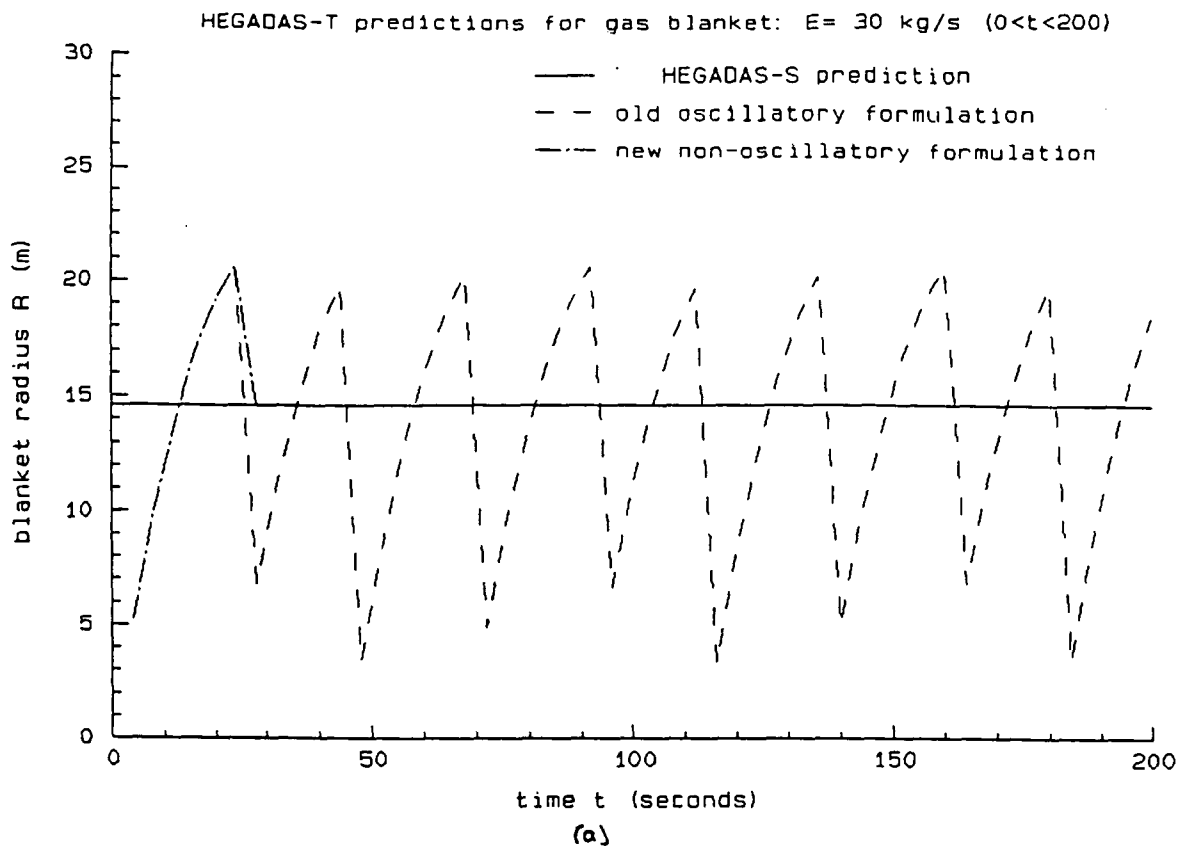


Fig. 7.14. Primary pool with radius $R_p = 3 \text{ m}$, spill rate $E = 30 \text{ kg/s}$ and spill duration = 200 seconds; HEGADAS-T predictions of gas-blanket dimensions;
 (a) blanket radius $R_g(t)$
 (b) blanket height $H_g(t)$

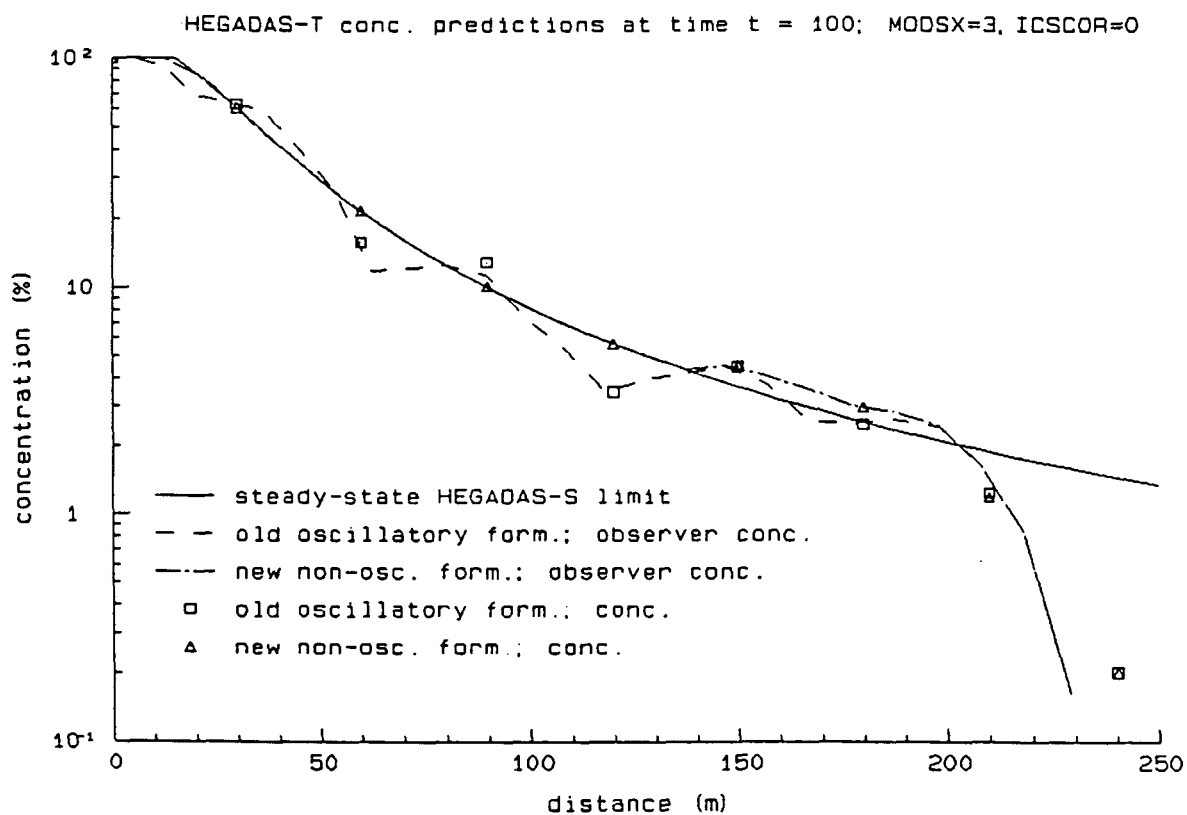


Fig. 7.15. Primary pool with radius $R_p = 3$ m, spill rate $E = 30$ kg/s and spill duration = 200 seconds; HEGADAS-T predictions at time $t = 100$ seconds of observer concentrations, and concentrations including the effects of downwind dispersion (Chatwin/Wilson formulation, MODSX=3; no cloud shape correction, ICSCOR=0)

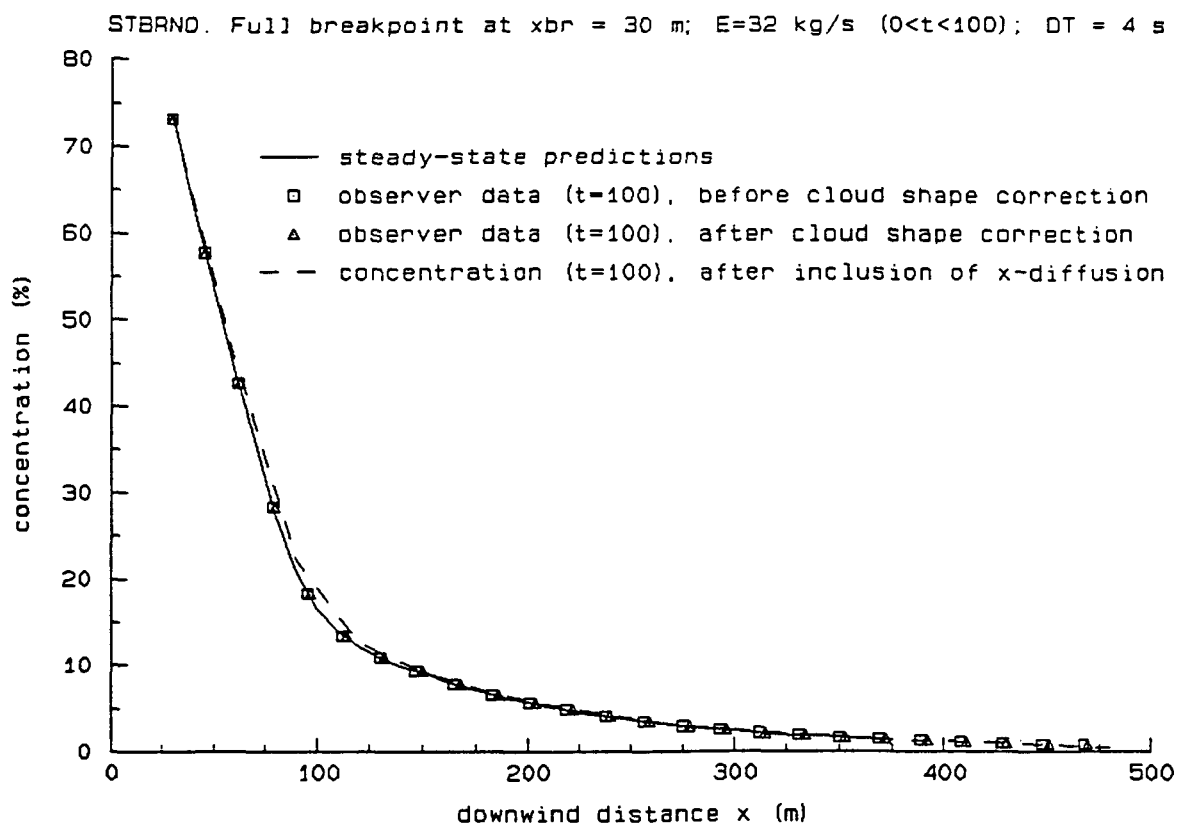


Fig. 7.16. HEGADAS-T predictions of center-line groundlevel concentration (% molar fraction) at time $t=100$ for a finite-duration vertical source at breakpoint $x_{br} = 30$ m ($E = 32$ kg/s, $0 < t < 100$) and HEGADAS-S predictions for a corresponding problem ($E = 32$ kg/s, $x_{br} = 30$ m)

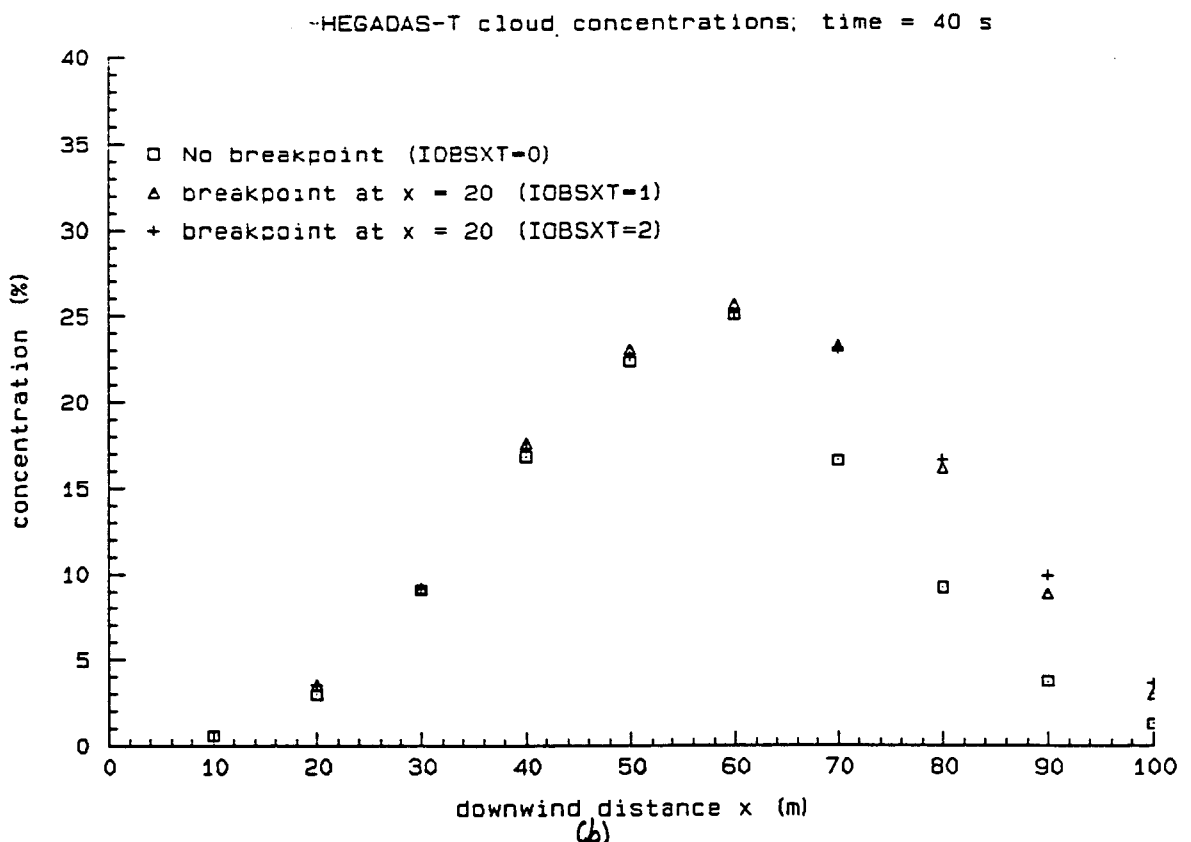
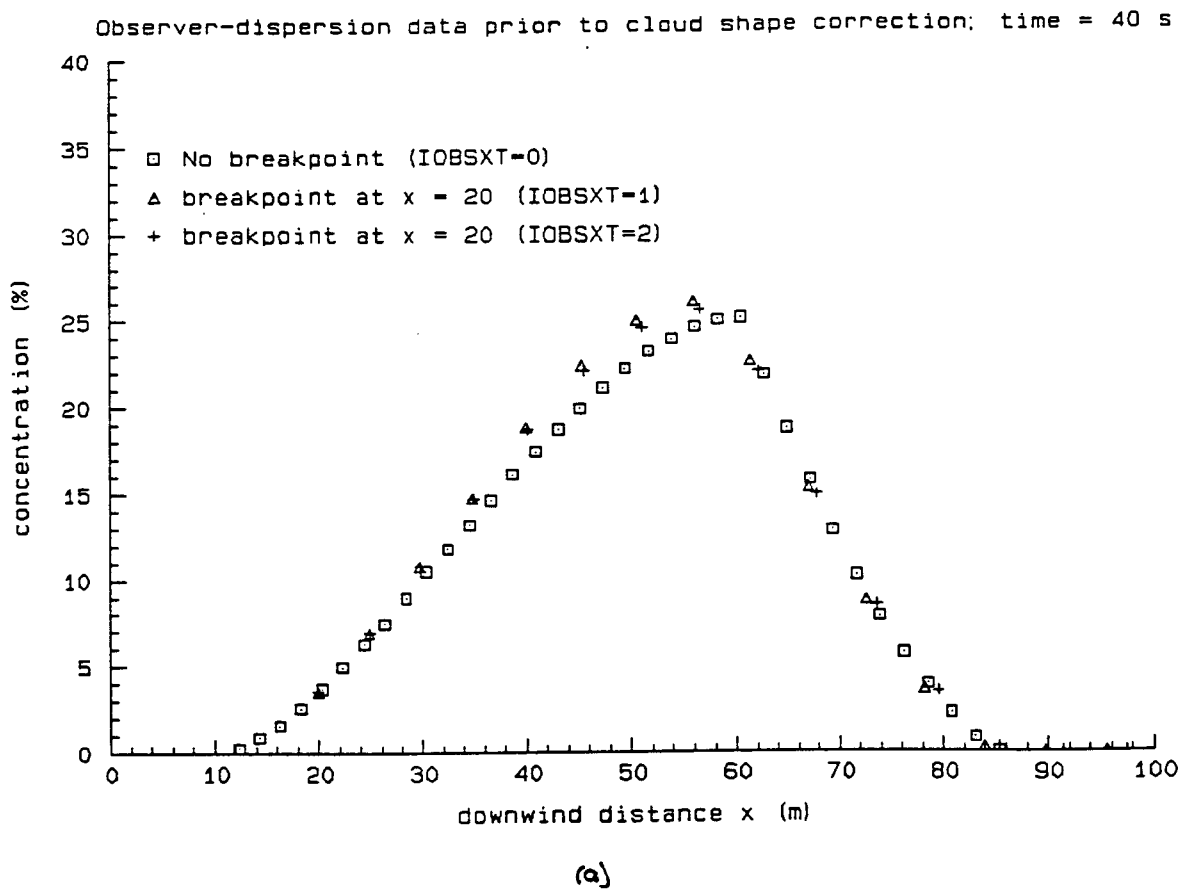


Fig. 7.17. Finite-duration steady-state gas release; source strength $E(t) = 30 \text{ kg/s}$, $0 < t < 20$ seconds; HEGADAS-T concentration predictions at time $t = 40$ of center-line groundlevel concentration (% molar fraction) for runs with primary pool data specified (IOBSXT=0) or data at breakpoint $x_{br} = 20 \text{ m}$ (observer-position formulas IOBSXT=1 or IOBSXT=2)
 (a) Observer concentrations prior to cloud shape correction
 (b) Cloud concentrations (including downwind diffusion)

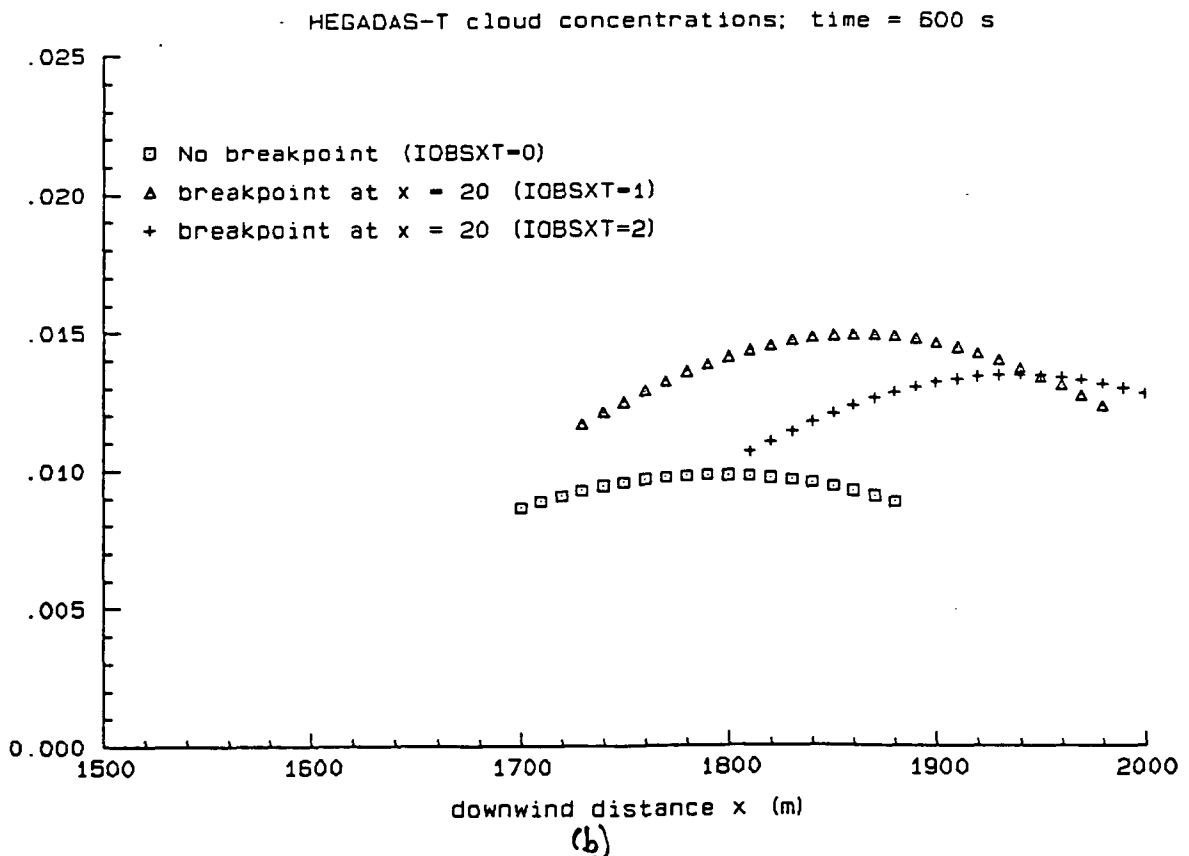
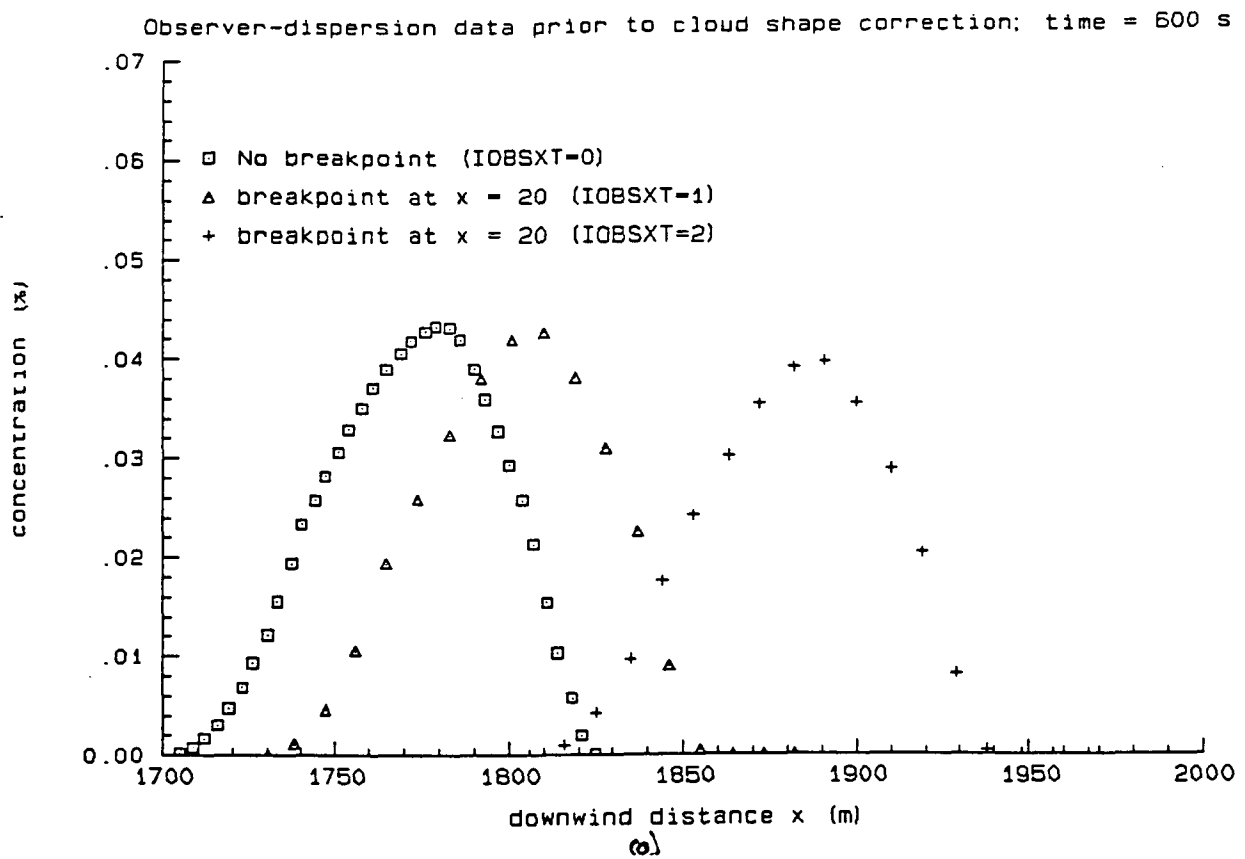


Fig. 7.18. Finite-duration steady-state gas release; source strength $E(t) = 30 \text{ kg/s}$, $0 < t < 20$ seconds; HEGADAS-T concentration predictions at time $t = 600$ of center-line groundlevel concentration (% molar fraction) for runs with primary pool data specified (IOBSXT=0) or data at breakpoint $x_{br} = 20 \text{ m}$ (observer-position formulas IOBSXT=1 or IOBSXT=2)
 (a) Observer concentrations prior to cloud shape correction
 (b) Cloud concentrations (including downwind diffusion)

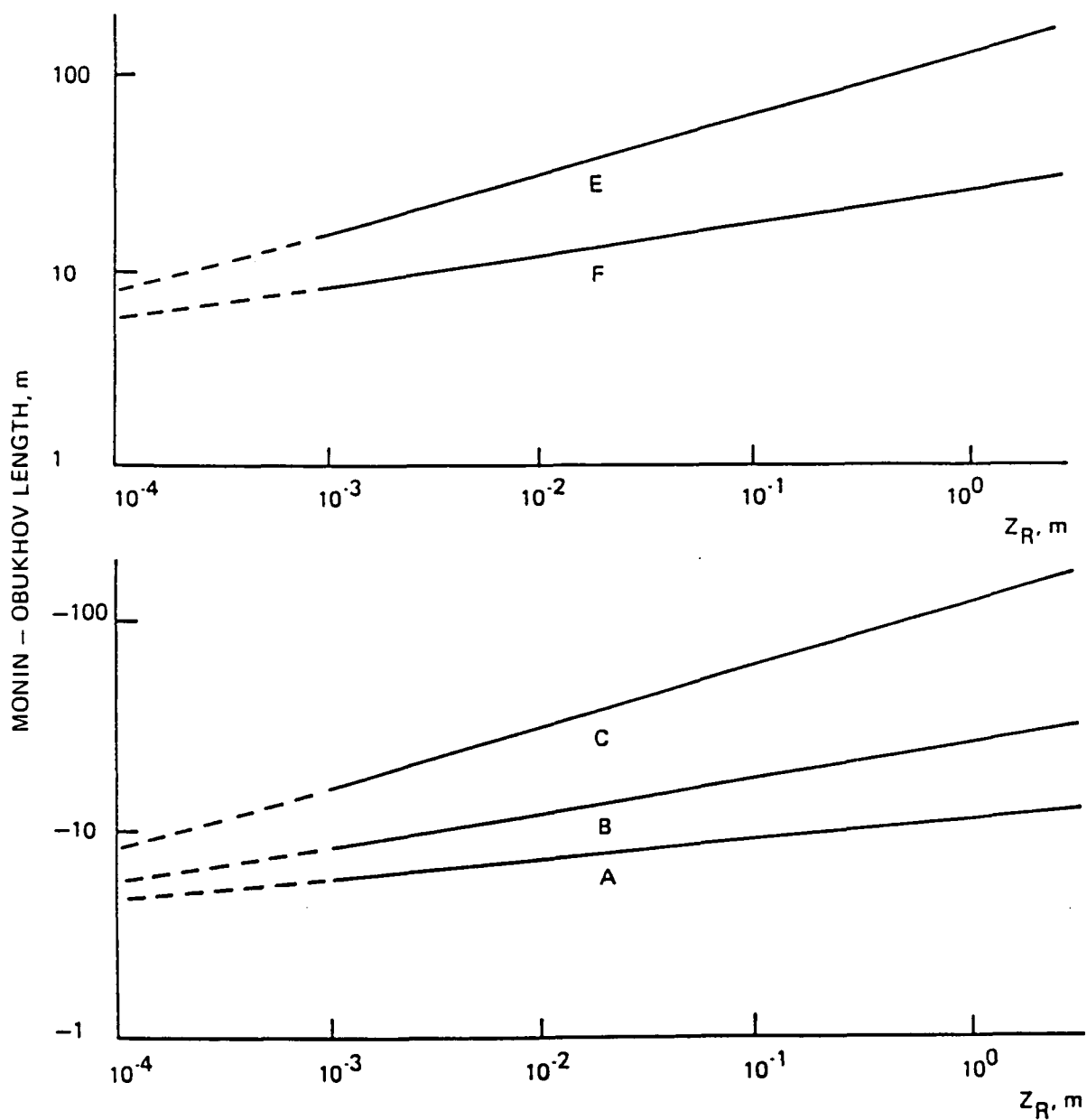


Fig. 7.19. The Monin-Obukhov length λ as a function of Pasquill stability class PQSTAB (= A,B,C,D,E,F) and surface roughness z_R [from Irwin (1979)]

8. SURFACE ROUGHNESS EFFECTS: COMPARISON OF HEGADAS PREDICTIONS WITH
WIND-TUNNEL DATA.

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8.1. Introduction

To use the HEGADAS¹ model to calculate dispersion in industrial settings requires input conditions substantially different from those in the Goldfish HF dispersion experiments used to evaluate HEGADAS version 5 and in other experiments used to validate earlier versions of HEGADAS. On an industrial site the flow over and around structures will generate stronger turbulence than the air-flow over the flat desert and this will lead to more rapid mixing and subsequent dilution of gas clouds.

HEGADAS assumes turbulence is generated by shear stress at the ground, and its affect on mixing is parameterized by the friction velocity, u_* . The friction velocity is, however, wind-speed dependent and when comparing the wind-field over different sites it is more usual to use as a parameter the surface roughness length, z_R , where the vertical wind profile is of the form:

$$U(z) = 2.5 u_* \ln(z/z_R) \quad (8.1)$$

and the wind speed at a given height, $U(10 \text{ m})$, is known. The roughness length is an aerodynamic parameter but, intuitively, it is a measure of the "roughness" of the ground being usually a factor 5 - 30 times smaller than the physical height of projections.

The roughness length at Frenchmann Flat, the site of the GOLDFISH experiments, is very small and in the range 0.00001 - 0.0003 m compared with 0.1 - 1.0 m in an industrial setting. Thus we would expect different cloud shapes and reduced dispersion distances for ground-level releases on an industrial site compared with the GOLDFISH experiments. Figure 8.1 illustrates that factor 10 increases in the surface roughness length parameter significantly decrease maximum plume concentrations. The release

¹In this section HEGADAS version 5 is referred to as HEGADAS.

conditions are appropriate to one of the experiments discussed in this section.

As surface roughness length increases, the basic processes that determine dispersion change from those assumed in the HEGADAS model. In particular, turbulence production is no longer limited to the ground surface but also takes place around the edges of structures which may extend through the depth of the gas cloud. The wind profile, equation 8.1, becomes undefined at heights smaller than the roughness length and the friction velocity, u_* , loses its utility as a measure of turbulence intensity. The limiting geometries in which the detailed flow around obstructions dominates dispersion are, however, not known and thus the limit of applicability of HEGADAS is also not known. Unfortunately, there are no full scale data that systematically describe the effect of roughness length on dispersion of HF or other dense gases.

In the absence of full scale data we have examined boundary-layer wind tunnel experiments of heavier than air gas (HTAG) dispersion, carried out by Petersen and Ratcliff (1988) on behalf of the American Petroleum Institute (API). Physical models of dense gas dispersion have been generally successful in modelling the full scale experiments at Thorney Island (Hall and Waters (1984), Davies and Inman (1987), Petersen and Ratcliff (1988)). Other full scale experiments involving dense gases have been complicated by changes in thermodynamic conditions during dilution. Meroney (1986) reviews the physical modelling of several field experiments in recommending guidelines for LNG dispersion simulations.

Petersen and Ratcliff used different sized obstacles, "roughness elements", to generate boundary layers with roughness lengths equivalent to between 0.015 and 0.525 m at full scale. The size of the roughness elements, at full scale, ranged from 1.3 to 5 m. These sizes are comparable with the depth of some dense gas clouds and large enough to admit the possibility that mixing in the wakes of the individual roughness elements determines dispersion.

We have compared HEGADAS calculations with data from these experiments to evaluate whether the effect of changing the surface roughness length in the model reproduces the observed differences in dispersion behaviour over the different wind-tunnel surfaces. We stress that, in view of the comments above, there was no a priori reason to assume validity of the model for this use or that, even if qualitative agreement was obtained, that input values of the surface roughness length should match wind-tunnel values.

We found that, while there remain differences between the HEGADAS model predictions and the HTAG database in a point-by-point examination of the data, there is overall agreement between predicted and measured concentrations using measured roughness lengths as input data. Thus we believe HEGADAS can be used to simulate releases into an atmospheric boundary layer with a surface roughness length of up to 0.5 m to an acceptable level of accuracy.

This finding, that dispersion among obstacles large compared with the initial cloud height depends upon the ambient turbulence intensity above the cloud, is at first surprising if one expects that only the local surface under the cloud influences its mixing. However, as mixing into dense gas clouds is predominantly via top entrainment, there must come a point, as the cloud dilutes, at which ambient turbulence becomes the dominant agent in the dilution. Some observations from the Thorney Island experiments are relevant in this context as these experiments were carried out in a boundary layer adjusting to a change in surface roughness. The detailed turbulence data from the experiments (Puttock (1987a)) show that the effective surface roughness, derived from velocity measurements, varied from 1.4 to 29 mm depending on wind-direction. For the planned wind direction there was only flat grass and sea upwind of the gas release point and the effective surface roughness was small. In some experiments there were trees and low buildings some 300m upwind of the release point and the effective surface roughness was larger. Model dispersion predictions (Puttock, 1987b) were consistently better in predicting dilution distances to 1% v when the effective roughness length, ie. appropriate to the measured ambient turbulence, was used in place of a value characteristic of the local surface.

This chapter describes the detailed comparison between the HEGADAS predictions and a subset of the HTAG database. As the study progressed we found that the description of gravity spreading originally in HEGADAS (version 4) did not properly describe all of the data and that this was unlikely to be an artifact of the wind-tunnel experiments. Several revisions to HEGADAS were made as we developed an improved model for the gravity spreading. It has not proved practical to describe all of the stages in the development of the model in this report however a summary of the major steps taken is given in Appendix A to this chapter. The model, as implemented in HEGADAS, is described in section 7.3.2. We will compare, for select cases, predictions made with HEGADAS and with HEGADAS version 4 that is described in Appendix 3.

8.2. The HTAG Database

The HTAG (Heavier Than Air Gas) database comprises the results of a series of experiments conducted by Petersen and Ratcliff for the API. under the heading "Effect of Homogeneous and Heterogeneous Surface Roughness on Heavier than Air Gas Dispersion". The description of these results used in this comparison with HEGADAS predictions was taken from report CPP 87-0417 dated August 1988. The report describes the experimental procedure, summarises experimental conditions and presents some of the results in graphical form. The gas concentration measurements themselves were supplied on an IBM format floppy disk labelled as Appendix G.

The HTAG measurements were made in an open-circuit wind tunnel using three source types and several different surface roughness configurations. Homogeneous roughness experiments were carried out to simulate full scale boundary layers with nominal surface roughness length, z_R , values of 3, 20 and 50 cm. The experimental conditions will be referred to generically in this report as R3, R20 and R50 respectively.

For the R3 and R20 experiments cubic roughness elements were laid out in regular formation with fixed orientation to the wind. For the R50

experiments the upwind roughness was arranged in regular rows with alternate rows face on to and oblique to the wind direction. Most experiments used the R3 and R50 configurations.

Heterogeneous roughness experiments were made with a model refinery structure set at different approaches to the wind. The effect of blocking structures, representing solid buildings, in conjunction with the refinery model was studied. Only near field concentration data were gathered and so these experiments have not been compared with HEGADAS predictions.

The effect of regular arrays of large structures, a tank farm, was also investigated. In these experiments the both the wind direction and the upwind surface roughness distribution were varied for a source upwind of the tanks. These data are not discussed in detail in this report. A short summary of the findings is given in Section 8.7.

The gases used in the experiments were blended to give three different source densities. The density ratios relative to air were 1.0 (passive dispersion), 1.4 and 4.0. Values of 3.9 and 4.2 were used for the densest gas in some of the runs. The source gases contained a hydrocarbon tracer amounting to some 6% by volume. The concentration of this tracer was measured using a flame ionization detector coupled to a gas chromatograph. The HTAG report does not clearly state the accuracy of the measurement. We believe the lowest concentration that can be measured to reasonable accuracy (< 25% error) is 6 ppmv or 0.01 % of the source tracer concentration. Concentrations smaller than 6 ppmv were reported for some of the experiments but we have excluded these from our HEGADAS comparisons.

Some of the experiments simulated stable wind conditions by cooling the wind tunnel floor. The average temperature difference between the tunnel air and the floor was 27 °C. The roughness elements were essentially two-dimensional and were made of chain (R3) and thin metal sheet (R20 & R50). These experiments are described briefly in Sections 8.2.1 and 8.7.

8.2.1 Scaling Considerations.

In this section we briefly examine the scaling criteria used in the wind tunnel simulations. We refer the reader to Snyder (1981) for a detailed discussion of wind tunnel modelling of the atmospheric boundary layer.

a) Richardson/Froude number

To simulate buoyancy correctly in dense gas dispersion it is necessary to preserve the bulk Richardson number of the flow:

$$Ri_* = g'H/u_*^2 \quad (8.2)$$

where $g' = g \Delta\rho/\rho$, g is the acceleration due to gravity, $\Delta\rho$ is a density difference and ρ the ambient density, H is a characteristic vertical length scale and u_* is a characteristic velocity here taken to be the friction velocity. The length scale factor selected for the HTAG experiments was 1:100, thus to maintain a constant Richardson number, $\Delta\rho$ and/or u_* must be modified. Density differences are sometimes exaggerated in plume dispersion studies as this allows higher flow velocities to be used (Snyder (1981)) but distorted density modelling was not used in the HTAG experiments. The velocity thus scales at 1:10 relative to the atmospheric boundary layer.

b) Reynolds Number.

With the above length and velocity scaling the Reynolds number, is 1000 times smaller in the model than at full scale. All laboratory studies rely on the assumption that the important characteristics of turbulent flow are independent of Reynolds number provided that this is sufficiently large (Snyder (1981)). Minimum Reynolds number criteria are easily met in studies of jet mixing or aerofoil flows but rough wall simulations of the atmospheric boundary layer are problematic due to the inherently low wind speeds of interest.

The thickness of the viscous sub-layer, δ , on a flat wall is proportional to the friction length, $\delta = 11 z_f$, (Monin and Yaglom (1987)):

$$\text{where:} \quad z_f = \nu/u_* \quad (8.3)$$

Taking values $\nu = 1.5 \times 10^{-5} \text{ m}^2/\text{s}$ for air, $u_* = 0.3 - 0.9 \text{ m/s}$ for the neutral atmospheric boundary layer conditions simulated in the HTAG experiments we obtain:

$$1.8 \times 10^{-4} < \delta < 5.5 \times 10^{-4} \text{ m} \quad (8.4)$$

(R50)
(R3)

for the viscous sub-layer thickness at full scale. In the wind-tunnel u_* is 10x smaller than at full scale and so the viscous sub-layer is a few millimeters thick. For the low roughness, R3, experiments the sampling height of 5 mm used in the HTAG gas concentration measurements lies just within the viscous sub-layer.

The relative height of the roughness elements to the friction length determines whether the wall is rough² and so whether the vertical velocity profile matches that in the atmosphere. For a fully rough boundary layer $h/z_f > 60$ (Monin and Yaglom (1987)). This ratio is equivalent to a minimum Reynolds number criterion based on the roughness element height. A boundary-layer is partially rough, i.e. influenced by surface elements if $h/z_f > 4$. In the wind-tunnel the obstacle height, h , ranged from 1.3×10^{-2} to $5 \times 10^{-2} \text{ m}$ so that:

$$26 < h/z_f < 320 \quad (8.5)$$

(R3)
(R50)

and on this basis the boundary layer was only fully rough for the R50 configuration.

²The following criteria are based on experiments with sand covered surfaces. It is not clear that they apply to sparsely distributed roughness elements on an otherwise smooth surface.

An alternative Reynolds number criterion (Snyder(1981), Petersen (1988)) is that:

$$u_* z_R / \nu > 2.5 \quad (8.6)$$

where z_R is the surface roughness length. This is equivalent to the criterion of Schlichting (1979) who cites a ratio of $h/z_f > 70$ (cf 60 above) for a fully rough wall when $h/z_R = 30$. For atmospheric boundary layers h/z_R depends on the physical characteristics of the roughness elements but is generally of order 10, thus the former criterion is the more conservative.

c) Peclet Number

There appear to be no well defined criteria describing the admissible ratio of molecular to turbulent diffusion in simulated atmospheric boundary layers. Molecular diffusion can have two effects. Firstly, it can act to smooth out local concentration fluctuations within the gas cloud. Secondly, if concentration gradients are sufficiently steep, diffusion can contribute significantly to total mass transfer. We consider both of these effects in turn.

Work by Crapper and Linden (1974) identified that molecular diffusion could affect the thickness of the density interface between two fluids. They defined a Peclet number in terms of the turbulence intensity and integral length scale and found that the density interface was broadened by molecular diffusion at Peclet numbers smaller than 200. If we assume that the obstacle height, h , is characteristic of a turbulence length scale it is appropriate to define:

$$Pe_* = u_* h / D \quad (8.7)$$

Taking, the molecular diffusivity $D = 1.1 \times 10^{-5} \text{ m}^2/\text{s}$, $0.3 < u_* < 0.9 \text{ m/s}$ and $1.3 < h < 5 \text{ m}$ at full scale we obtain:

$$35 \times 10^3 < Pe_* < 410 \times 10^3 \quad (8.8)$$

and in the model: $35 < Pe_* < 410$ (8.9)

(R3) (R50)

Comparing this with the criterion $Pe > 200$ for the neglect of molecular diffusion effects we see that in the low roughness experiments concentration gradients within the cloud may be smoothed by molecular diffusion and concentration fluctuations will be smaller than at full scale.

Turner (1968) studied entrainment across a density interface. He determined that molecular diffusion could contribute significantly to total mass transfer across the interface. The effect became more important with increasing density stratification. It is, however, not possible to derive a criterion from that work. An unpublished analysis by Mahieu (1984), reported by Puttock and Colenbrander (1985), does lead to a suitable criterion. Mahieu simulated dense gas releases in a wind-tunnel at different scales and observed how far the experiments could be scaled down before similarity failed. He also analysed wind-tunnel data from Meroney which could be interpreted as simulations of the same release at different scales. He found that the observations scaled correctly as long as:

$$Pe/Ri = U^3/g'D > 1500 \quad (8.10)$$

where U was the wind speed at a reference height of 10 cm in the wind-tunnels, and all experiments were performed at low roughness.

To use the criterion under conditions of higher roughness, however, the velocity scale should be a turbulence scale and not a convection scale. Britter and McQuaid (1988) substituted a friction velocity into (8.10) and suggested:

$$u_* > 0.6 (g'D)^{0.33} \text{ m/s} \quad (8.11)$$

as a criterion for neglecting molecular diffusion. This is equivalent to taking a limiting value of Pe_*/Ri_* , where both parameters take the cloud thickness as a length-scale. From this, taking $D = 1.1 \times 10^{-5} \text{ m}^2/\text{s}$, we find that u_* should satisfy:

$$\begin{aligned} u_* &> 0.02 \text{ m/s} & \text{for } (\Delta\rho/\rho) = 1.4 \\ u_* &> 0.04 \text{ m/s} & \text{for } (\Delta\rho/\rho) = 4 \end{aligned} \quad (8.12)$$

Comparing these values with the HTAG experiments we see that at high roughness (R50) u_* was normally 0.086 m/s and at low roughness (R3) 0.035 m/s. Thus the experiments should be free of diffusion effects, except possibly for the density ratio 4 experiments at low roughness which are at the borderline according to this criterion. We have looked for anomalies in that dataset, however, the results appear to be consistent with the findings from the other three sets of conditions.

We note that more work needs to be done on developing the diffusion criterion, in particular, because the ratio Pe_*/Ri_* is undefined in the limit as $(\Delta\rho/\rho) \rightarrow 0$ equation (8.11) is not valid for neutrally buoyant dispersion. A functional form $Pe_* / (1 + a Ri_*)^n$, as suggested by the dependence of total entrainment on Ri_* (Appendix 3), would have the correct limiting behaviour.

d) Monin-Obukov length

Some of the HTAG experiments were conducted under simulated stable stratification conditions. The vertical profiles of velocity and temperature in the atmospheric boundary layer are described in terms of the roughness length, friction velocity and the Monin-Obukov length, L , (Pasquill and Smith 1983). The effect of stable stratification is represented by the empirical functions Φ which appear in the boundary layer equations for velocity and excess temperature:

$$\frac{du}{dz} = \frac{u_*}{kz} \Phi_M \quad (8.13)$$

and

$$\frac{d\theta}{dz} = \frac{T_*}{kz} \Phi_H \quad (8.14)$$

where

$$\begin{aligned} \Phi_M &= 1 + 4.7 z/L & \text{for momentum} \\ \Phi_H &= 0.74 + 4.7 z/L & \text{for heat} \end{aligned} \quad (8.15)$$

are the relations used by Petersen ((1988) Appendix D) and

$$\begin{aligned}\Phi_M &= 1 + 6.9 z/L && \text{for momentum} \\ \Phi_H &= 1 + 9.2 z/L && \text{for heat}\end{aligned}\tag{8.16}$$

are used in HEGADAS. Thus to simulate the correct boundary layer velocity and temperature profiles the wind tunnel model should preserve the ratio z/L . As length is scaled by 100 the model Monin-Obukov length should also be reduced by a factor of 100.

The Monin-Obukov length is defined as:

$$L = - \frac{u_*^3}{k g \frac{\overline{T'w'}}{T_0}}\tag{8.17}$$

where k ($=0.41$) is the von Karman constant, g the acceleration due to gravity, T' and w' are temperature and vertical velocity fluctuations and T_0 is a reference temperature. The over bar denotes averaged values. The parameters g and T_0 are necessarily the same order of magnitude in the model as at full scale. The required scale reduction for L is 0.01 and u_* is 0.1 of the full scale value so that for similarity:

$$\overline{T'w'}_{\text{model}} = 0.1 \overline{T'w'}_{\text{atmosphere}}\tag{8.18}$$

now $\overline{T'w'} < (\overline{T'^2} \overline{w'^2})^{0.5}$ and $(\overline{w'^2})^{0.5}$ scales as u_* thus

velocity scaling provides the factor 0.1 and hence the temperature fluctuations in the model should be of the same order of magnitude as at full scale. The magnitude of the temperature fluctuations can be at most equal to the temperature difference across the boundary layer and so the model should preserve temperatures at their full scale values.

In the HTAG experiments the temperature difference maintained across the boundary layer was much greater than that found in the atmosphere as shown in Table 1 below. The calculated value of L is that which matches u_* to

the roughness length, z_R , in HEGADAS and ΔT is the corresponding temperature difference.

Run ID	roughness z_R m		calculated			measured	
			u_* m/s	L m	ΔT °C 0-10m	ΔT °C 0-10m	ΔT °C 2-10m
HT68	R3	.002	.14	26	1.6	37	8
HT72	R20	.176	.27	35	2.44	31	9
HT74	R50	.320	.45	200	0.7	30	6

Table 1. Stable boundary layer properties for some HTAG experiments.

Thus stable atmospheric stratification was not properly simulated. We would expect vertical mixing to be less in the wind tunnel than at full scale because of the greater stratification. This was found to be the case in the comparisons of HEGADAS predictions with the wind tunnel data. In all examples HEGADAS over-predicted entrainment and gave too low gas concentrations. The stable flow calculations have not been included in this report for this reason but the results are discussed briefly in section 8.7.

e) Low frequency turbulence and lateral cloud growth.

Whilst most of the important features of atmospheric boundary layer turbulence can be simulated in the wind tunnel there are differences in the low frequency components of the turbulence spectrum which are of particular significance for gas dispersion studies.

In the atmosphere, eddies exist which are large compared with the lateral plume dimension and these distort the plume as it convects. Thus "snap shots" of a plume taken at different times show changes in the instantaneous plume shape. For this reason it is conventional to describe parameters such as the plume width in terms of averaged values as would be observed by continuous measurement over a standard time. This time is usually in the range 10 - 60 minutes. We note that, except under conditions of extremely small wind direction fluctuations, the hourly

observed plume will be wider than the ten-minute plume and averaged concentrations will be lower.

In contrast, wind-tunnel flows are designed to minimise low frequency disturbances in order to improve the repeatability of measurements. Thus a wind tunnel plume will attain a steady-state shape on a time-scale sufficient to smooth out details of the turbulent mixing process. In the HTAG experiments steady state concentration averages were obtained with a minimum sampling time of about 1 minute. The concentration measurements used a sampling time of three minutes.

To examine the effect of differences in the low frequency turbulence between atmospheric and windtunnel dispersion we compare the widths of neutrally dense plumes at different distances from the source. The plume half-width, $W_h(x)$, is defined by:

$$W_h^2(x) = \frac{\int y^2 c(x,y) dy}{\int c(x,y) dy} \quad (8.19)$$

where $c(y)$ is concentration and y is the lateral distance from the plume centre-line. For a gaussian plume, $W_h = \sigma_y$, and correlations derived from field experiments exist to predict the variation with σ_y with distance from the release point. At distances up to a kilometer the full scale experimental data is well fitted by a power law, $\sigma_y = ax^b$ and at distances greater than a kilometer by the form, due to Briggs, $\sigma_y = ax/(1+bx)^{0.5}$ (Hanna et. al. (1982)). Typical values for the constants in the σ_y equations are discussed in section 7.3.1. As noted above, the value of σ_y is dependent upon the length of time over which the measurements are averaged. An empirical rule for converting between averaging times is (TNO (1980)):

$$\sigma_y(t) = \sigma_y(600)(t/600)^{0.2} \quad (8.20)$$

where time, t , is measured in seconds and $\sigma_y(600)$ is a "standard" 10-minute average value.

The lateral concentration profiles of neutrally buoyant gas clouds released at ground level is Gaussian and it is generally assumed that the cloud half-width, W_h , will be the same as σ_y for elevated plumes. We note that W_h will be different for dense gas clouds because of gravity spreading.

Figure 8.2 compares the HTAG measured plume half-widths for neutrally buoyant releases, in this case $W_h = \sigma_y$, with the power law σ_y function for atmospheric dispersion under neutrally stratified conditions. The correlation is based on field data with an averaging time of 10 minutes and corresponds to the Pasquill-Gifford curve for stability class D (Section 7.3.1). To illustrate the possible range of full scale values that could arise through averaging time effects we also show the corresponding curves for 3 and 30 minute averages. The HTAG data are classified into point and small area sources as described in section 8.2.2.

Most of the HTAG data are for distances smaller than 160 m (at full scale) from the source and as such give little information about the change in σ_y with downstream distance. We note that there is a lot of scatter in this data and it is not well described by a single correlation. Very close to the origin, < 40 m, the measured σ_y values for the area sources are consistently greater than the full scale correlation. This is due to the finite source size, the correlation being valid for a point source. At distances greater than 160 m the HTAG data deviate significantly from the full scale correlation with the plume width increasing much more slowly with distance from the source. A regression line through the small area source data gives:

$$\text{the power law:} \quad \sigma_y = 0.63x^{0.6} \quad (8.21)$$

$$\text{or the Briggs formulation:} \quad \sigma_y = 0.238x/(1+0.0411x)^{0.5} \quad (8.22)$$

both equations being an equally good fit to the data. One set of point source data in Figure 8.2, those for run HT86, showed smaller values of σ_y these were correlated by:

$$\sigma_y = 0.16x^{0.786} \quad (8.23)$$

Thus the wind tunnel experiments do not properly simulate the "expected" lateral growth of neutrally buoyant gas clouds. As described above this is because large scale plume meander, which arises in the atmosphere through wind direction fluctuations, effectively broadens the path traced by the plume. The wind tunnel reproduces the essential turbulent mixing process, and so correctly models plume dilution and the local plume width, but cannot reproduce plume meander.

We observe that the full scale plume behaviour would be far better described by taking explicit account of meander by defining the probability (fraction of time) that any location in the plume path would be exposed to gas. The average concentration at a point would then be given by the probability of exposure multiplied by the actual plume concentration. The latter corresponds to the concentration measured in the wind-tunnel.

The rate of plume growth in the far field is accounted for in HEGADAS by specifying σ_y as an input parameter to the model. The measured value, equation (8.21) was used.

8.2.2 Source conditions

For ease of reference, in this and in following sections, all dimensions will be expressed as their full scale equivalent. The scale factor for length is 100 and for velocity it is 10. We note that the results of the comparison with HEGADAS are independent of whether model scale or full scale dimensions are used.

Three source types were used and are described as: point, small area and large area.

The point source was a straight pipe of diameter 0.24 m. Gas was injected into the tunnel horizontally from a height of 0.24 m in the streamwise direction. The volume flow rate for the initial tests was .248 m³/s increasing to 6.683 m³/s in three stages in later tests. The exit velocities thus ranged from 5.48 to 148 m/s. We would expect jet momentum

to affect the initial development of these plumes. The higher flow rate experiments are not compared with model predictions because HEGADAS takes no account of source momentum, horizontal or vertical, and its effect on mixing.

In the HEGADAS simulations the point source was treated as a ground level area source, square in cross-section, and of equal area to the pipe exit.

The small area source was circular with diameter 5.08 m. The source gas was injected vertically with an exit velocity of 0.55 m/s which is 10% of the reference wind speed at 10 m height. At the greatest flow rate the injection velocity increased to 1.6 m/s. The ratio of the exit velocity, U_e , to the friction velocity, u_* , ranged from 0.64 - 4.57. We note that Hall and Waters (1989) find that discharge momentum can affect downwind dispersion from area sources at ratios U_e/u_* as small as 0.1. The emerging source flow acts as a blockage, vortex shedding from which influences dispersion. We might therefore expect parameters such as σ_y to vary with source emission rate, although no such dependence could be properly distinguished from the data. The small area source was again treated as a square of equivalent area in the HEGADAS simulations.

The large area source was a composite of 9 small area sources arranged in a square array. The exit velocity was 0.124 m/s and the ratio with u_* ranged from 0.14 - 0.35. In the HTAG report the source was described as having an effective width of 22 m and was modelled as such.

8.2.3 Surface Features and the Ambient Wind.

The data from which the wind velocity profile is derived is not fully described in the HTAG report. Appendix E of the HTAG report lists values of the logarithmic profile parameters z_R and u_* together with the index, n , of a power law fit:

$$U \propto z^n \quad (8.24)$$

to the vertical velocity profile. Appendix G, the data disk containing details of each run, gives a reference velocity for each experiment. This was usually close, within 6%, in value to the wind speed at 10 m height given in Tables 3 and 4 of the report which describe the target conditions for each run. In making the HEGADAS predictions we have used the z_R values given in Appendix E and assumed the reference velocity in Appendix G to be that at 10 m. The resulting friction velocity u_* , and power law index α calculated by HEGADAS (cf Appendix 3) do not always agree with the values of u_* and n given in Appendix E as shown in Table 2. We would expect n and α to differ because the power law fit to the logarithmic velocity profile depends on the range of heights over which the agreement is optimized. HEGADAS emphasises the lowest 10 m of the boundary layer whilst the HTAG study appears to fit the lowest 40 m.

For heterogeneous roughness the logarithmic velocity profile is not a good approximation to the wind profile, especially in the near wake of the refinery model, Petersen and Ratcliff (1988) Appendix I. We will not consider the heterogeneous roughness experiments in this study.

Configuration	z_R (m)	U_{10} (m/s)	HTAG		HEGADAS	
			U_* (m/s)	n (-)	U_* (m/s)	α (-)
R3	.015	5.6	.35	.17	.35	.2
		2.7	.17	.17	.17	.2
R20	.182	5.7	.56	.27	.58	.33
R50	.525	5.7	.86	.35	.78	.42
		3.3	.50	.35	.45	.42

Table 2. Wind Profile Parameters

8.3 HEGADAS Model Use

8.3.1 Input Data

This section assumes familiarity with the HEGADAS input data file and, together with the HTAG report provides the information needed to reproduce the HTAG simulations.

The HEGADAS model was run with heat transfer and water vapour transfer options turned off (ISURF = 2). Material properties then enter only through the chosen molecular weight.

The source was assumed square and the input source lengths were chosen to match the experimental source area. These were:

Source type	Source length, m
Point	0.213
Small area	4.502
Large area	22.0

Table 3. Source Lengths.

We note that these input source lengths are in fact nominal since the mass flow rates were sufficiently large for HEGADAS to create a virtual source. We refer the reader to the description of the HEGADAS "gas blanket" given in Appendix 3.

The reference height for the velocity profile was set at 10 m. The nominal reference velocity and surface roughness for the homogeneous roughness runs were:

Run. I.D.	z_R , m	u_{10} , m
R3	0.015	5.6
R20	0.182	5.6
R50	0.525	5.6

Table 4. Roughness lengths

The air, ground and gas temperatures were set to 20 °C.

The built-in values for the lateral plume dispersion coefficient, σ_y , were not used because, as discussed above, the wind tunnel simulations do not reproduce plume meander which is an ad hoc component of the standard σ_y correlation formulae. A power law for σ_y derived from the HTAG experiments with neutral density clouds was therefore used as input. The model parameters as they appear in the input file were:

```
CROSSW =1      (flag to use an input power law)
           0.63 (constant  $\delta$  in power law)
           0.6  (exponent  $\beta$  in power law)
```

The laboratory in which the HTAG experiments were conducted is sited above sea level such that the ambient pressure is lower than the 1 atm assumed in the HEGADAS model by a factor 0.85. HEGADAS is not intended to be run at other than 1 atm pressure, however, we made some test calculations that showed that predictions using 0.85 and 1 atm ambient pressure gave similar results provided the mass release rate of gas was kept constant. We used the HEGADAS standard pressure of 1 atm for the HTAG simulations and adjusted the volume gas release rate to maintain the mass flow.

The assumed densities and molecular weights are given in Table 5 and were referenced to dry air at 20 °C.

Density Ratio	Density kg/m ³	Molecular wt g/mol
1	1.204	28.96
1.4	1.686	40.5
3.9	4.696	113
4.2	5.06	122

Table 5. Gas Properties

The mass flux of released gas was calculated from the above densities, the source area and the volumetric flow of gas for the HTAG runs

was reduced 15% to account for the changed atmospheric pressure. For the experiments used in this report the volume flow rates, at 20 °C, were:

Source type	Run I.D.	Corrected volume flow rate m ³ /s @ 1 atm
Point	86 - 91	0.63
Small area	138 - 143	18.7
Large area	47 - 52	51.0

Table 6. Gas Flow Rates

8.4 Modifications made to the HEGADAS model

A major finding of this study has been that the gravity spreading formula originally used in HEGADAS version 4 and generally accepted for plume spread over smooth ground and for small ambient wind speeds did not properly describe spreading under the HTAG conditions. A revised spreading formula which takes into account the effect of ambient turbulence (cf section 7.3.2 and Appendix 8.A) has been developed and incorporated into HEGADAS. Before considering the comparison between HEGADAS and the HTAG data it is appropriate to highlight the reasons for amending the model and the effect of the changes that have been made.

Figure 8.3 shows plume centre-line concentrations and plume half-widths, W_h , as defined by equation (8.19), calculated using HEGADAS version 4 (dashed lines) and HEGADAS version 5 (solid lines). The calculations are made for two small area source experiments. The roughness distribution is R3 and the density ratio for the two cases is 1.4 and 3.9. The experimental data are shown as points: the squares denote the plume half-width and the triangles the maximum plume concentration.

If we compare the HEGADAS-4 (dashed lines) calculations with the data we see that the plume width is greatly over-predicted at distances greater than 80 m from the source, and the error increases with the release gas density. The predicted centre-line concentrations are lower than the measured values as a consequence of the over-predicted plume width.

The experimental data suggest that the initial stages of plume spread are correctly predicted but that the rate of lateral spread changes quite abruptly at about 80 m downstream for these cases. Thereafter the cloud spreads very slowly. The changes made to the gravity spreading law and incorporated into HEGADAS comprise a criterion for this transition and a formula for the post transition spreading rate. The solid lines in Figure 8.3 show the new HEGADAS calculations are identical those of HEGADAS version 4 up to the transition point and thereafter give much better agreement with the measured plume widths. The new HEGADAS predicted concentrations are concomitantly in better agreement with the data than those of version 4.

One unknown factor in HEGADAS-5 is the rate of spread immediately following transition. This is controlled by an adjustable parameter, C_D , in the HEGADAS input file. A value $C_D = 5$ has been found to give the best agreement with the wind tunnel data. The sensitivity of the calculations to C_D is discussed in Appendix 8.A. We note that setting $C_D = 0$ in the input data file forces HEGADAS-5 to use the HEGADAS-4 gravity spreading formulation.

Complete full scale validation of the revised gravity spreading model (independent that is of the GOLDFISH comparisons described in Chapter 9) has not been possible, mainly because few full scale steady experiments have large enough release rates for the effect to be pronounced. Figure 8.4 shows results for test 54 of the SHELL MAPLIN SANDS LPG spill experiments. This was a continuous release into a low wind speed. The distance to LFL (lower flammability limit) was significantly underpredicted by HEGADAS-2 (Colenbrander and Puttock (1983)) and the reason for this has never been explained. The dashed lines are predictions made in 1982 and the solid lines are HEGADAS-5. Agreement with data at sensor heights of 0.6 and 1.6 m is much better with the revised gravity spreading model. The data at 2.4 m are apparently less well predicted but examination of the data shows that the difference between maximum and averaged measured concentrations was small at the lower sensor heights but large at 2.4 m. Thus we infer that the averaged concentrations, shown in Figure 8.4, at 2.4 m were depressed by intermittency.

8.5 Model Data Comparison

We report a subset of the comparisons made between the HTAG database and HEGADAS predictions. To demonstrate as complete a test of the model as possible we have taken those experiments which report concentrations over the greatest range of downwind distances. Runs of each source type have been included. These runs are not necessarily those which are best modelled, and include those which are worst modelled, by HEGADAS. The runs are:

Source Type	I.D.	Downstream Range
Large Area:	HT47 - HT52	40 - 320 m
Small Area	HT138 - HT143	40 - 640 m
Point	HT86 - HT91	20 - 320 m

Table 7. Experiments used in this comparison with HEGADAS

In making the comparison between the HEGADAS predictions and the HTAG data we wish to provide both a quantitative measure of goodness of fit and a qualitative impression of the agreement between the predicted and measured cloud shapes. It has not proved practical to reproduce each measured cross-wind and vertical concentration profile in comparison with its modelled equivalent. Instead we present graphs of the:

- decay of concentration at ground-level in the flow direction,
 - increase in cloud half-width with downstream distance,
- to give a qualitative impression of the predictions together with a graph of:
- predicted vs measured concentration at each sampling point
- to give a quantitative measure of agreement.

HEGADAS predicts ground-level concentrations, an assumed vertical concentration is then used to calculate concentrations at different heights. The HTAG "ground-level" measurements were actually made at a scale height of 0.5 m, however, the sampling method introduces some ambiguity into the data comparison. The sampling rate was such that the

measuring probe sampled gas from a region larger than the probe diameter. As a consequence, the sampling process involved spatial averaging of concentration because the sampled gas was a mixture of gas from different heights. Meroney (1986) cites a similar problem in his review of wind tunnel simulations.

It is not possible to correct for this process because the samples were taken from a region in which velocity and density change significantly across the sampling cross-section. We can see, however, that errors will be smallest where the vertical concentration gradient at the ground is small. The measured concentrations can at most equal the ground-level concentration and so, as an approximation, we compare HEGADAS predictions both at ground-level and at the sampling height with the data. The difference between these predictions indicates where the change in concentration with height is significant and where the potential for error is greatest.

The minimum concentration for which predictions have been compared is 0.01% of the source gas. This corresponds to 6 ppmv tracer concentration in the HTAG experiments. We believe lower concentrations to be subject to rapidly increasing error.

8.6 Results

8.6.1 Large Area Sources

Figure 8.5 shows the results of the model predictions for run HT47 which was a neutrally buoyant release over the R3 roughness distribution. Figure 8.5 and subsequent figures comprise three graphs.

- Top left is shown the predicted and measured plume half-width and the maximum plume concentration. The predicted concentrations are for heights $z=0$ and $z=0.5$ m and the data were measured at $z=0.5$ m.
- Top right is shown the experimental data that make up the "ground-level" cross-sectional concentration profiles. The data

points at each downwind position have been joined using a cubic-spline interpolation scheme to aid interpretation. These lines do not represent HEGADAS predictions. In this case the measured profiles are gaussian in shape from 90 m downwind as expected of a neutral density release.

- Bottom right is shown a point-by-point comparison of the predicted and measured concentrations at both cross-wind and vertical locations for all downwind distances. This graph indicates how well the model replicates the plume cross-sectional profile. The graph was constructed by reading the x,y,z positions of the measuring points from the HTAG data file and modifying the y position to take account of the drift of the plume centre-line. The required HEGADAS concentration was then calculated. We have distinguished data comprising the cross-wind profiles from vertical profile measurements made at y=0. We note that the vertical profiles are generally not on the plume centre-line. The point-by-point comparison includes a solid line, indicating perfect agreement, and dashed lines indicating a factor two deviation from agreement. We also note that, because concentrations can change by an order of magnitude when moving small distances across the plume, small differences between predicted and measured plume shape appear as very large errors in predicted to measured concentration on this graph.

The figure caption also includes the geometric mean ratio of the predicted to measured concentration, both for the horizontal profiles and for the vertical profiles. More detailed statistics are given at the end of this section.

These three figures together give an overall impression of both the qualitative and quantitative agreement between the model and the data. The predicted plume width using the input σ_y correlation derived from the small-area releases is in good agreement with the data. The plume has a finite size at the source due to the gas blanket and this is in agreement with the data. Centre-line concentrations are overpredicted by a constant factor. The point-by-point comparison of the data shows that all points

lie within a factor of two of agreement with horizontal concentrations overpredicted by 34 % on average.

Figure 8.6 shows the corresponding results for run HT48 which was density ratio 1.4 and roughness R3. Predicted plume widths are much greater than measured which leads to very large differences in concentration at the cloud edges. The difference in plume widths is difficult to reconcile with the run conditions. A comparison with Figure 8.5 shows that the experimental data are very similar to those for the neutral density release of run HT47. The plume widths are virtually identical up to 160 m from the source and concentrations are also nearly the same. We would expect the dense gas plume to be significantly broadened by gravity spreading. In comparison the corresponding releases over R50 roughness, where gravity spreading should be less important due to more rapid mixing, do show significant changes in cloud shape as do the small area source experiments.

Figure 8.7 shows results for run HT49 which was density ratio 4.2 and roughness R3. The plume shape is quite well predicted by HEGADAS but the centre-line concentration at 320 m is seriously underpredicted. The measured concentration profile at 40 m is very irregular, thereafter the plume adopts a slab-like concentration profile. The point-wise comparison of data shows a majority of point within a factor of two of agreement but there is a large degree of scatter, mostly arising from the 320 m station. It is possible that, at this low roughness and for this size of plume, the boundary layer downwind of the source is laminarizing so that entrainment into the cloud is less than that assumed by HEGADAS.

Figure 8.8 shows results for run HT50 which was density ratio 1 and roughness R50. Overall agreement is quite good although the centre-line concentration is slightly over predicted. Most of the data were predicted to within a factor two.

Figure 8.9 shows results for run HT51, density ratio 1.4 and R50 roughness distribution. There are relatively few experimental data points above 0.01% concentration. Centre-line concentrations are underpredicted

by a factor of two but the change in concentration with distance is correctly predicted. The plume is markedly wider than that for the density ratio 1 release and the width is modelled correctly.

Figure 8.10 shows results for run HT52, density ratio 4.2 and R50 roughness distribution. The experimental data share the features of the corresponding experiment over the R3 roughness distribution. The plume reaches a half width of 50 m close to the source and thereafter changes very little. There appears to be very little entrainment into the gas cloud between 40 and 160 m from the source with the peak concentration hardly changing. The concentration starts to decrease after 160 m but the data are insufficient to establish a trend. HEGADAS correctly predicts the plume width and the transition point to slow spreading but centre-line concentrations are underpredicted at distances greater than 80 m. Most of the predictions lie within a factor two of the data.

A summary of the large area source results is given in Table 8.8. The table shows the geometric mean ratio of predicted to measured concentration and the number of data points used in the comparison. The mean ratio of predicted to measured concentration must be considered in relation to the scatter of the data. The uncertainty in estimating the mean is measured by the standard error which (to 95% confidence) is twice the standard deviation divided by the square root of the number of samples.

It is important to remember that the model comparison has been made using a single realization of each experiment. It is probable that different results would be found if the model were compared with the average of several repeats of each of the experiments.

We have no data to estimate the repeatability of the HTAG experiments but understand that point-wise repeatability of dense gas dispersion experiments is generally better than a factor two. Assume that, in repeats of the experiments, the measurements differ at each point by less than a factor of 2, such that:

$\log_{10} \left(\frac{\text{true concentration}}{\text{measured concentration}} \right)$ is normally distributed with standard

deviation $\log_{10}(\sqrt{2})$. Then for a single experiment, comprising say 23 data points, compared with average of many experiments, the mean ratio of "true" to measured concentration would be determined to within a factor of $2^{1/\sqrt{23}}$.

Thus, to give a measure of the significance of the spread of the data, we include in the table the standard error expected when comparing a single experiment with a perfect model.

The results are divided into horizontal "ground-level" concentrations, marked H, and vertical concentrations marked V.

RUN	CONDITIONS			MEAN RATIO	NO OF DATA	STD ERR EXP	STD ERR CALC
HT47	1.0	R3	H	1.34	23	1.17	1.16
HT48	1.4	R3	H	5.42	23	2.35	1.16
HT49	4.2	R3	H	0.66	22	1.38	1.16
HT50	1.0	R50	H	0.85	27	1.32	1.14
HT51	1.4	R50	H	0.72	11	1.27	1.23
HT52	4.2	R50	H	0.53	26	1.79	1.15
HT47	1.0	R3	V	0.89	18	1.15	1.18
HT48	1.4	R3	V	0.60	9	1.65	1.26
HT49	4.2	R3	V	0.3	5	4.14	2.23
HT50	1.0	R50	V	0.98	18	1.10	1.18
HT51	1.4	R50	V	0.58	19	1.26	1.17
HT52	4.2	R50	V	0.55	15	1.36	1.19

Table 8.8. Summary of Large Area Source results.

The results for run HT48 are clearly different from those for the other experiments. As run HT48 had the same cloud shape and concentrations as the neutral density run HT47, whereas the higher roughness runs HT51 and HT50 were clearly different, it is probable that HT48 used a release gas density ratio of 1 rather than the intended 1.4. This would bring the data into line with the predictions.

If we compare the standard errors for the horizontal profiles, H, we see that the data scatter is largest for the two density ratio 4.2 releases. In both cases we suspect that the gas cloud is significantly modifying the flow field and this factor is not taken into account by

HEGADAS. In both cases HEGADAS, on average, underpredicts concentrations by 34% for the R3 experiments and 47% for the R50 experiments. We note that this difference is substantially smaller than the factor 5 difference in measured concentrations between the two experiments.

For the the neutrally buoyant releases HEGADAS consistently overpredicts the R3 roughness data by about 34% using the measured input conditions. The R50 data is underpredicted by 15% although the standard error is quite large. The effect of the increase in roughness was to reduce measured concentrations by a factor of 3 and HEGADAS has described this effect well. The density ratio 1.4 release over R50 roughness is underpredicted by 28 %.

The vertical profile results are not expected to be particularly well modelled by HEGADAS but, nevertheless, it is of interest to compare the model results. We have to discard run HT48 because of doubts over the run conditions and run HT49 because there are insufficient data. We see that the neutral density releases are very well modelled by the assumed HEGADAS profile with the mean ratio of predicted to measured concentration being 89 % (R3) and 98 % (R50). In both cases the standard error is smaller than the repeatability estimate. This agreement is much better than would be expected since, in HEGADAS, the vertical profile depends on the ground level concentration and in both cases the ground level concentration (actually the concentration at 0.5 m height) is less well predicted than the vertical profiles. The dense gas results are limited to the R50 roughness and in both cases concentrations are underpredicted by a fraction consistent with the ground level results.

8.6.2 Small Area Sources

Figure 8.11 shows results for run HT138, density ratio 1 and R3 roughness distribution. The plume width has been fitted to these data as described in section 8.1.1. Centre-line concentrations are in very good agreement with the data and overall the pointwise comparison with the measurements is very good.

Figure 8.12 shows results for run HT139, density ratio 1.4 and R3 roughness. The effect of the increase in source gas density on cloud spreading is very marked in contrast with the large area source results for run HT48. This would seem to confirm that the latter data are suspect. The plume width is slightly under-predicted and centre-line concentrations over-predicted by a small amount. The point-wise comparison is good with most calculated concentrations being within a factor two of the measurements. The difference in cloud width causes predictions at the cloud edges to be smaller than the measurements.

Figure 8.13 shows results for run HT140, density ratio 3.9, R3 roughness. The plume width is correctly predicted as is the rate of decrease of concentration with distance from the source. The actual centre-line concentrations are slightly underpredicted. One of the measured concentrations at 160 m from the source is clearly wrong and shows up as an outlier in the point-wise comparison with data.

Figure 8.14 shows results for run HT141, density ratio 1, R50 roughness. The HEGADAS calculations are everywhere in good agreement with the data.

Figure 8.15 shows results for run HT142, density ratio 1.4, R50 roughness. The cloud width is smaller than that for the R3 roughness experiment, HT139, and is well predicted. Centre-line concentrations are very well predicted and the point-wise comparison with the data shows good overall agreement.

Figure 8.16 shows results for run HT143, density ratio 3.9, R50 roughness distribution. The experimental data are very irregular and do not conform to expected profiles. This appears in the point-wise comparison of the predictions with the data as horizontal bands where the HEGADAS cloud is flat-topped and the prediction is constant whereas the measured concentration varies by up to a factor of 4. Despite this additional scatter the overall performance of the model is good. The plume width and centre-line concentrations are well predicted.

The small area source experiments are summarized in Table 8.9. The horizontal profiles are better predicted than those for the large area sources. The standard error is generally small and comparable with repeatability estimate. The geometric mean ratio of predicted to measured is within 22% of agreement for all of the runs and there is no significant difference between the R3 and R50 experiments. For reference, increasing roughness from R3 to R50 decreased measured concentrations by a factor of 3 for density ratio 1, a factor 4 for density ratio 1.4 and a factor 6 for density ratio 3.9. The vertical concentration profiles were also substantially in agreement with data.

RUN	CONDITIONS			MEAN RATIO	NO OF DATA	STD ERR EXP	STD ERR CALC
HT138	1.0	R3	H	1.22	27	1.22	1.14
HT139	1.4	R3	H	0.78	39	1.16	1.12
HT140	3.9	R3	H	0.84	44	1.16	1.11
HT141	1.0	R50	H	1.00	23	1.13	1.16
HT142	1.4	R50	H	0.91	31	1.17	1.13
HT143	3.9	R50	H	1.03	42	1.22	1.11
HT138	1.0	R3	V	0.76	24	1.16	1.15
HT139	1.4	R3	V	1.06	13	1.41	1.21
HT140	3.9	R3	V	1.02	7	3.25	1.30
HT141	1.0	R50	V	1.11	27	1.10	1.14
HT142	1.4	R50	V	1.19	28	1.08	1.14
HT143	3.9	R50	V	1.02	21	1.21	1.16

Table 8.9. Summary of Small Area Results

8.6.3 Point Sources

The point source results are not expected to agree well with HEGADAS predictions because, by virtue of the release type, the entrainment into the cloud will be dominated by jet mixing which HEGADAS does not model.

The point source flow rates were significantly smaller than for the area sources and the influence of the source gas density on dispersion is relatively small. For neutrally buoyant releases the plumes over low

roughness were markedly narrower than those for area sources, Figure 8.2. Over high roughness the plume width was the same as for the area sources, perhaps indicating that jet momentum decayed faster at the higher ambient turbulence intensity. In the following comparisons the input σ_y parameters for the R3 experiments were determined by fitting a power law to the measured plume width for run HT86. The small area source σ_y was used for the R50 experiments.

Figure 8.17 shows results for run HT86, density ratio 1 and R3 roughness distribution. The experimental data show significant drift of the cloud and non-uniformity of concentrations at 240 m. The decrease in concentration with distance from the source is very rapid and, against expectation, is quite well predicted by HEGADAS.

Figure 8.18 shows results for run HT87, density ratio 1.4 and R3 roughness distribution. The experimental data are almost identical to the previous case and there is little evidence of gravity spreading. Model agreement with the data is however slightly better although the pointwise comparison shows more scatter due to irregularities in the measured profiles.

Figure 8.19 shows results for run HT88, density ratio 3.9 and R3 roughness distribution. Here there is some evidence of cloud broadening due to source gas density and the effect is well modelled by HEGADAS. Centre-line concentrations are very well predicted. Again the point-wise data comparison shows a lot of scatter due to the shape of the measured profiles.

Figure 8.20 shows results for run HT89, density ratio 1 and R50 roughness distribution. The plume width is greater than for the R3 experiments and the rate of decrease of centre-line concentration faster. Using the small area source correlation for σ_y , HEGADAS predictions are in excellent agreement with the measurements. The measured cross-wind profiles are not perfectly gaussian in shape and this leads to some scatter in the point-by-point data comparison.

Figure 8.21 shows results for run HT90, density ratio 1.4 and R50 roughness distribution. The measured concentrations are not very different from those of the neutrally buoyant release except very close to the source, possible due to the increase in exit momentum that accompanies the increase in source gas density. The HEGADAS predictions are essentially the same as for run HT89 and agreement with the data is consequently equally good.

Figure 8.22 shows results for run HT91, density ratio 3.9 and R50 roughness distribution. The increase in source gas density has less effect on the measurements than for the R3 experiment. The cloud width is the same but concentrations are slightly greater. HEGADAS calculations are in good agreement with the data at distances greater than 40 m from the source.

The point source results are summarized in Table 8.10.

RUN	CONDITIONS			MEAN RATIO	NO OF DATA	STD ERR EXP	STD ERR CALC
HT86	1.0	R3	H	1.09	25	1.20	1.15
HT87	1.4	R3	H	0.94	25	1.26	1.15
HT88	3.9	R3	H	0.97	34	1.26	1.13
HT89	1.0	R50	H	0.76	28	1.15	1.14
HT90	1.4	R50	H	0.67	25	1.23	1.15
HT91	3.9	R50	H	0.74	26	1.25	1.14
HT86	1.0	R3	V	0.95	10	1.15	1.25
HT87	1.4	R3	V	1.08	8	1.42	1.28
HT88	3.9	R3	V	0.83	4	1.28	1.41
HT89	1.0	R50	V	1.68	10	1.37	1.25
HT90	1.4	R50	V	1.64	9	1.76	1.26
HT91	3.9	R50	V	2.08	8	1.64	1.28

Table 8.10. Summary of Point Source Results.

The point source horizontal plane data are remarkably well predicted by HEGADAS considering that much of the plume entrainment must have taken place through jet entrainment. The scatter on the data is enhanced by including measurements made at 20 and 40 m in the point-wise data comparison, positions where source effects dominate the plume

profiles. For the R3 roughness the average prediction was in agreement with the data. There was virtually no difference between the density ratio 1.4 and neutrally buoyant releases. Concentrations for the density ratio 3.9 releases were a factor of two greater. Over R50 roughness concentrations were on average underpredicted by up to 33 %, the data comparison being strongly influenced by the near source results. The effect of changing roughness was to decrease measured concentrations by a factor of 3 for neutral density, a factor 5 for density ratio 1.4 and a factor 6 for density ratio 3.9.

No real conclusion can be drawn from the vertical concentration profile comparisons since the data are sparse and are mostly near to the source. The assumed HEGADAS profile does not describe the concentration profile across a horizontal jet.

8.7 Observations on other HTAG experiments

The HTAG database included stable flow simulations and dispersion across a tank farm. These data have been compared with HEGADAS predictions as part of this study but, for reasons of space, we restrict our description of this work to the major findings.

A major difficulty with the stable flow simulations was determining appropriate input data. As discussed in section 8.1.1 the thermal stratification achieved in the wind tunnel was somewhat greater than that found in the atmosphere and so the effect of stratification on vertical entrainment and on the wind profile was not well represented by the correlations implicit in HEGADAS. The surface roughness lengths for the stable flows were also rather less than those for neutral density, possibly because the roughness elements were planar rather than cubic and may have been less efficient turbulence generators. Lower wind speeds were also used in the experiments. These factors introduce concern as to whether the boundary-layer was properly rough. The comparison with HEGADAS predictions showed that, for all conditions, plume concentrations were underpredicted. This implies the entrainment rate in HEGADAS was too large for these conditions, as would be expected from the discussion above.

We note that the large area source, density ratio 4.2 clouds under neutrally stratified flow were also thought to cause flow laminarization. The vertical stratification in these cases due to the presence of the cloud would be greater than the thermal stratification in the stable flow experiments. This implies that very large and dense gas clouds could modify the wind speed profile and friction velocity. HEGADAS predictions are sensitive to the assumed stability class (chapter 10, section 10.2.2) and so this area should be investigated.

The tank farm dispersion experiments were of interest as an example of a situation problem in which the roughness element size first increased in the flow direction and then decreased. The data showed, on entry to the tank farm, evidence of gas channelling between the model tanks. For dense gas releases this opposed gravity spreading. Further inside the tank farm the flow could divide around tanks such that the plume width on exit was a strong function of wind direction. The changes in plume width were not necessarily accompanied by changes in concentration. These two features could not be adequately described using the breakpoint formulation in HEGADAS. It is not possible to make the plume width smaller to represent channelling neither is it possible to have clouds of two different widths with the same gas concentrations.

Although it was unfortunate not to be able to test the effect on dispersion of changing the roughness length in the wind direction against data, the data comparison shows that HEGADAS should not be used to calculate dispersion where significant blockage of the flow is likely to occur.

8.8 Summary and Conclusions

In this work:

HEGADAS predictions have been compared with a set of boundary layer wind tunnel experiments of dense gas dispersion carried out by CPP Inc. on behalf of the API. These experiments simulate full scale atmospheric boundary layers with a surface roughness length between

0.015 and 0.525 m using regular arrays of cubic obstacles of full scale side length of 1.3 and 5 m.

The wind-tunnel modelling criteria have been briefly reviewed. Over low roughness the modelled boundary layer was only partially rough thus the detailed flow near the wall may differ from full-scale. The lateral spread of neutrally buoyant plumes was smaller than would be expected in full scale experiments.

The HEGADAS calculations were carried out as a practical exercise to test whether dispersion in these high roughness boundary layers could be predicted by varying the surface roughness length in the model. It must be emphasised that the assumptions in HEGADAS apply only to boundary layers where the roughness element size is small compared with the depth of the dense gas cloud. These conditions were not met by the HTAG experiments.

We found, taking the small-area releases as representative of practice, that:

HEGADAS predictions were in good overall agreement with the HTAG data for neutrally buoyant releases. The average ratio of predicted to measured concentration was within 25% for both roughness boundary layers. The measured concentrations were a factor 3 different in the two boundary layers.

For dense gas releases, the gravity driven plume spread underwent a transition close to the source. This behaviour was consistent with laboratory studies of gravity current collapse. A model for this process was formulated and a criterion for transition developed and incorporated into HEGADAS.

With the revised gravity spread formulation HEGADAS correctly predicted the dispersion of density ratio 1.4 and 3.9 releases into the two boundary layers to within, on average, 25 %. The measured

concentrations differed by a factor 4 for density ratio 1.4 and a factor 7 for density ratio 3.9 between the two boundary layers.

With the revised gravity spread formulation HEGADAS correctly predicted the distance to LFL for MAPLIN SANDS spill 54, a high Richardson number release, poorly predicted by earlier versions of HEGADAS.

We conclude that:

- 1) With the changes made to HEGADAS, dispersion calculations can be carried out using a roughness length up to 0.5 m
- 2) The model should not be used in circumstances where the flow is likely to become strongly blocked, i.e. where obstructions are large enough to affect the trajectory of the cloud.

APPENDIX 8.A DEVELOPMENT OF THE GRAVITY SPREADING MODEL

In this section we give a brief overview of the stages passed through in the development of the new gravity spreading model incorporated into HEGADAS-5. The model, as implemented in HEGADAS-5, is described in Chapter 7, section 7.3.2.

The basis of our approach has been the proposal, due to Linden and Simpson (1986, 1988), that the spreading of a dense gas cloud under the action of gravity can proceed at one of two rates, dependent upon the structure of the interface between the dense gas and the fluid into which the cloud is spreading. The preferred mode of spread is that of a gravity current with the front velocity given by:

$$U/u_* = C_E (g'H)^{0.5}/u_* = C_E Ri^{0.5} \quad (A.1)$$

This rate has typically been determined by lock-exchange experiments in which the gravity current spreads into fluid at rest or by counter-flow experiments in which the gravity current is opposed by a steady flow Simpson and Britter (1979). In such experiments the gravity current can be maintained by extremely small density differences and there is a step change in density across the interface between the dense and external fluids.

In the lock-exchange experiments of Linden and Simpson (1986, 1988) the working fluids were made turbulent by injecting air bubbles through the bottom of the test tank. This turbulence resembles the action of top entrainment in a convecting dense gas cloud. The experiment showed that the turbulence destroyed the gravity current interface between the dense and ambient fluids. The fluids were then separated by a diffuse region which maintained its structure as it propagated into the ambient fluid at a much lower velocity (a factor of approximately 1/8) than the corresponding gravity current. When the stirring was stopped the gravity current reformed.

Linden and Simpson proposed that, after transition, the rate of advance of the dense fluid was determined by a balance between turbulent dissipation and the (assumed linear) pressure gradient across the zone. For a steady boundary layer flow this can be written:

$$\frac{d}{dz} K \frac{du}{dz} = - \frac{g'(H-z)}{L} \quad (\text{A.2})$$

where H is the depth of the dense gas layer, L the lateral extent of the diffuse zone and K is the turbulent diffusivity. In their experiments L was equal to the displacement of the edge of the dense fluid from its starting position.

Linden and Simpson solved equation (A.2) and averaged the velocity over the channel depth to get an expression for the spreading velocity after transition. To predict the transition position in their experiments, which corresponded to the dense fluid travelling the distance, L , they proposed that the transition point occurred when the ratio of the two spreading velocities was constant and equal to one. Their analysis gave qualitatively correct results but they found the constant was about 2.6.

We proposed that something similar happens in the lateral spreading of a convecting dense gas cloud. To describe conditions after transition we derived the solution to equation (2) using the eddy diffusivity K appropriate to the neutrally stratified external flow:

$$K = k u_* z$$

This gave equation (A.3) as an expression for the spreading velocity averaged over the cloud depth, H :

$$u = \frac{1}{3} \frac{g' H^2}{k L u_*} \quad (\text{A.3})$$

We needed to identify the length-scales H and L . The cloud height corresponds naturally to the HEGADAS parameter H_{eff} . The

length-scale L is the thickness the diffuse edge of the dense fluid, post collapse, and so we identified this with σ_y by analogy with the development of the edges of the HEGADAS cloud profile. To complete the model we assumed a smooth transition from gravity current to diffuse cloud spreading by choosing the mechanism that gave the lowest spreading velocity when evaluated from local conditions. This was equivalent to taking the ratio of the two velocities to be constant and equal to one.

This model greatly improved agreement between HEGADAS predictions and the HTAG results, however, transition to diffuse spreading took place too early and cloud widths were underpredicted. We found that we could optimise agreement by varying the ratio of the velocities at transition but the overall results were unsatisfactory.

We reconsidered our approach and identified three areas in which the analysis could be improved.

Firstly, we had neglected the effect of density stratification inside the cloud on momentum transfer. It is more realistic to assume that an internally driven flow will be so affected. The eddy diffusivity will reduce as stratification, parameterised by the bulk Richardson number Ri_* , increases and turbulence is damped. The exact dependence of K on Ri_* is however uncertain.

Secondly, the choice of σ_y for the characteristic length-scale, L , in equation (A.3) was inappropriate. After transition this length-scale would more properly be of order of the half-width of the cloud.

Finally, we needed to examine critically the criterion used to change between the two modes of cloud spreading.

To take account of the effect of stratification on the turbulent diffusivity within the cloud we assumed the same Richardson number dependence used in HEGADAS for mass diffusion so that:

$$K = k u_* z / (1 + .8 Ri_*)^{0.5} \quad (A.4)$$

and the solution to equation (A.2) becomes:

$$\frac{u}{u_*} = \frac{1}{3k} R_i (1 + 0.8 Ri_*)^{\frac{1}{2}} \frac{H}{L} \quad (A.5)$$

We further assumed that the ratio of the length-scales H/L is proportional to the HEGADAS length-scale ratio H_{eff}/B_{eff} with a proportionality constant $1/C_D$.

We then re-evaluated the ratio of the spreading velocities, A_t , calculated using equations (A.1) and (A.5) to see whether the assumption that this was constant was better met than before. The results are shown in Table A.1 where:

$$A_t = \frac{B_{eff} / H_{eff}}{(R_i (1 + 0.8 Ri_*))^{\frac{1}{2}}} \quad (A.6)$$

RUN No	Est. Trans'n Point m	H_{eff} m	B_{eff} m	Ri_* -	Ri -	A_t -	B_{eff}/H_{eff}
HT139	70	1.09	29.1	3.69	3.55	7.12	27
HT140	80	0.68	49.9	13.80	10.88	6.46	74
HT142	50	3.45	28.0	0.77	0.76	7.32	8
HT143	35	1.48	44.4	5.30	4.39	6.25	30
HT48	----- RUN NOT USED -----						
HT49	130	0.81	93.6	23.80	17.49	6.18	116
HT51	60	3.54	38.7	1.50	1.46	6.09	11
HT52	60	1.87	80.1	8.01	6.42	6.21	43

Table A.1 Ratio of spreading velocities, A_t , at the estimated transition point.

Results for Run HT48 were not used because of uncertainties in the data, section 8.6.1. We see that the ratio A_t is indeed remarkably constant given the variation in both Richardson number and the ratio of the cloud width to height. Thus the assumption that A_t is constant appears to be a good criterion for transition. The average value of A_t is 6.5 and this value has been used in HEGADAS.

The rate of spreading after transition is dependent upon the value chosen for the proportionality constant C_D . Figure 8.A.1. shows the effect of changing C_D on plume width and centre-line concentration for run HT140. For reference purposes the value $C_D=0$ corresponds to the gravity current formulation of HEGADAS-4. The value $C_D=1$ is equivalent to assuming that the ratio of the length-scales in the diffuse cloud equation (A.6) is equal to the ratio of H_{eff} to B_{eff} . The calculations are relatively insensitive to C_D values greater than 1. A value of 5 gave the best overall fit to the HTAG data and is recommended as a default value in HEGADAS-5.

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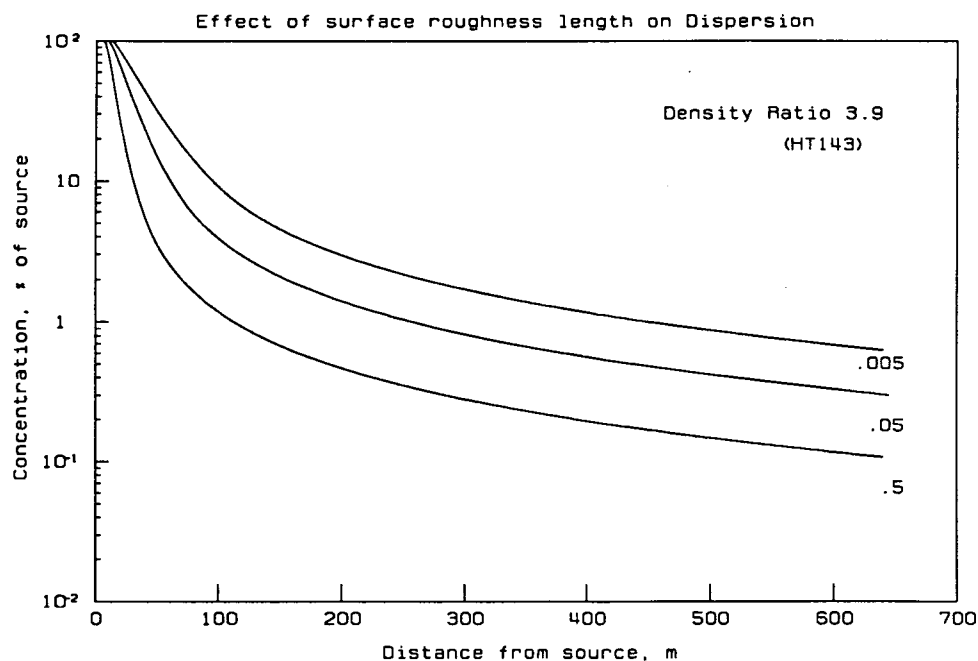


FIGURE 8.1 Effect of changing surface roughness length on dispersion

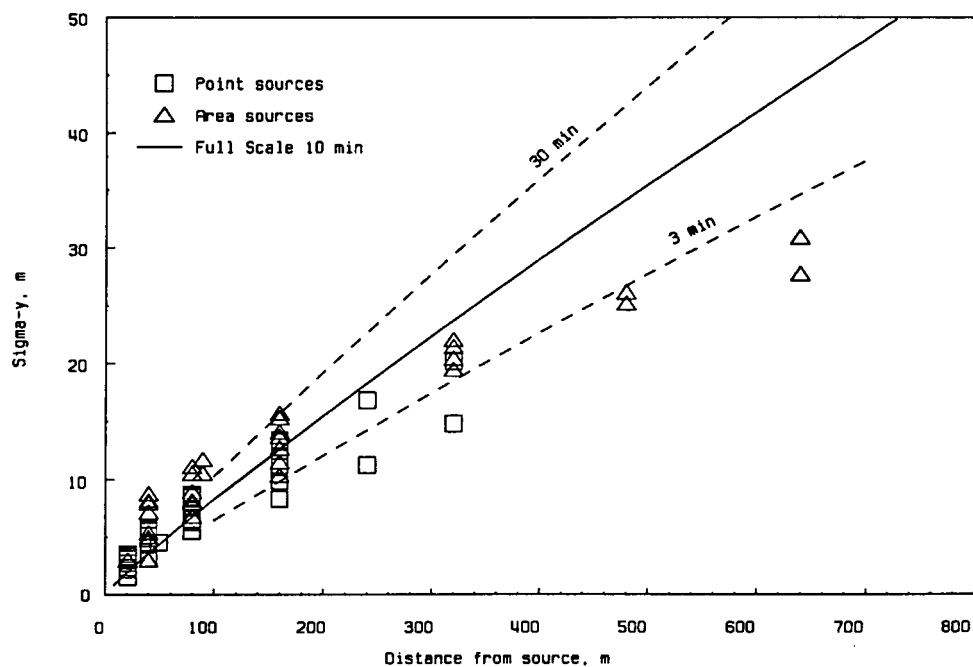


FIGURE 8.2

Comparison between wind tunnel measurements of sigma-y (neutrally buoyant releases) and the Pasquill-Gifford D-Stability curve as represented in HEGADAS for different averaging times.

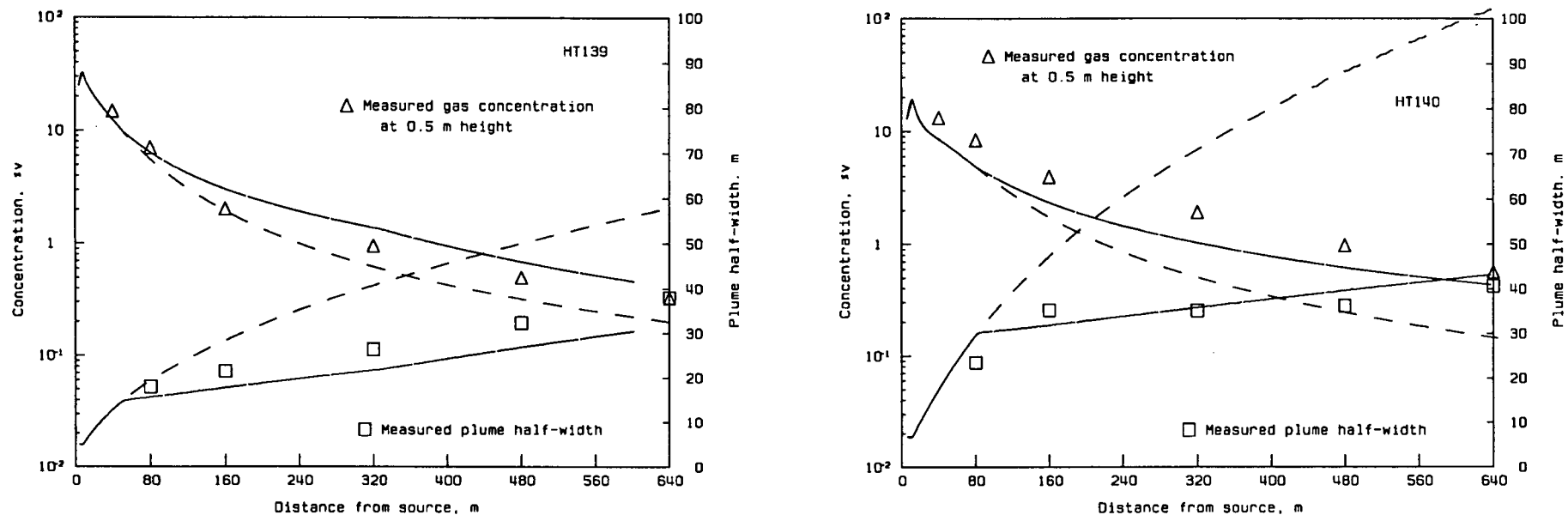


FIGURE 8.3

Effect of changing the gravity spreading formulation in HEGADASS to describe the plume spread observed in the course of the HTAG dispersion experiments. The dashed lines show the plume widths and centerline concentrations predicted by the original HEGADAS model. The HTAG data (squares) show a sharp reduction in the plume spread at about 80 m. The solid lines show the revised HEGADAS model predictions that take this into account.

Above left density ratio 1.4 and above right density ratio 3.9.

Results are for the R3 roughness distribution.

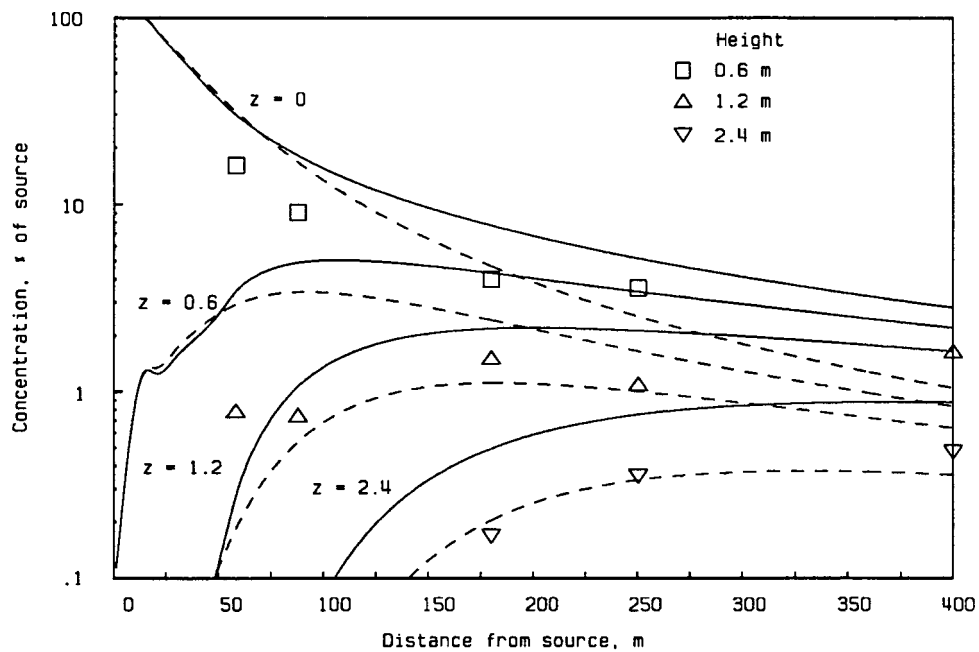
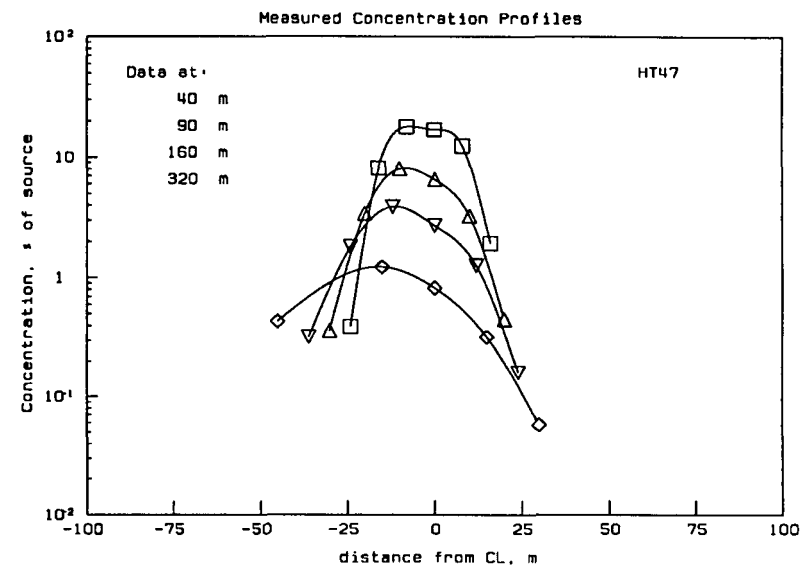
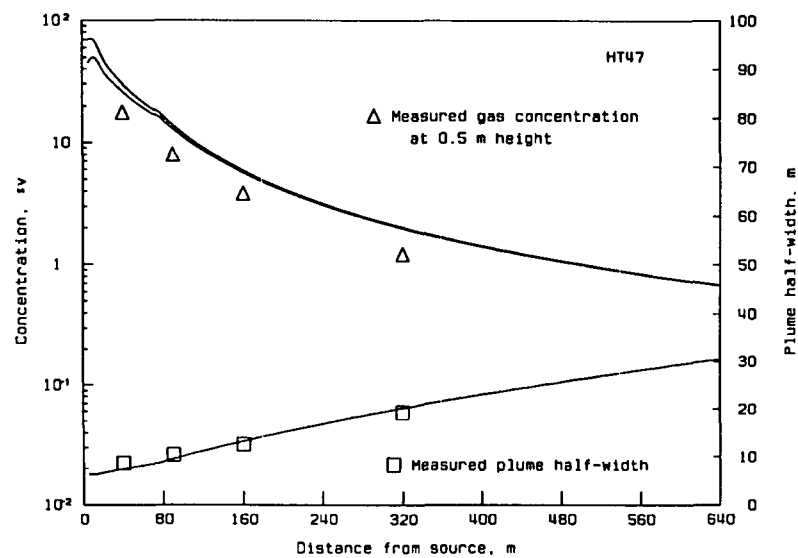


FIGURE 8.4

Comparison between the revised HEGADAS model (solid lines) and data from Maplin sands spill 54 (LPG). The dashed lines denote previous HEGADAS (1982) calculations for this experiment. The measured concentrations at 2.4 m height are probably low because of intermittency.



8. SOURCE TYPE : LARGE AREA
 DENSITY RATIO : 1
 ROUGHNESS : R3

ABOVE : COMPARISON BETWEEN HEGADAS CALCULATED AND MEASURED PLUME CENTERLINE CONCENTRATIONS AND PLUME HALF-WIDTH. PREDICTED CONCENTRATIONS ARE AT $z=0$ AND $z=0.5$ M, DATA ARE AT $z=0.5$ M.

TOP RIGHT : MEASURED CROSSWIND PROFILES AT DIFFERENT DOWNWIND LOCATIONS. LINES ARE SPLINE FIT TO AID INTERPRETATION.

BOTTOM RIGHT : POINT-BY-POINT COMPARISON OF CALCULATED AND MEASURED CONCENTRATIONS. DASHED LINES SHOW FACTOR TWO DEVIATION FROM AGREEMENT.

MEAN RATIO OF PREDICTION TO DATA:

HORIZONTAL: 1.34
 VERTICAL : 0.89

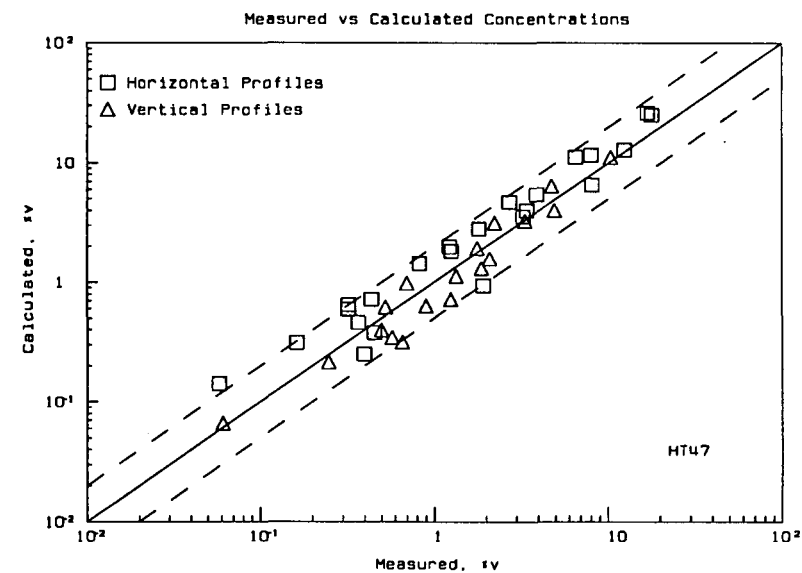
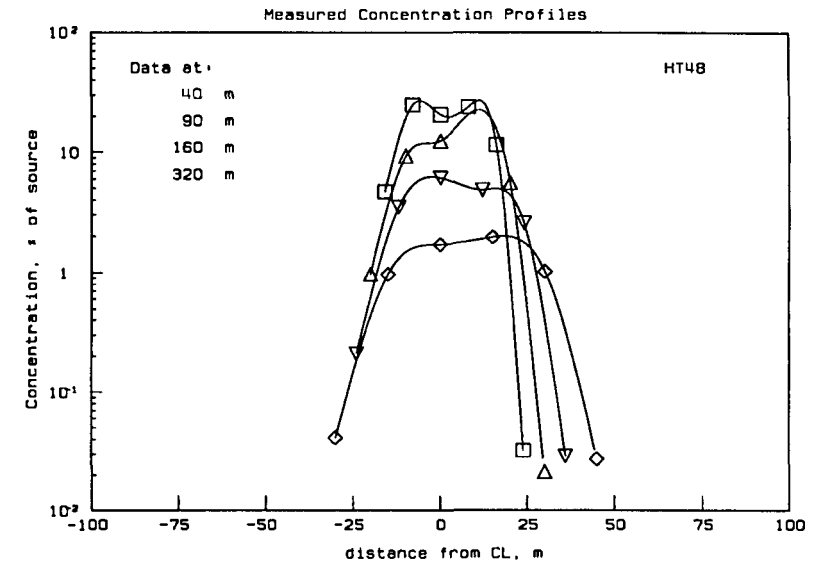
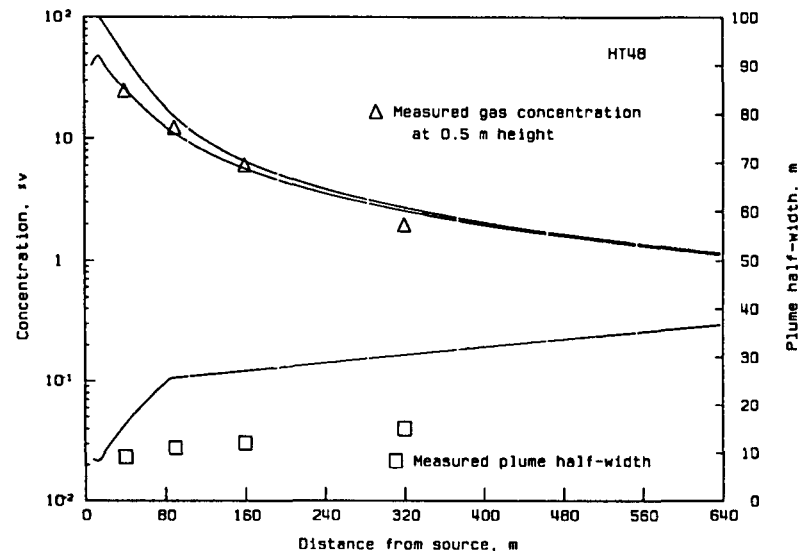


FIGURE 8.5 **RUN HT47**



SOURCE TYPE : LARGE AREA
DENSITY RATIO : 1.4
ROUGHNESS : R3

ABOVE : COMPARISON BETWEEN HEGADAS CALCULATED AND MEASURED PLUME CENTERLINE CONCENTRATIONS AND PLUME HALF-WIDTH. PREDICTED CONCENTRATIONS ARE AT $Z=0$ AND $Z=0.5$ M, DATA ARE AT $Z=0.5$ M.

TOP RIGHT : MEASURED CROSSWIND PROFILES AT DIFFERENT DOWNWIND LOCATIONS. LINES ARE SPLINE FIT TO AID INTERPRETATION.

BOTTOM RIGHT : POINT-BY-POINT COMPARISON OF CALCULATED AND MEASURED CONCENTRATIONS. DASHED LINES SHOW FACTOR TWO DEVIATION FROM AGREEMENT.

MEAN RATIO OF PREDICTION TO DATA:

HORIZONTAL: 5.42
VERTICAL : 0.60

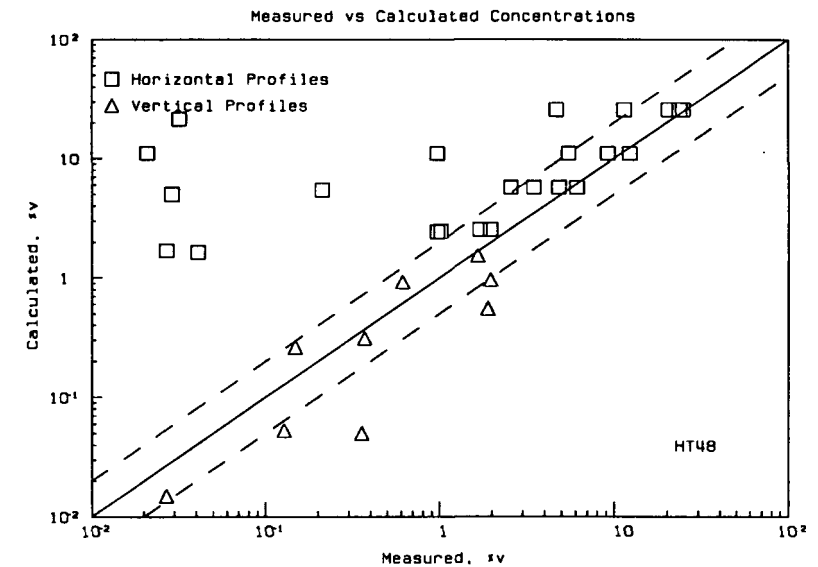
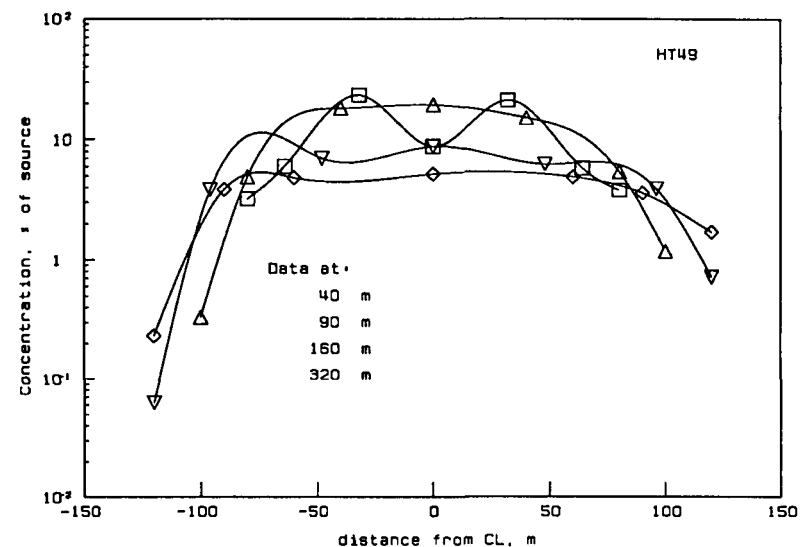
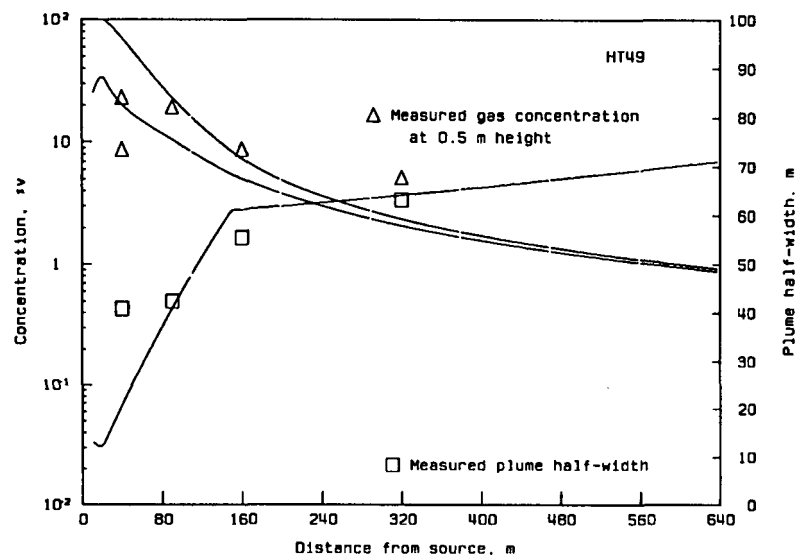


FIGURE 8.6 RUN HT48



SOURCE TYPE : LARGE AREA
 DENSITY RATIO : 4.2
 ROUGHNESS : R3

ABOVE : COMPARISON BETWEEN HEGADAS CALCULATED AND MEASURED PLUME CENTERLINE CONCENTRATIONS AND PLUME HALF-WIDTH. PREDICTED CONCENTRATIONS ARE AT $z=0$ AND $z=0.5$ M, DATA ARE AT $z=0.5$ M.

TOP RIGHT : MEASURED CROSSWIND PROFILES AT DIFFERENT DOWNWIND LOCATIONS. LINES ARE SPLINE FIT TO AID INTERPRETATION.

BOTTOM RIGHT : POINT-BY-POINT COMPARISON OF CALCULATED AND MEASURED CONCENTRATIONS. DASHED LINES SHOW FACTOR TWO DEVIATION FROM AGREEMENT.

MEAN RATIO OF PREDICTION TO DATA:
 HORIZONTAL: 0.66
 VERTICAL : 0.30

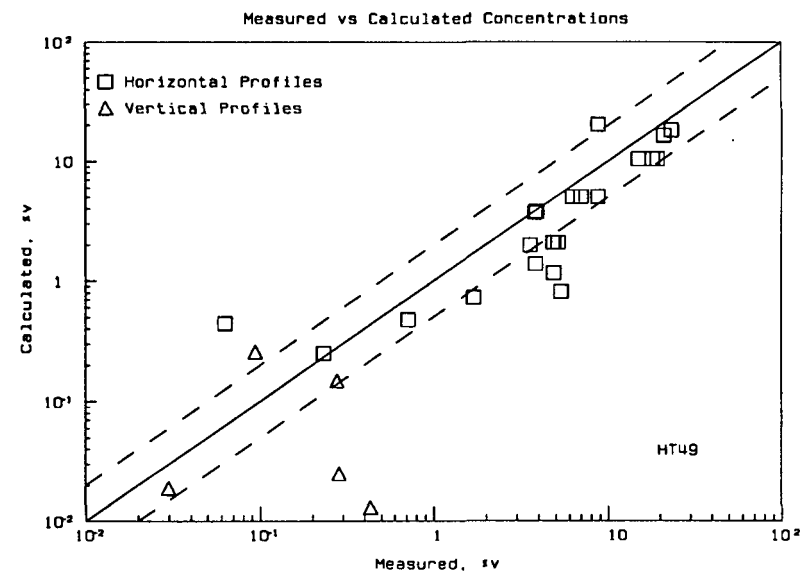
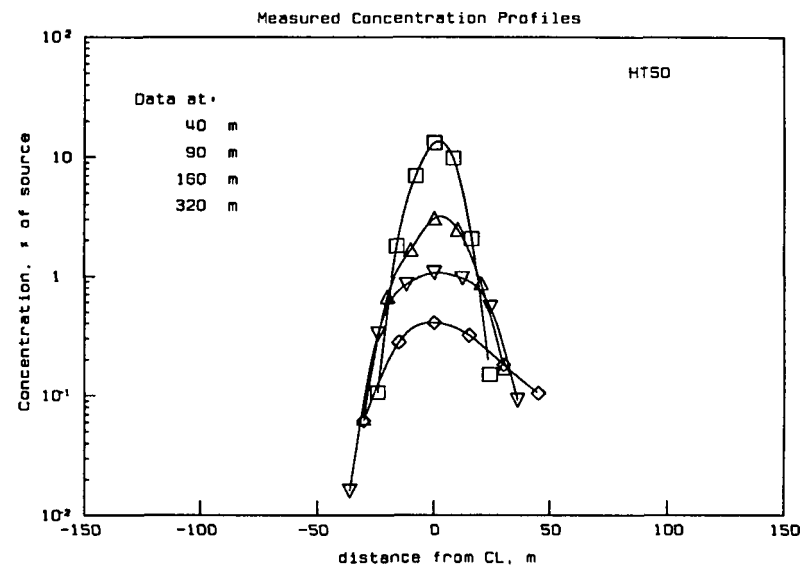
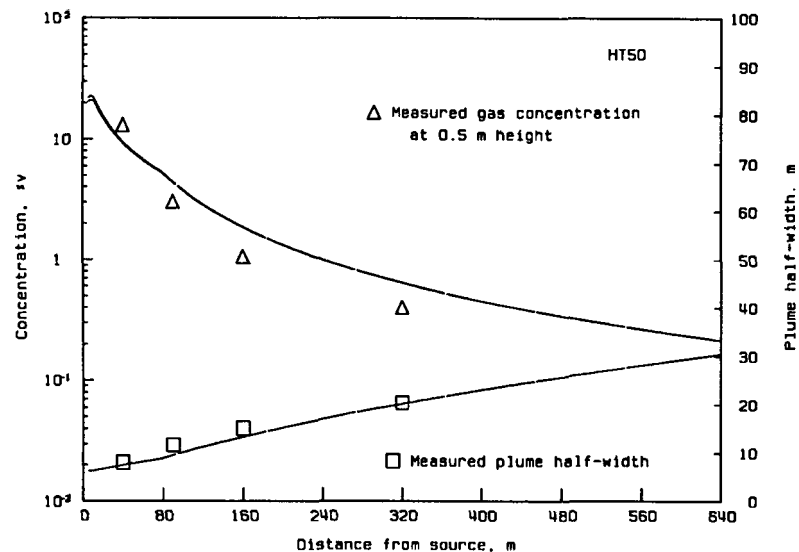


FIGURE 8.7 **RUN HT49**



SOURCE TYPE : LARGE AREA
 DENSITY RATIO : 1
 ROUGHNESS : R50

ABOVE : COMPARISON BETWEEN HEGADAS CALCULATED AND MEASURED PLUME CENTERLINE CONCENTRATIONS AND PLUME HALF-WIDTH. PREDICTED CONCENTRATIONS ARE AT $Z=0$ AND $Z=0.5$ M, DATA ARE AT $Z=0.5$ M.

TOP RIGHT : MEASURED CROSSWIND PROFILES AT DIFFERENT DOWNWIND LOCATIONS. LINES ARE SPLINE FIT TO AID INTERPRETATION.

BOTTOM RIGHT : POINT-BY-POINT COMPARISON OF CALCULATED AND MEASURED CONCENTRATIONS. DASHED LINES SHOW FACTOR TWO DEVIATION FROM AGREEMENT.

MEAN RATIO OF PREDICTION TO DATA:
 HORIZONTAL: 0.85
 VERTICAL : 0.98

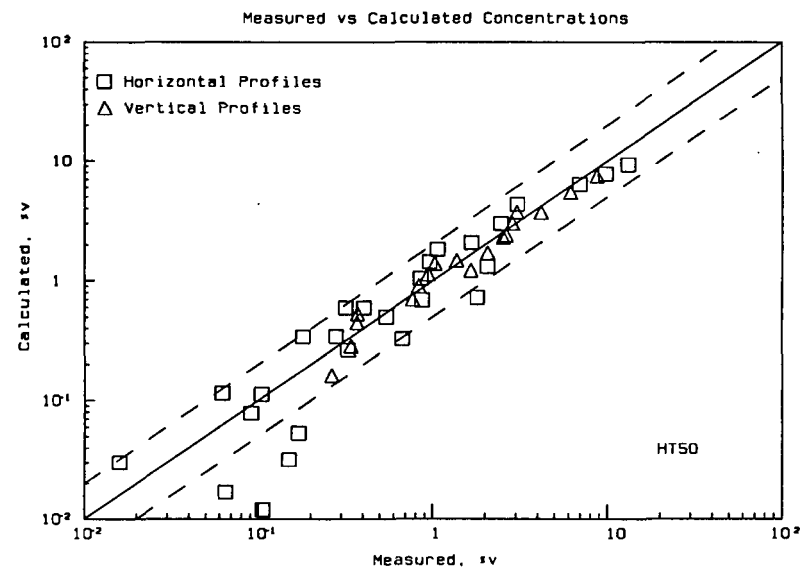
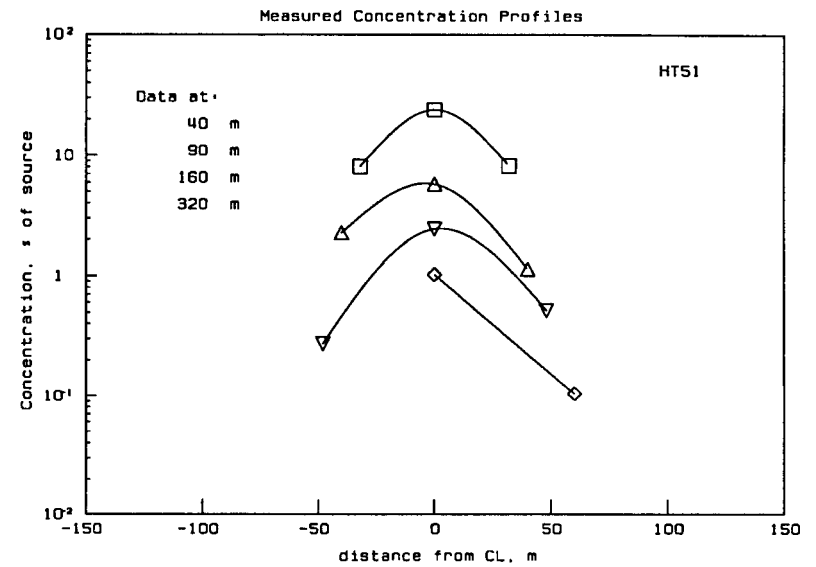
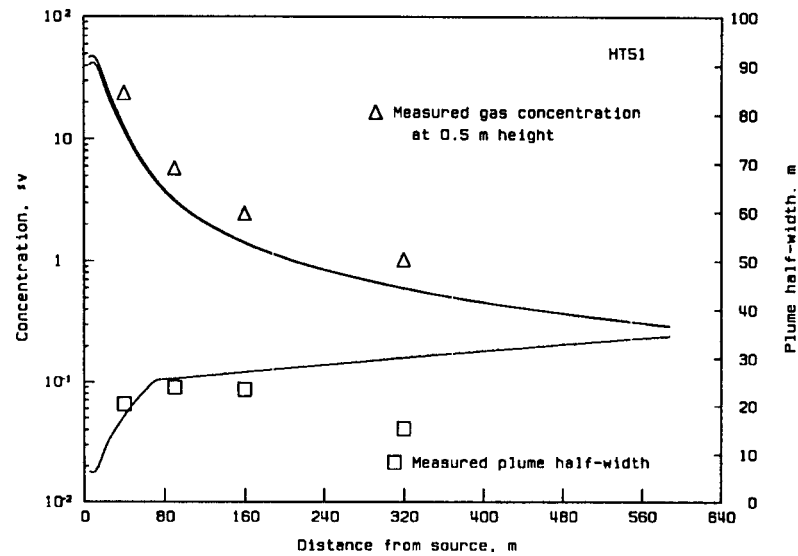


FIGURE 8.8 RUN HT50



SOURCE TYPE : LARGE AREA
DENSITY RATIO : 1.4
ROUGHNESS : R50

ABOVE : COMPARISON BETWEEN HEGADAS CALCULATED AND MEASURED PLUME CENTERLINE CONCENTRATIONS AND PLUME HALF-WIDTH. PREDICTED CONCENTRATIONS ARE AT $Z=0$ AND $Z=0.5$ M, DATA ARE AT $Z=0.5$ M.

TOP RIGHT : MEASURED CROSSWIND PROFILES AT DIFFERENT DOWNWIND LOCATIONS. LINES ARE SPLINE FIT TO AID INTERPRETATION.

BOTTOM RIGHT : POINT-BY-POINT COMPARISON OF CALCULATED AND MEASURED CONCENTRATIONS. DASHED LINES SHOW FACTOR TWO DEVIATION FROM AGREEMENT.

MEAN RATIO OF PREDICTION TO DATA:
HORIZONTAL: 0.72
VERTICAL : 0.58

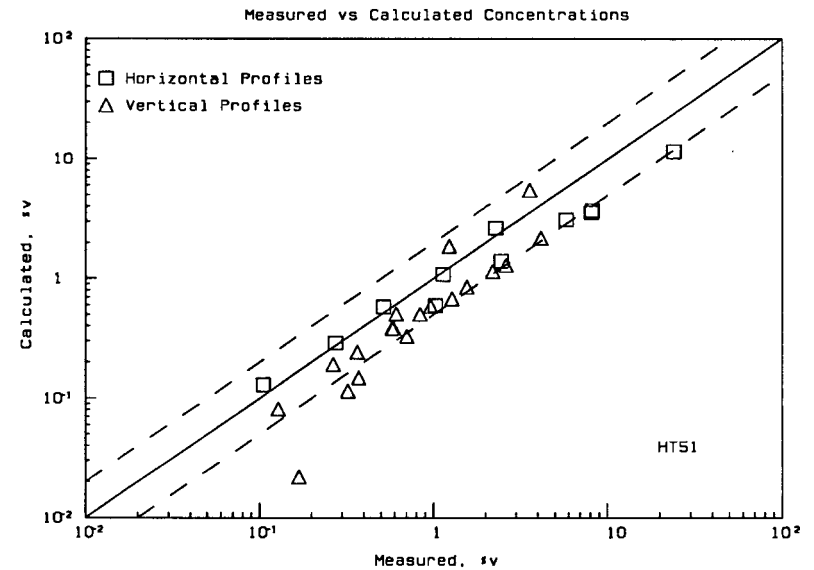
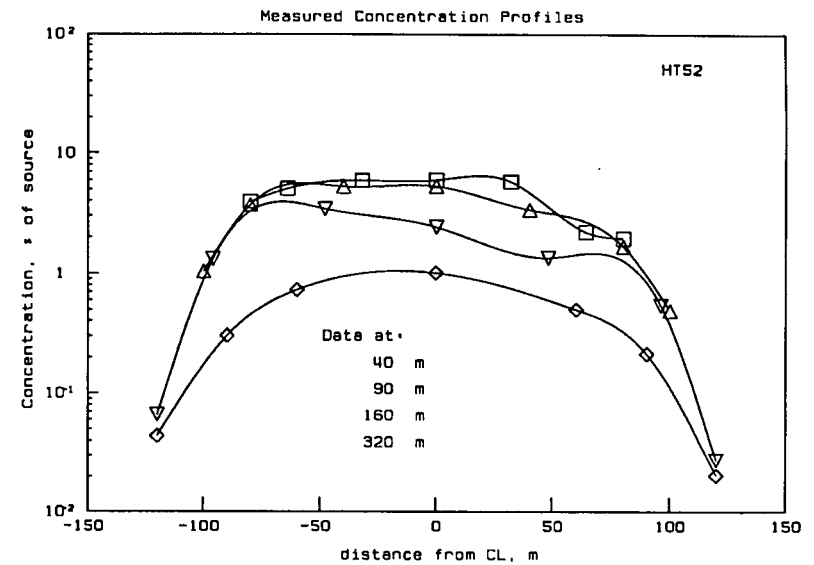
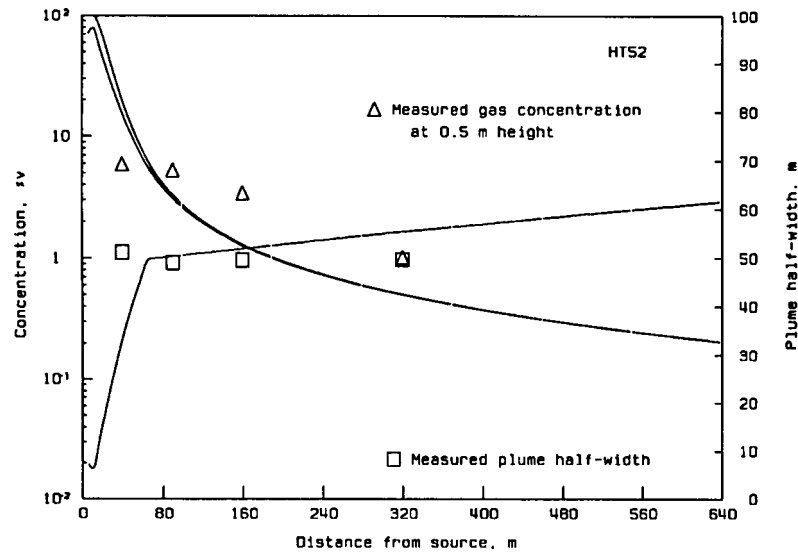


FIGURE 8.9 RUN HT51



SOURCE TYPE : LARGE AREA
DENSITY RATIO : 4.2
ROUGHNESS : R50

ABOVE : COMPARISON BETWEEN HEGADAS CALCULATED AND MEASURED PLUME CENTERLINE CONCENTRATIONS AND PLUME HALF-WIDTH. PREDICTED CONCENTRATIONS ARE AT $z=0$ AND $z=0.5$ M, DATA ARE AT $z=0.5$ M.

TOP RIGHT : MEASURED CROSSWIND PROFILES AT DIFFERENT DOWNWIND LOCATIONS. LINES ARE SPLINE FIT TO AID INTERPRETATION.

BOTTOM RIGHT : POINT-BY-POINT COMPARISON OF CALCULATED AND MEASURED CONCENTRATIONS. DASHED LINES SHOW FACTOR TWO DEVIATION FROM AGREEMENT.

MEAN RATIO OF PREDICTION TO DATA:

HORIZONTAL: 0.53
VERTICAL : 0.55

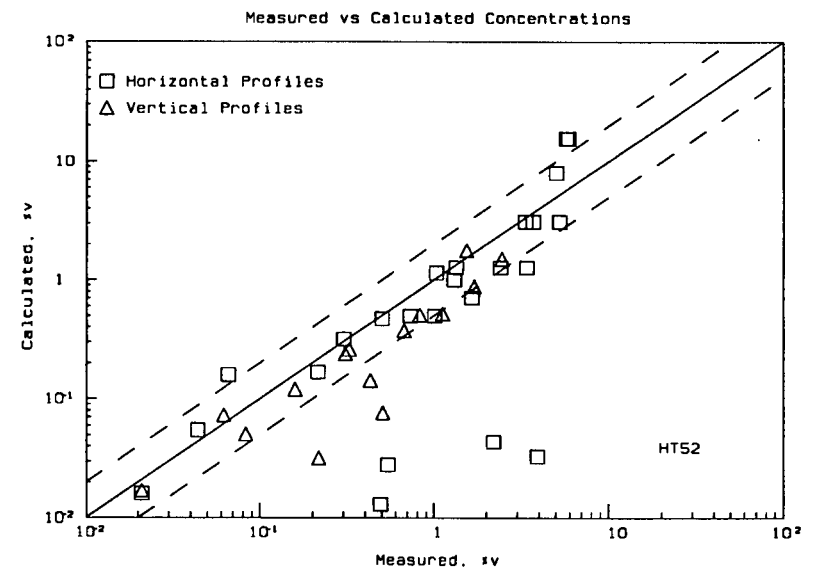
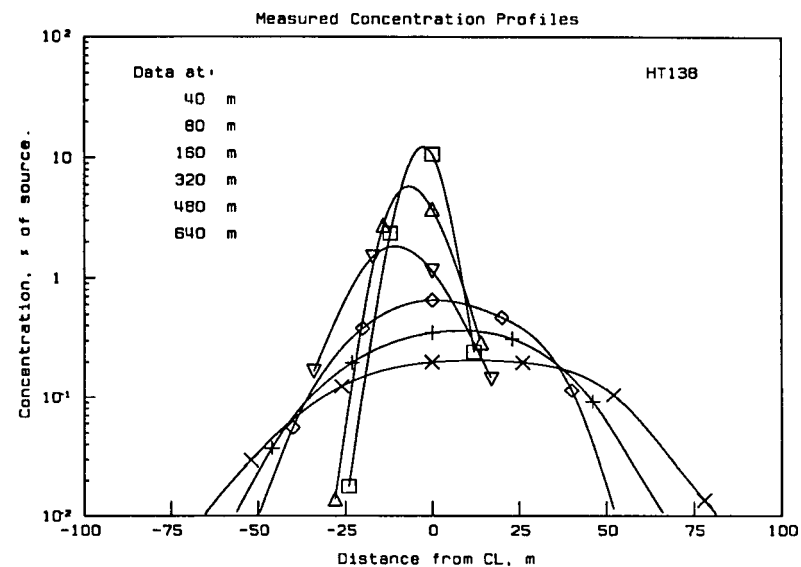
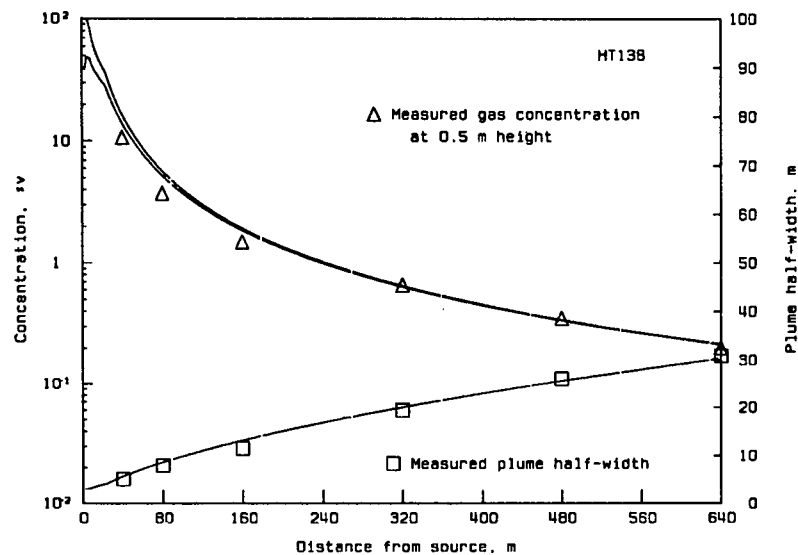


FIGURE 8.10 RUN HT52



SOURCE TYPE : SMALL AREA
 DENSITY RATIO : 1
 ROUGHNESS : R3

ABOVE : COMPARISON BETWEEN HEGADAS CALCULATED AND MEASURED PLUME CENTERLINE CONCENTRATIONS AND PLUME HALF-WIDTH. PREDICTED CONCENTRATIONS ARE AT $Z=0$ AND $Z=0.5$ M, DATA ARE AT $Z=0.5$ M.

TOP RIGHT : MEASURED CROSSWIND PROFILES AT DIFFERENT DOWNWIND LOCATIONS. LINES ARE SPLINE FIT TO AID INTERPRETATION.

BOTTOM RIGHT : POINT-BY-POINT COMPARISON OF CALCULATED AND MEASURED CONCENTRATIONS. DASHED LINES SHOW FACTOR TWO DEVIATION FROM AGREEMENT.

MEAN RATIO OF PREDICTION TO DATA:
 HORIZONTAL: 1.22
 VERTICAL : 0.76

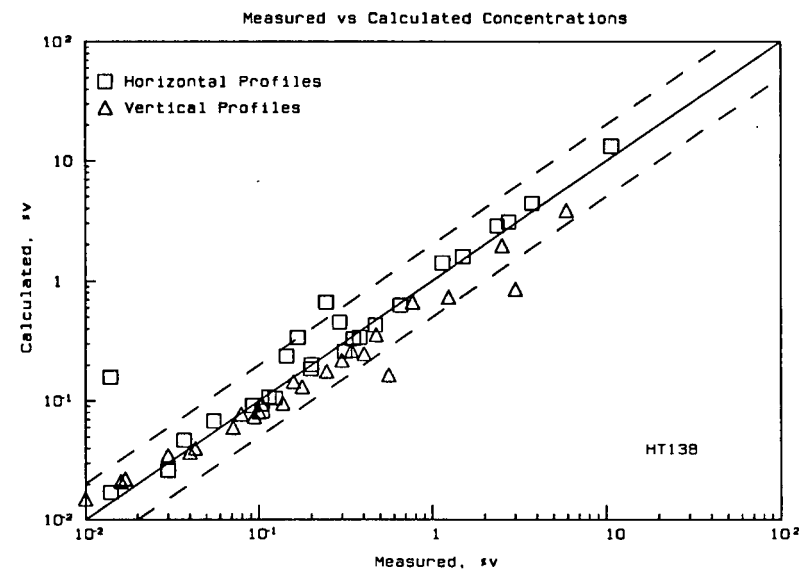
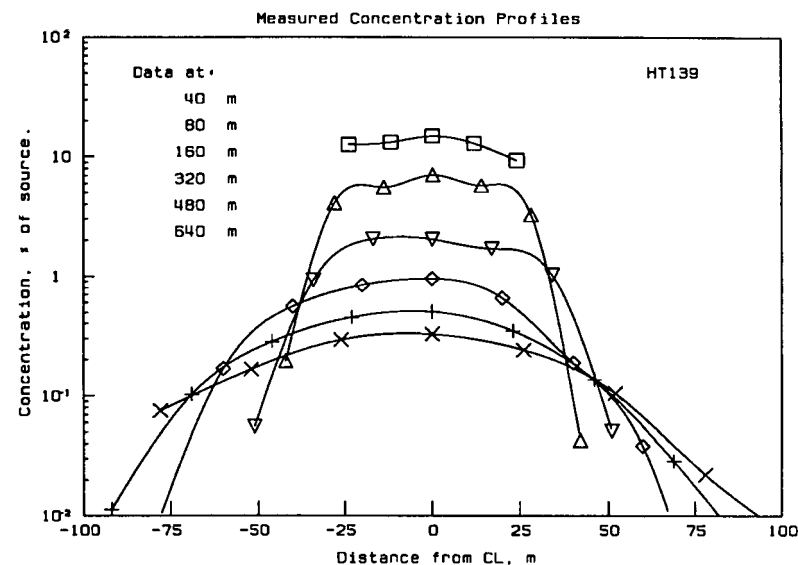
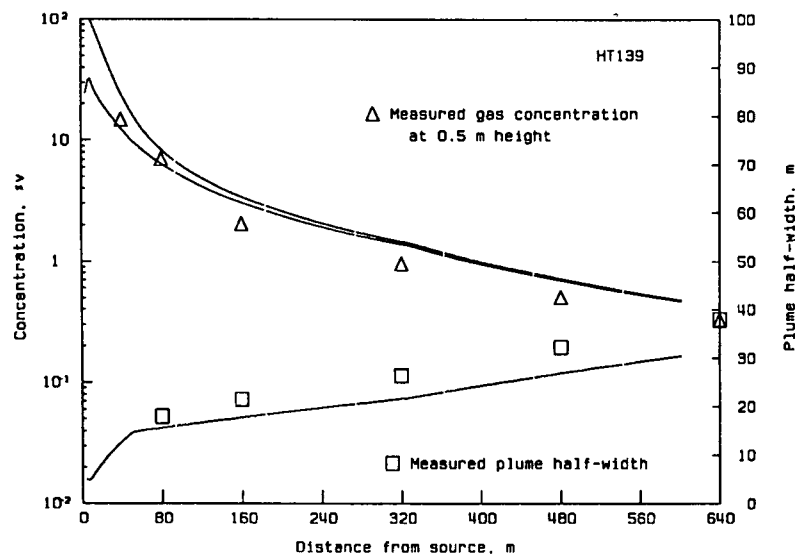


FIGURE 8.11 **RUN HT138**



SOURCE TYPE : SMALL AREA
 DENSITY RATIO : 1.4
 ROUGHNESS : R3

ABOVE : COMPARISON BETWEEN HEGADAS CALCULATED AND MEASURED PLUME CENTERLINE CONCENTRATIONS AND PLUME HALF-WIDTH. PREDICTED CONCENTRATIONS ARE AT $Z=0$ AND $Z=0.5$ M, DATA ARE AT $Z=0.5$ M.

TOP RIGHT : MEASURED CROSSWIND PROFILES AT DIFFERENT DOWNWIND LOCATIONS. LINES ARE SPLINE FIT TO AID INTERPRETATION.

BOTTOM RIGHT : POINT-BY-POINT COMPARISON OF CALCULATED AND MEASURED CONCENTRATIONS. DASHED LINES SHOW FACTOR TWO DEVIATION FROM AGREEMENT.

MEAN RATIO OF PREDICTION TO DATA:
 HORIZONTAL: 0.78
 VERTICAL : 1.06

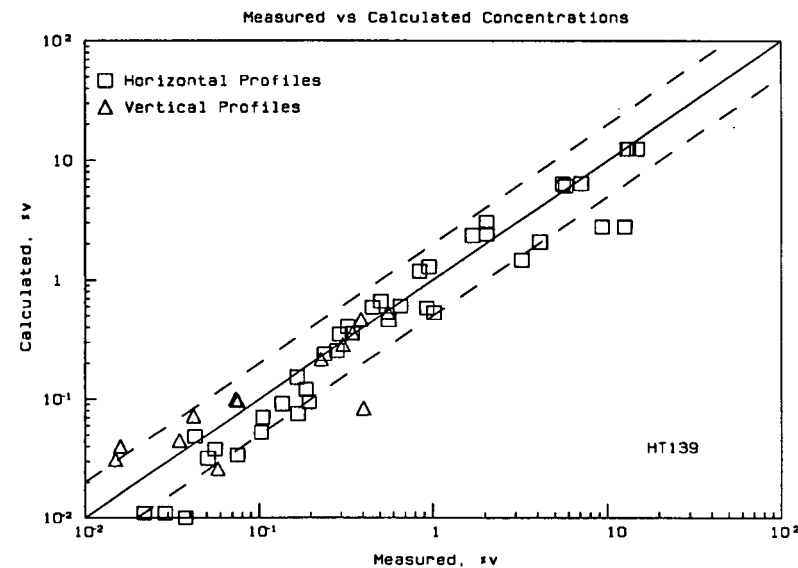
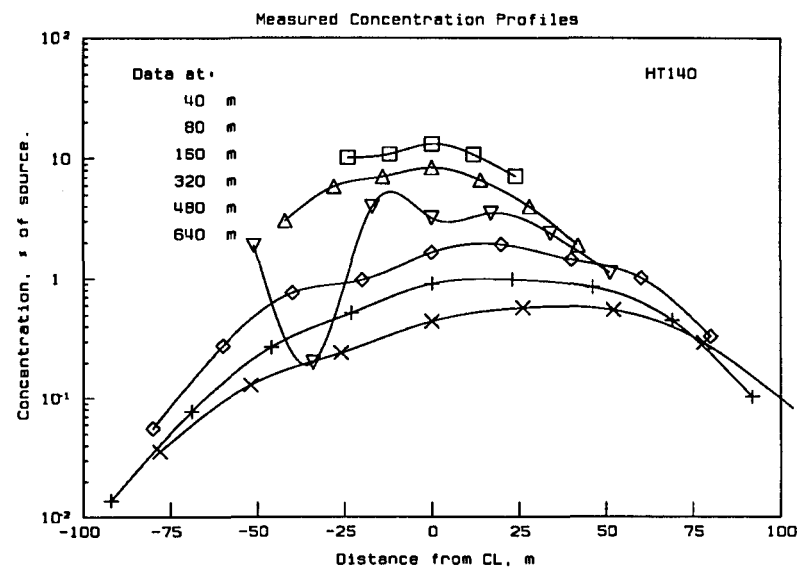
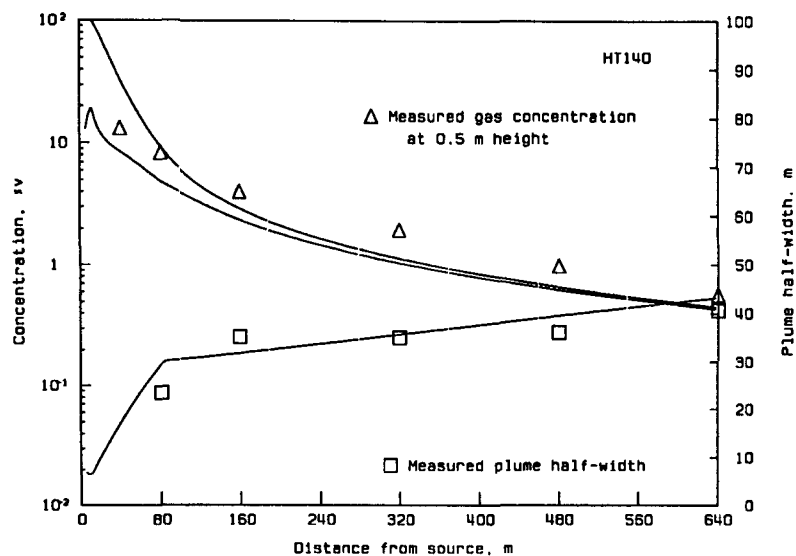


FIGURE 8.12 RUN HT139



SOURCE TYPE : SMALL AREA
 DENSITY RATIO : 3.9
 ROUGHNESS : R3

ABOVE : COMPARISON BETWEEN HEGADAS CALCULATED AND MEASURED PLUME CENTERLINE CONCENTRATIONS AND PLUME HALF-WIDTH. PREDICTED CONCENTRATIONS ARE AT $Z=0$ AND $Z=0.5$ M, DATA ARE AT $Z=0.5$ M.

TOP RIGHT : MEASURED CROSSWIND PROFILES AT DIFFERENT DOWNWIND LOCATIONS. LINES ARE SPLINE FIT TO AID INTERPRETATION.

BOTTOM RIGHT : POINT-BY-POINT COMPARISON OF CALCULATED AND MEASURED CONCENTRATIONS. DASHED LINES SHOW FACTOR TWO DEVIATION FROM AGREEMENT.

MEAN RATIO OF PREDICTION TO DATA:
 HORIZONTAL: 0.84
 VERTICAL : 1.02

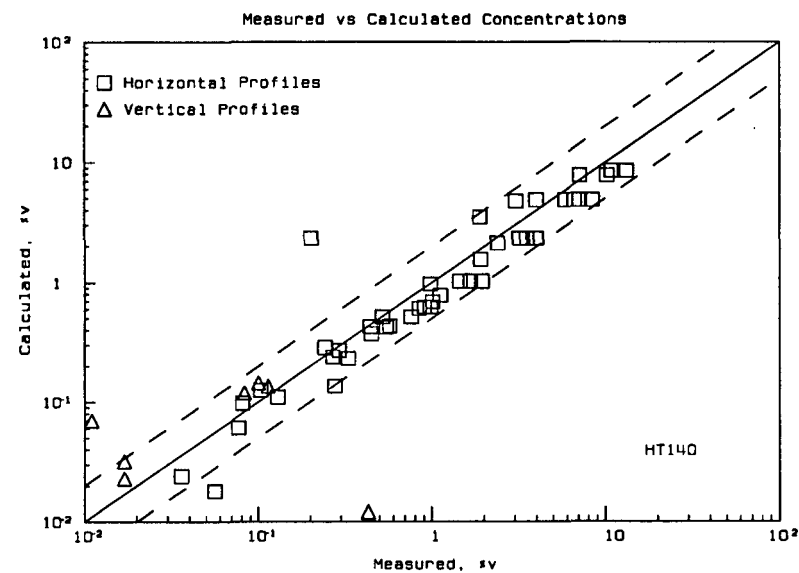
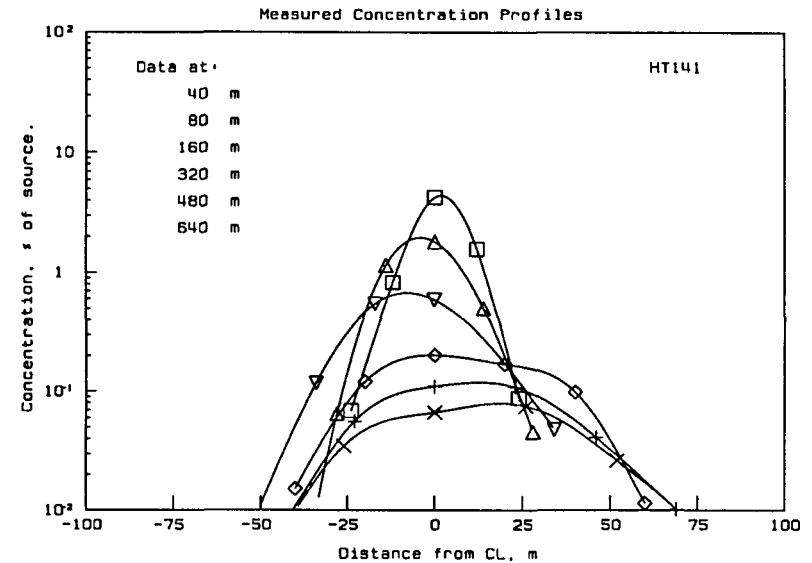
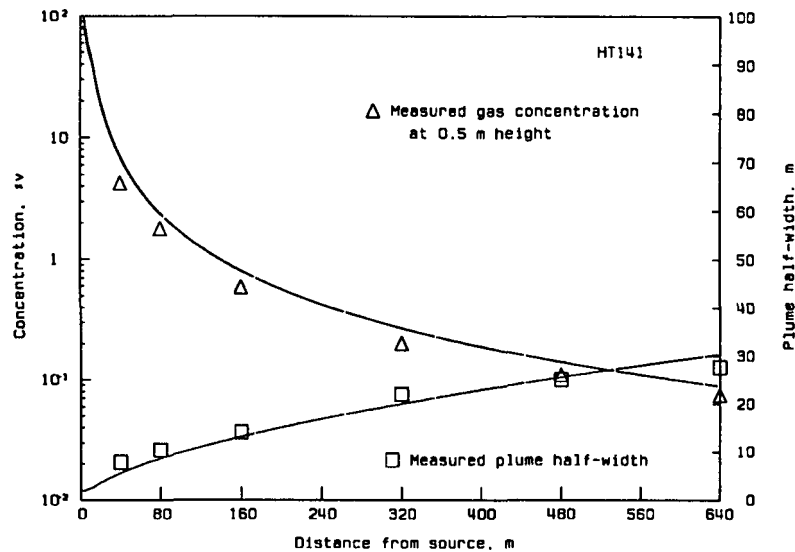


FIGURE 8.13 **RUN HT140**



SOURCE TYPE : SMALL AREA
 DENSITY RATIO : 1
 ROUGHNESS : R50

ABOVE : COMPARISON BETWEEN HEGADAS CALCULATED AND MEASURED PLUME CENTERLINE CONCENTRATIONS AND PLUME HALF-WIDTH. PREDICTED CONCENTRATIONS ARE AT $Z=0$ AND $Z=0.5$ M, DATA ARE AT $Z=0.5$ M.

TOP RIGHT : MEASURED CROSSWIND PROFILES AT DIFFERENT DOWNWIND LOCATIONS. LINES ARE SPLINE FIT TO AID INTERPRETATION.

BOTTOM RIGHT : POINT-BY-POINT COMPARISON OF CALCULATED AND MEASURED CONCENTRATIONS. DASHED LINES SHOW FACTOR TWO DEVIATION FROM AGREEMENT.

MEAN RATIO OF PREDICTION TO DATA:
 HORIZONTAL: 1.00
 VERTICAL : 1.11

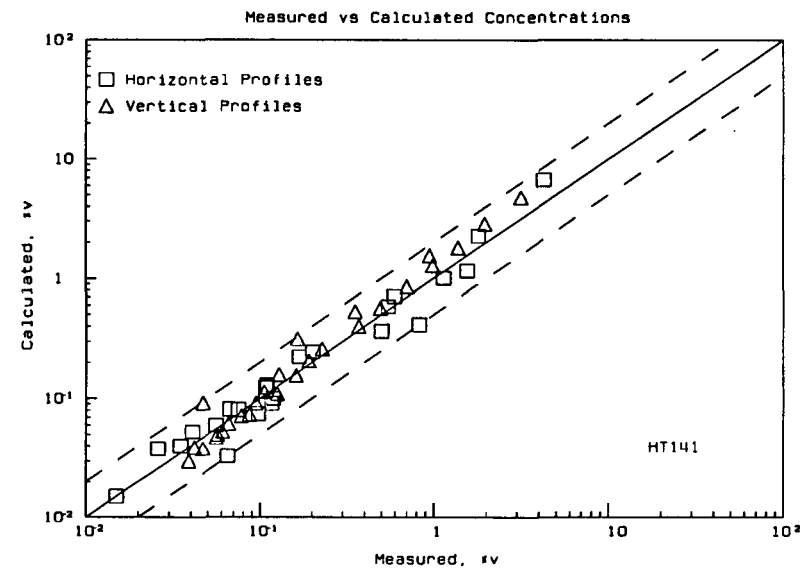
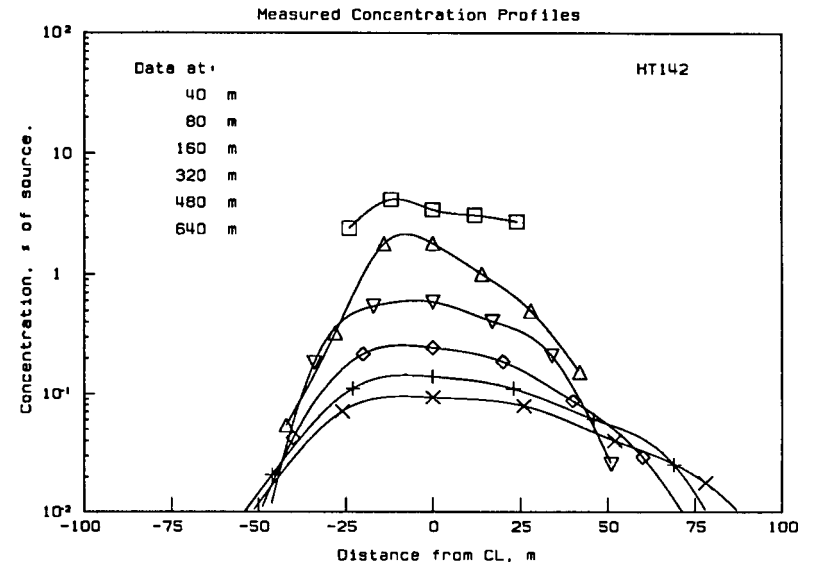
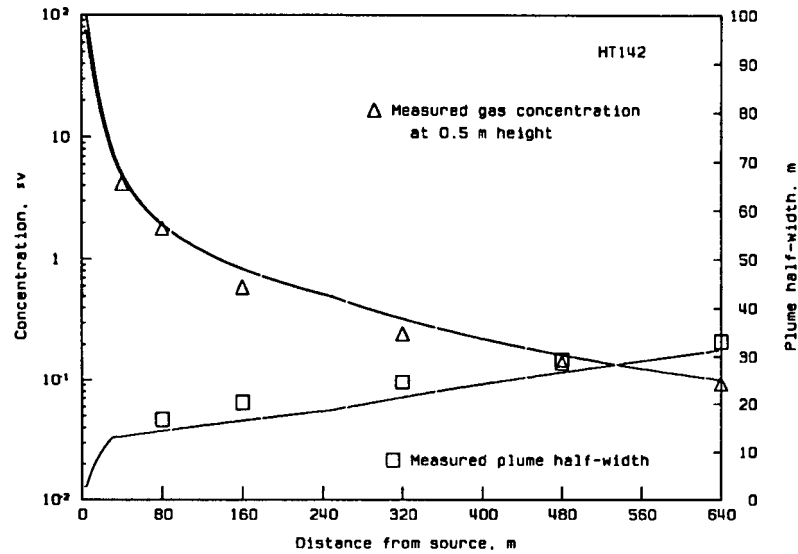


FIGURE 8.14 RUN HT141



SOURCE TYPE : SMALL AREA
 DENSITY RATIO : 1.4
 ROUGHNESS : R50

ABOVE : COMPARISON BETWEEN HEGADAS CALCULATED AND MEASURED PLUME CENTERLINE CONCENTRATIONS AND PLUME HALF-WIDTH. PREDICTED CONCENTRATIONS ARE AT Z=0 AND Z=0.5 M, DATA ARE AT Z=0.5 M.

TOP RIGHT : MEASURED CROSSWIND PROFILES AT DIFFERENT DOWNWIND LOCATIONS. LINES ARE SPLINE FIT TO AID INTERPRETATION.

BOTTOM RIGHT : POINT-BY-POINT COMPARISON OF CALCULATED AND MEASURED CONCENTRATIONS. DASHED LINES SHOW FACTOR TWO DEVIATION FROM AGREEMENT.

MEAN RATIO OF PREDICTION TO DATA:
 HORIZONTAL: 0.91
 VERTICAL : 1.19

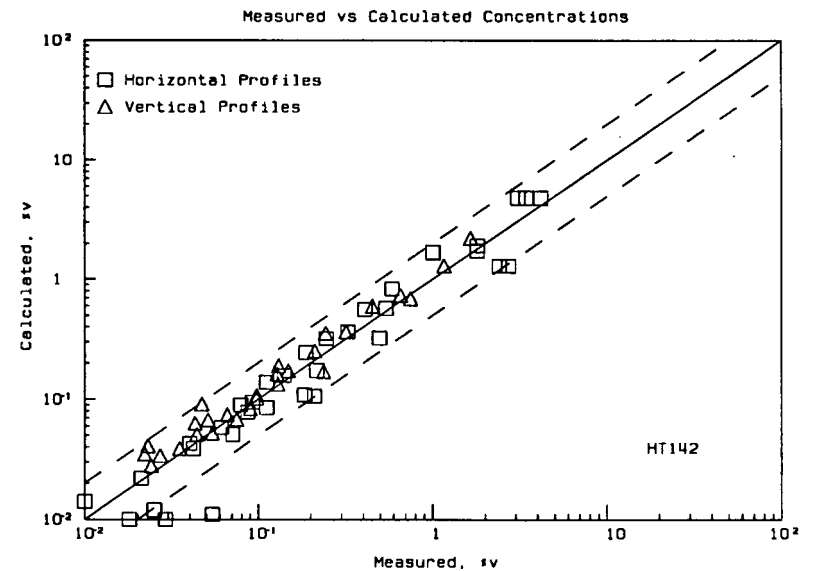
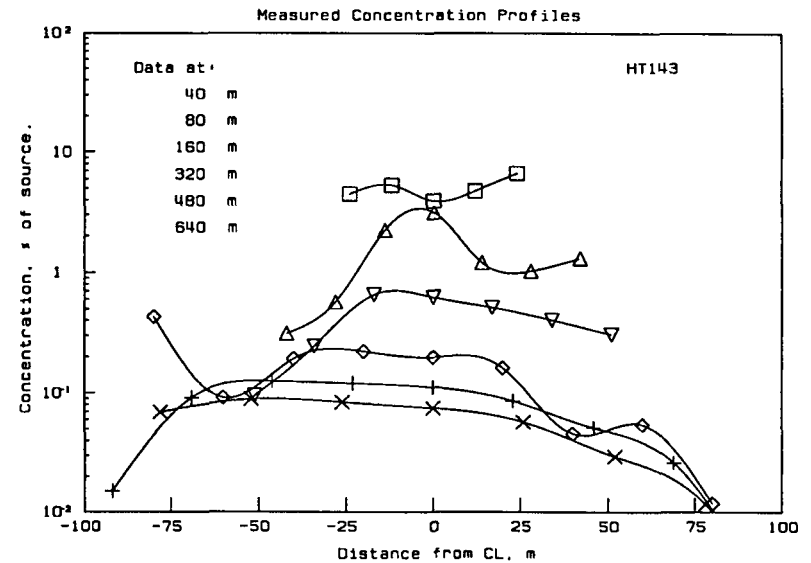
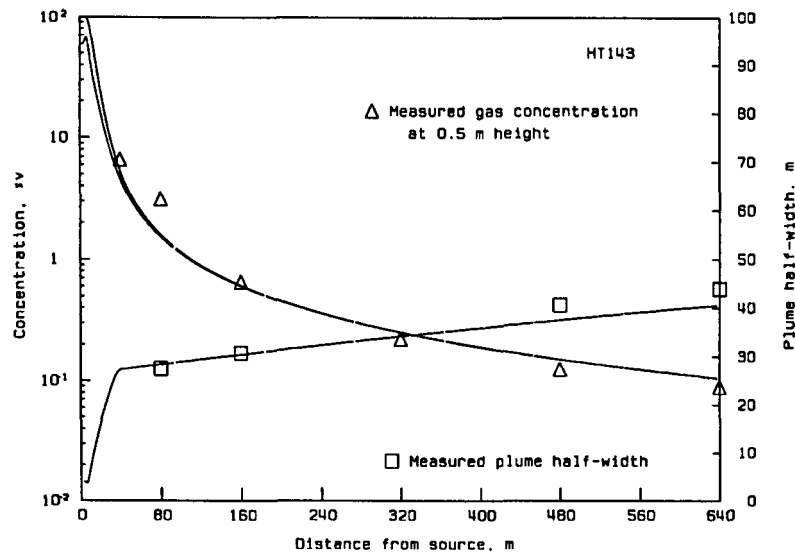


FIGURE 8.15 **RUN HT142**



SOURCE TYPE : SMALL AREA
 DENSITY RATIO : 3.9
 ROUGHNESS : R50

ABOVE : COMPARISON BETWEEN HEGADAS CALCULATED AND MEASURED PLUME CENTERLINE CONCENTRATIONS AND PLUME HALF-WIDTH. PREDICTED CONCENTRATIONS ARE AT $Z=0$ AND $Z=0.5$ M, DATA ARE AT $Z=0.5$ M.

TOP RIGHT : MEASURED CROSSWIND PROFILES AT DIFFERENT DOWNWIND LOCATIONS. LINES ARE SPLINE FIT TO AID INTERPRETATION.

BOTTOM RIGHT : POINT-BY-POINT COMPARISON OF CALCULATED AND MEASURED CONCENTRATIONS. DASHED LINES SHOW FACTOR TWO DEVIATION FROM AGREEMENT.

MEAN RATIO OF PREDICTION TO DATA:

HORIZONTAL:	1.03
VERTICAL :	1.02

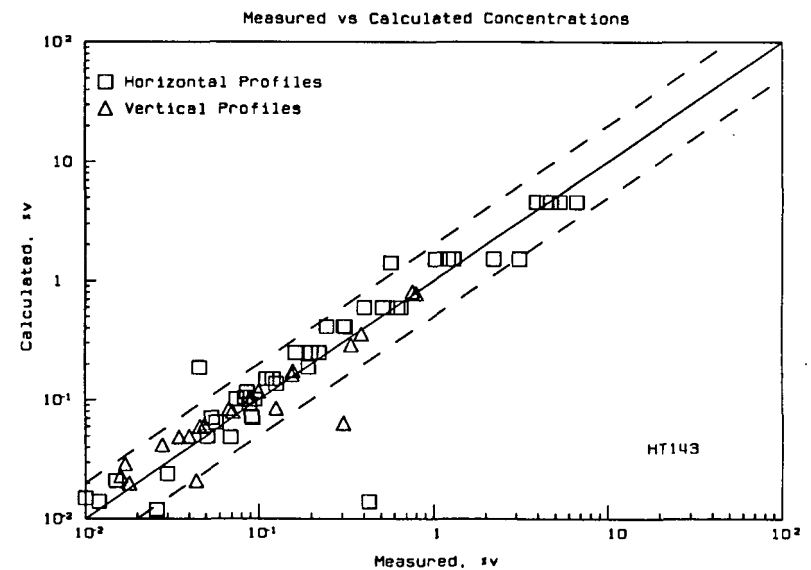
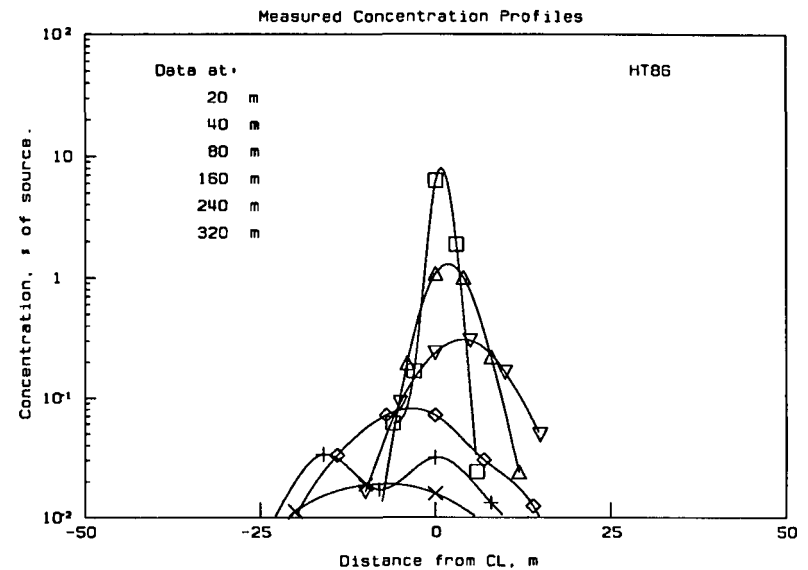
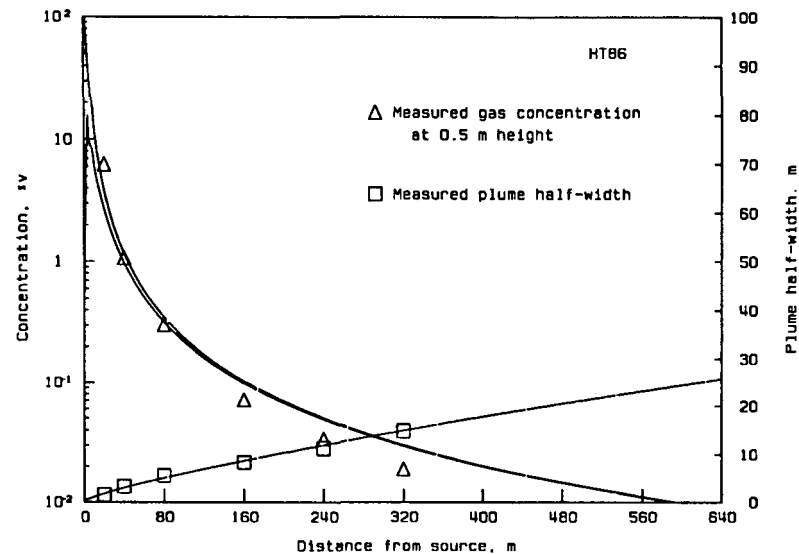


FIGURE 8.16 **RUN HT143**



SOURCE TYPE : POINT
DENSITY RATIO : 1.0
ROUGHNESS : R3

ABOVE : COMPARISON BETWEEN HEGADAS CALCULATED AND MEASURED PLUME CENTERLINE CONCENTRATIONS AND PLUME HALF-WIDTH. PREDICTED CONCENTRATIONS ARE AT Z=0 AND Z=0.5 M, DATA ARE AT Z=0.5 M.

TOP RIGHT : MEASURED CROSSWIND PROFILES AT DIFFERENT DOWNWIND LOCATIONS. LINES ARE SPLINE FIT TO AID INTERPRETATION.

BOTTOM RIGHT : POINT-BY-POINT COMPARISON OF CALCULATED AND MEASURED CONCENTRATIONS. DASHED LINES SHOW FACTOR TWO DEVIATION FROM AGREEMENT.

MEAN RATIO OF PREDICTION TO DATA:
HORIZONTAL: 1.09
VERTICAL : 0.95

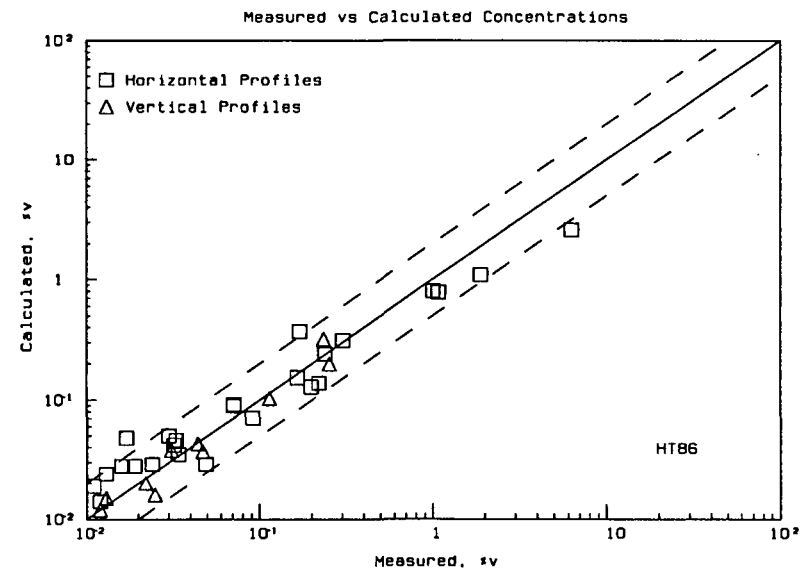
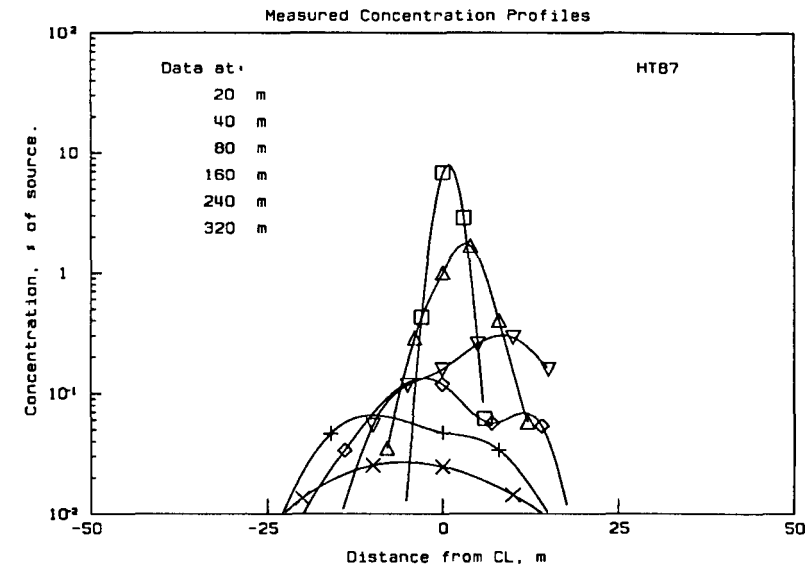
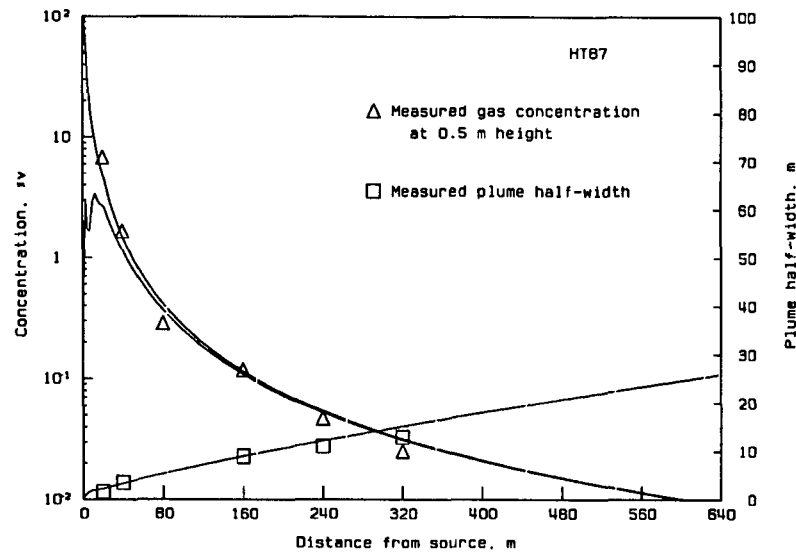


FIGURE 8.17 **RUN HT86**



SOURCE TYPE : POINT
 DENSITY RATIO : 1.4
 ROUGHNESS : R3

ABOVE : COMPARISON BETWEEN HEGADAS CALCULATED AND MEASURED PLUME CENTERLINE CONCENTRATIONS AND PLUME HALF-WIDTH. PREDICTED CONCENTRATIONS ARE AT $Z=0$ AND $Z=0.5$ M, DATA ARE AT $Z=0.5$ M.

TOP RIGHT : MEASURED CROSSWIND PROFILES AT DIFFERENT DOWNWIND LOCATIONS. LINES ARE SPLINE FIT TO AID INTERPRETATION.

BOTTOM RIGHT : POINT-BY-POINT COMPARISON OF CALCULATED AND MEASURED CONCENTRATIONS. DASHED LINES SHOW FACTOR TWO DEVIATION FROM AGREEMENT.

MEAN RATIO OF PREDICTION TO DATA:

HORIZONTAL:	0.94
VERTICAL :	1.08

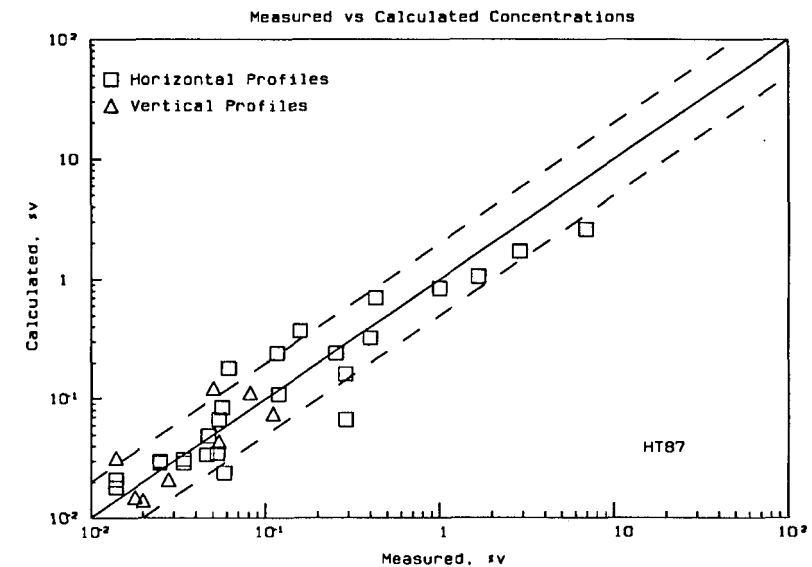
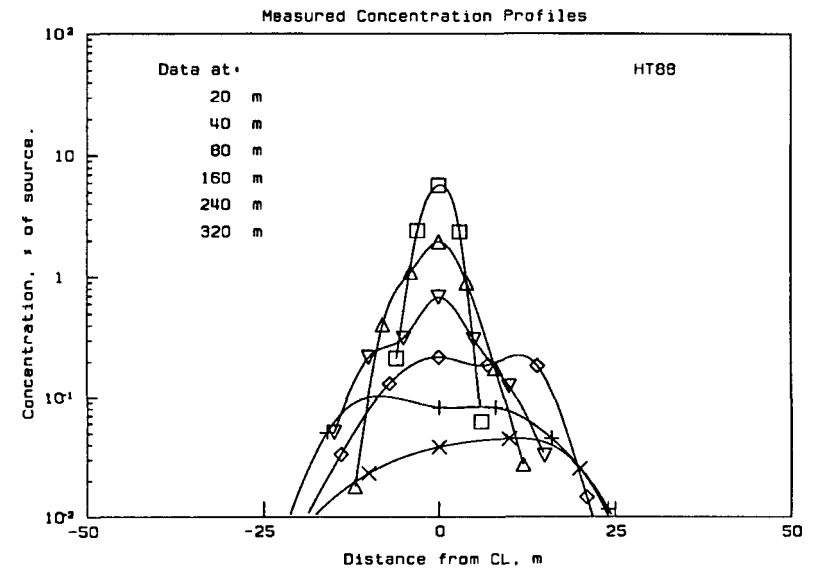
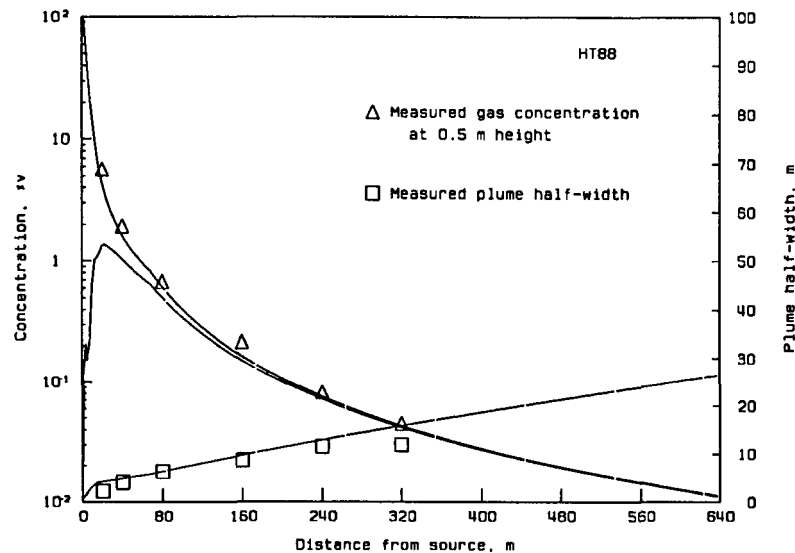


FIGURE 8.18 RUN HT87



SOURCE TYPE : POINT
DENSITY RATIO : 3.9
ROUGHNESS : R3

ABOVE : COMPARISON BETWEEN HEGADAS CALCULATED AND MEASURED PLUME CENTERLINE CONCENTRATIONS AND PLUME HALF-WIDTH. PREDICTED CONCENTRATIONS ARE AT Z=0 AND Z=0.5 M, DATA ARE AT Z=0.5 M.

TOP RIGHT : MEASURED CROSSWIND PROFILES AT DIFFERENT DOWNWIND LOCATIONS. LINES ARE SPLINE FIT TO AID INTERPRETATION.

BOTTOM RIGHT : POINT-BY-POINT COMPARISON OF CALCULATED AND MEASURED CONCENTRATIONS. DASHED LINES SHOW FACTOR TWO DEVIATION FROM AGREEMENT.

MEAN RATIO OF PREDICTION TO DATA:
HORIZONTAL: 0.97
VERTICAL : 0.83

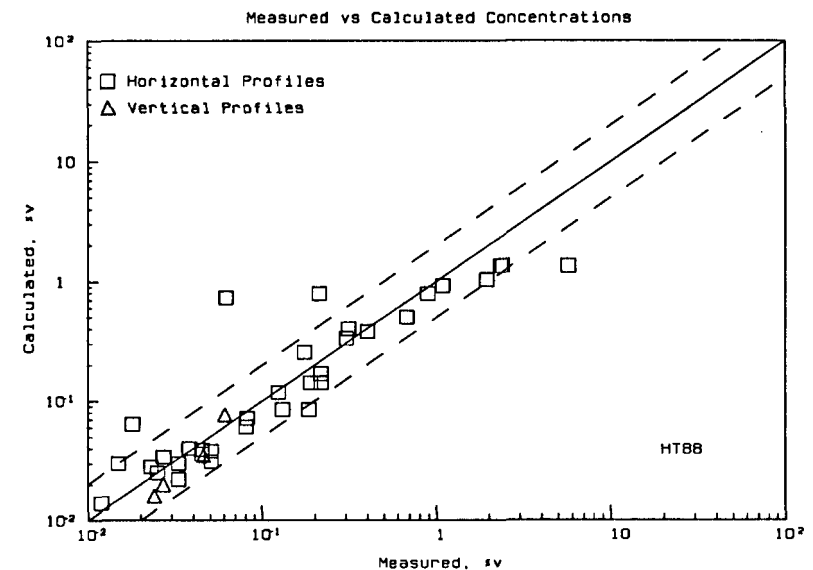
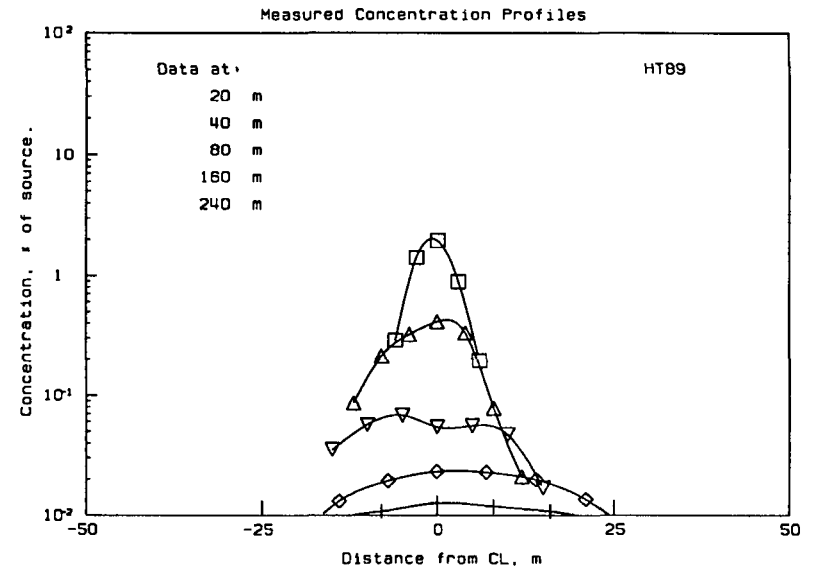
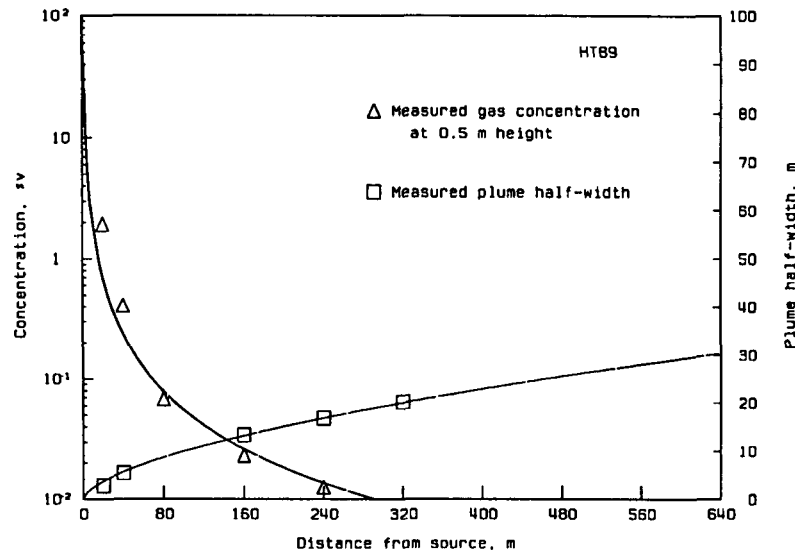


FIGURE 8.19 **RUN HT88**



SOURCE TYPE : POINT
 DENSITY RATIO : 1.0
 ROUGHNESS : R50

ABOVE : COMPARISON BETWEEN HEGADAS CALCULATED AND MEASURED PLUME CENTERLINE CONCENTRATIONS AND PLUME HALF-WIDTH. PREDICTED CONCENTRATIONS ARE AT $z=0$ AND $z=0.5$ M, DATA ARE AT $z=0.5$ M.

TOP RIGHT : MEASURED CROSSWIND PROFILES AT DIFFERENT DOWNWIND LOCATIONS. LINES ARE SPLINE FIT TO AID INTERPRETATION.

BOTTOM RIGHT : POINT-BY-POINT COMPARISON OF CALCULATED AND MEASURED CONCENTRATIONS. DASHED LINES SHOW FACTOR TWO DEVIATION FROM AGREEMENT.

MEAN RATIO OF PREDICTION TO DATA:
 HORIZONTAL: 0.76
 VERTICAL : 1.68

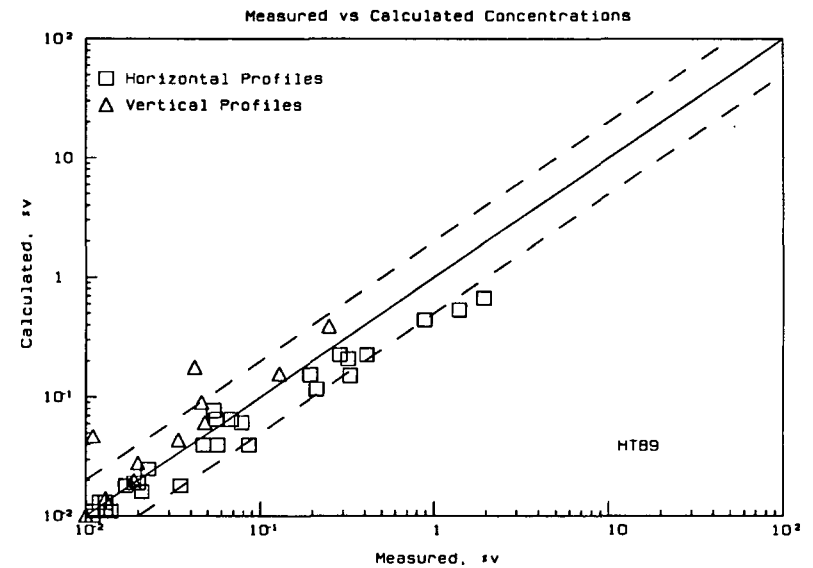
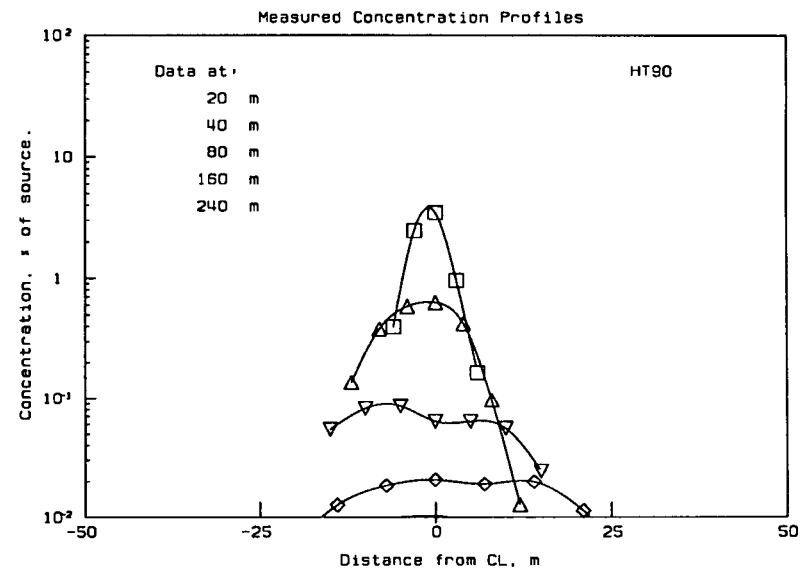
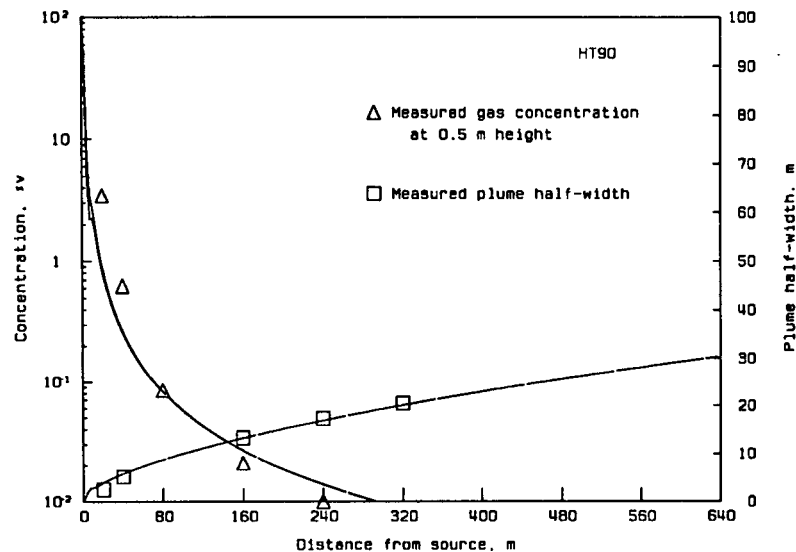


FIGURE 8.20 RUN HT89



SOURCE TYPE : POINT
 DENSITY RATIO : 1.4
 ROUGHNESS : R50

ABOVE : COMPARISON BETWEEN HEGADAS CALCULATED AND MEASURED PLUME CENTERLINE CONCENTRATIONS AND PLUME HALF-WIDTH. PREDICTED CONCENTRATIONS ARE AT $Z=0$ AND $Z=0.5$ M, DATA ARE AT $Z=0.5$ M.

TOP RIGHT : MEASURED CROSSWIND PROFILES AT DIFFERENT DOWNWIND LOCATIONS. LINES ARE SPLINE FIT TO AID INTERPRETATION.

BOTTOM RIGHT : POINT-BY-POINT COMPARISON OF CALCULATED AND MEASURED CONCENTRATIONS. DASHED LINES SHOW FACTOR TWO DEVIATION FROM AGREEMENT.

MEAN RATIO OF PREDICTION TO DATA:
 HORIZONTAL: 0.67
 VERTICAL : 1.64

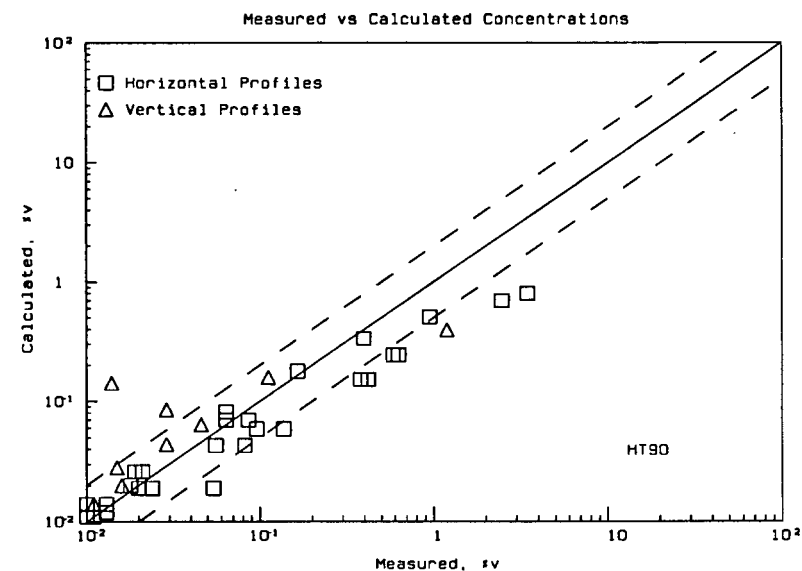
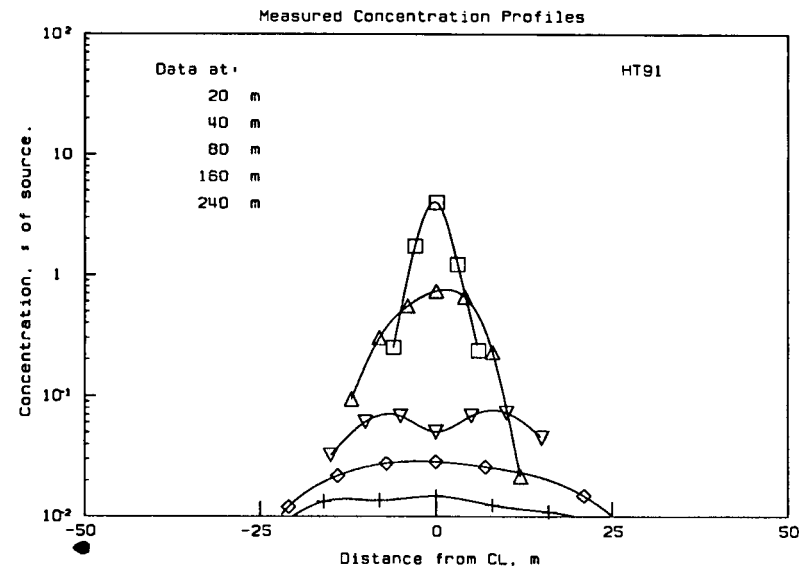
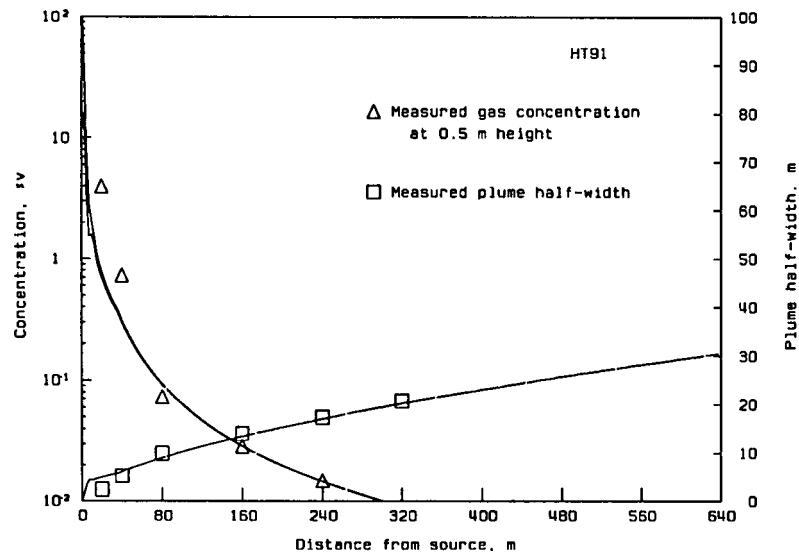


FIGURE 8.21 **RUN HT90**



SOURCE TYPE : POINT
 DENSITY RATIO : 3.9
 ROUGHNESS : R50

ABOVE : COMPARISON BETWEEN HEGADAS CALCULATED AND MEASURED PLUME CENTERLINE CONCENTRATIONS AND PLUME HALF-WIDTH. PREDICTED CONCENTRATIONS ARE AT Z=0 AND Z=0.5 M, DATA ARE AT Z=0.5 M.

TOP RIGHT : MEASURED CROSSWIND PROFILES AT DIFFERENT DOWNWIND LOCATIONS. LINES ARE SPLINE FIT TO AID INTERPRETATION.

BOTTOM RIGHT : POINT-BY-POINT COMPARISON OF CALCULATED AND MEASURED CONCENTRATIONS. DASHED LINES SHOW FACTOR TWO DEVIATION FROM AGREEMENT.

MEAN RATIO OF PREDICTION TO DATA:

HORIZONTAL:	0.74
VERTICAL :	2.08

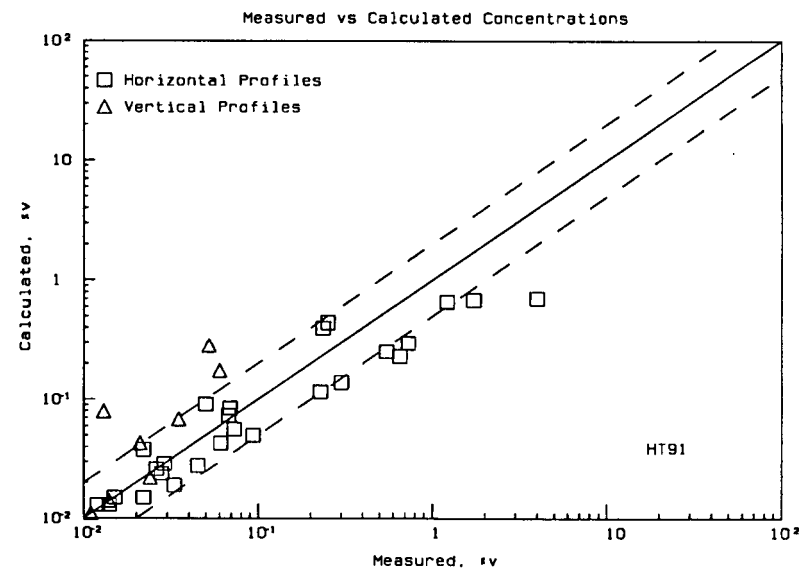


FIGURE 8.22 **RUN HT91**

9. SIMULATION OF THE GOLDFISH EXPERIMENTS BY THE PROGRAMS
HFPLUME AND HEGADAS

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9.3. Steady-state dispersion calculations for Goldfish experiments	9.11
9.4. Transient dispersion calculations for Goldfish 1 experiment	9.15
9.5. Discussion and conclusions	9.19
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9.1. Introduction

In this chapter the first three "Goldfish" experiments are simulated by the programs HFPLUME and HEGADAS. The predicted concentrations from the simulations are compared to the observed concentrations. As an introduction, we present a discussion of that data used in the development of the models and of the process of validation.

It is worth stressing that at no stage in the development of HEGADAS have field data on dense gas dispersion been used to calibrate, or tune, the model. The model parameters are derived from laboratory experiments which try to study the individual processes in isolation, or from field experiments on passive dispersion. The combined effect of these processes has then been validated against field data and found to be satisfactory, except when a particular process was missing from the model (i.e. water vapour transfer from the sea surface). In that case, laboratory experiments were performed to study that process in isolation, and changes made to the model physics. Model performance was then found to be improved when the revised model was re-evaluated against the field data.

There are sufficient differences between the laboratory experiments on entrainment and their use in the model that one could not be certain of their applicability without validating the entire model against experimental field data. Thus the validation studies are essential. However, in the process of developing HEGADAS we have found that we have not had to adjust laboratory-derived parameters in order to achieve agreement with field data.

The origins of specific aspects of the HEGADAS formulation are as follows. The vertical entrainment relation is based on laboratory studies of mixing into dense layers (Appendix 3, Section 3). The early rate of gravity spread of a dense cloud is supported by many observations; the value 1.15 for the coefficient C_E was derived by van Ulden (1984), from a wide range of observations. The criterion for gravity current collapse is obtained from the wind tunnel data of Petersen and Ratcliff (1989); the values of the lateral-spreading velocity ratio A_L obtained over a wide

range of experimental conditions are remarkably constant (Section 7.3.2); such a finding adds confidence that this is an appropriate formulation. collapse of gravity spreading, the rate of lateral spreading is inversely proportional to the parameter C_D (also derived from the same experiments). It has been found, however, that dispersion predictions are generally rather insensitive to the value of this parameter. The formulae for σ_y , from which the rate of change of S_y is derived, come from atmospheric data on passive dispersion (section 7.3.1).

The surface heat transfer relations used in HEGADAS are standard formulae (Appendix 3, Section 5.1). The approach used for surface water vapour transfer into cold clouds dispersing over water is that of Rosner (1967) (Appendix 3, Section 5.2). Laboratory experiments validate this approach. The coefficient "a" in the convective entrainment formulation was derived from the same series of laboratory experiments (Appendix 3, Section 5.3). The HF thermodynamic model is that of Schotte (1988), validated against laboratory data on mixing of HF and moist air.

The HFPLUME and PLUME models, just as HEGADAS, are the synthesis of many component submodels; each is (as far as practicable) physically based and has been separately validated. Several submodels are common to HFPLUME/PLUME and HEGADAS; HFPLUME/PLUME may be said to "inherit" experimental validation from HEGADAS. Such inherited mechanisms are: heavy gas entrainment, gravity slumping, gravity current collapse, post-collapse spreading, and (positive) buoyancy enhanced entrainment within grounded clouds. The HF thermodynamic submodel in HFPLUME, while common, differs marginally in formulation and has been separately validated (Chapter 2).

Mechanisms unique to the HFPLUME and PLUME models include jet entrainment, crosswind entrainment, and the description of (airborne) plume path. Entrainment within gas jets is well established with the "top-hat" coefficient 0.08 reported (Keffer and Baines, 1963). In respect of two-phase "flashing" jets the predictions of the jet model have been validated against large scale experiments involving the release from pressurised storage of liquified propane gas (Appendix 1, McFarlane (1988), Cowley and Tam (1988)).

In respect of crosswind entrainment the asymptotic form of the correlation and the coefficient value of 0.60 are those suggested by Briggs (1975, 1984) on the basis of extensive wind tunnel and atmospheric dispersion data on buoyant plumes. Specifically this coefficient value underpins his formula for buoyant plume rise. The PLUME model has been tested against (but not fitted to) an extensive set of wind tunnel data (Petersen, 1986) on the path of buoyant gas jets released upwards and at right angles to an imposed (uniform) wind. These data are well represented by the PLUME entrainment form.

Hoot, Meroney, and Peterka (1973) carried out an extensive (wind tunnel) study of the release of dense gas perpendicular to an imposed wind. These data are not well represented by the (buoyant plume) entrainment formulation; but may be fitted by making allowance for an effect of density upon dense ascending or buoyant descending plumes (Boussinesq approximation). A single parameter fit to plume rise-height data produces satisfactory results for the downwind displacement of maximum plume rise. In addition predictions of ("top-hat") leading edge and plume centre-line touchdown sensibly and symmetrically bracket visible leading edge touchdown as correlated by Hoot, Meroney and Peterka (1973). Exact validation is not possible owing to uncertainties in the interpretation of the "visible plume edge". PLUME is also successful in predicting the observed (wind tunnel) behaviour of hot-air jets directed downwards, perpendicular to an uniform air stream (Li, Leijdens and Ooms, 1986).

Results have previously been published on the comparison of HEGADAS predictions with field data on the dispersion of propane (Puttock et al., 1982) and liquefied natural gas (Puttock, 1987a). Predicted results using HEGADAS in combination with an instantaneous-release front-end model HEGABOX have also been compared with the Thorney Island freon/air releases (Puttock, 1987b).

This chapter contains comparisons of the predictions of the HFPLUME and HEGADAS models with the experimental results of the Goldfish experiments on the dispersion of HF releases. The results provide a validation of the HFPLUME and HEGADAS models.

The Goldfish experiments were conducted at the liquefied gaseous spill test facility in the USA during the summer of 1986. See Blewitt (1988) for a detailed description of these experiments. Section 9.2 includes a summary of the experimental conditions and the experimental results.

In this Chapter, the first three Goldfish experiments are abbreviated to Goldfish 1, Goldfish 2, and Goldfish 3, respectively.

In Section 9.3 steady-state calculations for Goldfish 1, Goldfish 2 and Goldfish 3 are discussed. First, results are presented of the flash data and near-source dispersion data calculated by HFPLUME. Secondly, results of the dispersion data calculated further downwind by HEGADAS-S are given.

In Section 9.4 transient calculations for Goldfish 1 are presented. These calculations are performed by HEGADAS-T to determine the dispersion data as function of downwind distance and time. Input to the HEGADAS-T run are chosen to be the flash data and the near-source transition data derived from the steady-state HFPLUME analysis of the Goldfish 1 experiment mentioned above.

9.2. Experimental conditions and experimental results

Experimental conditions (input to programs)

The Goldfish experiments were conducted at the U.S. Department of Energy liquefied gaseous spill test facility during the summer of 1986. They involved the release of anhydrous HF as a horizontal liquid jet. The HF was released on flat terrain with a very low surface roughness. In this chapter only the first three Goldfish experiments are discussed. The last three tests, which examined the effectiveness of water spray mitigation systems, are not applicable for model evaluation and will not be considered.

In the Goldfish tests the release conditions were configured to simulate a high pressure release, as would result from the acid rich portion of an HF alkylation unit. The major findings of the experiments was that approximately 20% of the released liquid HF flashed and the remaining 80% was transported downwind as an liquid aerosol (aqueous HF-fog), which subsequently evaporated. There was no liquid pool formed in the experiments.

Table 9.1 includes a list of the parameters characterising the experiments Goldfish 1, Goldfish 2 and Goldfish 3. These parameters include reservoir data (storage conditions for the anhydrous HF), pipe-exit plane data (dimensions of an assumed pipe-break, pressure at pipe-break), ambient data (atmosphere data, surface roughness) and the averaging time for measurement of the concentrations.

In Table 9.1 it is indicated to which of the programs HFFLASH, HFPLUME and HEGADAS the parameters must be input. The "note" column in Table 9.1 refers to the following notes.

1. The values of the reservoir data, release duration, ambient temperature, ambient windspeed, and atmospheric stability class are taken from Table 3.1 in Blewitt (1988).

2. The values quoted for the orifice pressure and the HF release rate correspond with the steady-state values taken from Figures 3.1-3 in Blewitt (1988).
3. See Table 3.2 in Blewitt (1988) for the quoted values of the orifice diameter.
4. The values of the orifice height are taken from Blewitt (1989).
5. In HEGADAS the ambient pressure P_a is always assumed to be 1 atm, and therefore does not need to be input.
6. The values of relative humidity for the Goldfish 1, Goldfish 2 experiments are derived from measured Dewpoint temperatures given in Table 3.1 in Blewitt (1988). A precise value of the relative humidity for Goldfish 3 is not available. The appropriate choice for this value is discussed in the paragraphs below.

In the Goldfish 3 experiment, an attempt was made to increase the humidity at the release point. This was done by having a pond of water extending 600 meters upwind of the release point and also water sprays close upwind; see Blewitt (1988) for further details. Since much of the water vapour in the air was evaporated from the pond on the surface, there was a significant vertical gradient of humidity in the air downwind of the pond. This is confirmed by examination of the temperature lapse rate data near the ground surface. These data indicate a warming of the atmosphere as a function of height. This phenomenon was caused by the cooling of the atmosphere by the water being evaporated. Unfortunately, the humidity was only measured at ten metres elevation, and so the value measured, 16%, is not representative of the humidity in the HF plume nearer the surface.

Since the thermodynamics of the mixing of moist air and HF are well established, it would be possible to determine the humidity of the air mixed into the plume from the observed temperature and concentration at one point. For a given HF concentration, the temperature is a strong

function of the humidity. This cannot be done directly close to the point of release since there were no coincident measurements of concentration and temperature. We can, however, extrapolate the concentration measurements from 300 m to 200 m. The resulting estimate of concentration at 200 m is 2.5% compared to 1.84% measured at 300 m (Table 9.2). There is some uncertainty in this value, but it certainly appears to be between 2% and 3%. The measured temperature was 32°C; see Table 9.3.

Examining the relation between temperature and concentration shows that, for the temperature to be 32°C at a concentration of 2.5% requires an ambient relative humidity of about 35%. This result is extremely insensitive to any errors in the concentration estimate since the temperature versus concentration curves are flat in this region. We have therefore used a value of 35% for the relative humidity in our Goldfish 3 simulations.

As the plume dispersed further downwind, the air entrained would be less and less affected by the water pond, and so have decreasing humidity. We have tried a sensitivity run in which a change was made to a lower humidity further downwind, but we found no significant effect on the results. For the low humidity of the GOLDFISH trials, it is the air humidity in the early stages of dilution which affects dispersion.

7. Blewitt (1989) gives a review of available data for the surface roughness z_R on Frenchman Flats:

- Estimates of z_R 1.5 km downwind of the Goldfish spill point range from 5×10^{-6} m in spring (wet surface) to 10^{-4} m in fall (dry and cracked surface). During the Goldfish experiments the surface was dry but not cracked.
- The estimate of z_R near the spill point for conditions similar to those during the Goldfish experiments is $z_R = 3 \times 10^{-4}$, which is higher than the above estimates because of the spill test equipment.

From the above it follows that a surface roughness $z_R = 3 \times 10^{-4}$ near the spill point and z_R slightly less than 10^{-4} at 1500 m downwind of the spill point seem to be reasonable estimates of z_R for the Goldfish experiments. The intermediate roughness $z_R = 2 \times 10^{-4}$ is adopted in the HFPLUME and HEGADAS runs.

8. The observations for the crosswind dispersion coefficient σ_y discussed in Section 7.3.1 give little guidance as to what should be done for the abnormally low roughness at the Frenchman Flat site. There are no corresponding experimental observations of σ_y for sites with a roughness length as low as 0.0002 m.

Fortunately, measurements of the standard deviation of wind direction σ_θ were made during the Goldfish experiments. σ_y is closely determined by σ_θ , according to a formula of Pasquill(1973) which is independent of surface roughness and stability. Essentially surface roughness, atmospheric stability and averaging time affect σ_θ directly, and σ_y indirectly through their effects on σ_θ . Pasquill's formula is

$$\sigma_y = \sigma_\theta f(x) x$$

where the values of $f(x)$ are given in Table 9.4, and σ_θ is in radians. Taking the one-minute average $\sigma_\theta = 4$ degrees as an example, gives the values shown in Table 9.4. It can be seen that the original HEGADAS power-law and Briggs formula (corresponding to Pasquill-stability class D and averaging time $t_{av} = 60$ seconds) give a good fit up to $\sigma_y = 42$ m ($x=1000$ m), but not beyond.

The expression $\sigma_y = 0.17 x^{0.79}$ results from fitting δ, β in the power-law $\sigma_y = \delta x^\beta$ to the data for $\sigma_\theta f(x)x$ at $x = 400, 1000, 2000, 4000$ m). It is seen from Table 9.4 that this gives a very good fit from about $\sigma_y = 15$ m onwards (less than 10 % error).

$\sigma_y = 15$ m corresponds to a plume half-width $B_{eff} = (\pi/2)^{1/2} \sigma_y = 19$ m. It is seen from Table 9.6a that, owing to early gravity-spreading, nearly all the plume development in the Goldfish 3 release occurs in the

region $x > 300$ m in which $\sigma_y > 22.4$ m. Therefore in the Goldfish simulations we shall use $\sigma_y = \delta x^\beta$, with $\delta = (\sigma_\theta/4.0)0.17$ and $\beta = 0.79$. Hereby σ_θ is evaluated by averaging the measured σ_θ -values over all times and over the positions $(x,y) = (-1000,0)$, $(1000,-3)$, $(1600,0)$, $(2300,0)$ and $(3000,0)$. Thus $\sigma_\theta = 4.4, 5.1, 4.9$ degrees and $\delta = 0.19, 0.22, 0.21$ is found for the Goldfish 3, Goldfish 2 and Goldfish 1 experiments, respectively.

9. As mentioned in note 8, the values of δ, β are not derived from the Pasquill-stability class and the averaging time, but they are determined from measured σ_θ values, using the same averaging times for the concentration data. Hence in the Goldfish runs the averaging time is not used as input to HEGADAS-S.

Experimental results

In the experiments HF-concentration measurements were made at the distances $x = 300, 1000, 3000$ m downwind of the release point. At each of these downwind distances measurements were made at heights $z = 1, 3, 8$ m and a range of crosswind distances y . Measurements of the cloud temperature were made at the distances $x = 20, 40, 60, 100, 200$ and 1000 m downwind of the release point; see Figure 2.3 in Blewitt (1988) for the crosswind locations of the temperature sensors.

Results for the concentration and temperature measurements are summarized in Figures 9.1-9.5 and Tables 9.2 and 9.3.

1. Figures 9.1 and 9.2 (taken from Blewitt, 1988) include results for the measured concentration for Goldfish 1 and Goldfish 3, respectively. For each of the downwind distances $x = 300, 1000, 3000$, the concentration (in ppm) at the height $z=1$ is given as a function of the crosswind distance y and the time t .
2. Figures 9.3, 9.4 and 9.5 depict the crosswind concentration profiles measured at $x = 300, 1000, 3000$, respectively. These profiles are taken at times which most closely seem to represent steady-state.

3. The model is intended to predict the ensemble average behaviour of plumes under the given conditions, i.e. the average result when many experiments are performed under nominally identical mean conditions. For a steady release, we can take the mean of the observations obtained during the time period when concentrations were steady. The figures for c_{AV} in Table 9.2 are estimates of the mean centre-line concentration for each experiment and measuring distance. This is taken from the centre-line concentration obtained at each measuring time. Because of slight wind-direction changes, this may not come from the same sensor position (crosswind) at each time. The averaging time of the individual measurements was 60s, and it is still appropriate to compare with model predictions at sixty-second averaging, because we have not averaged the data further at fixed locations.
4. In Blewitt (1988) tables are included for the measured cloud temperature differences (30-second average) from ambient as a function of time. The data in these tables are summarized by Figures 4.23-4.26 in Blewitt (1988). After "smoothing" of the data, the maximum temperature difference was used as the measured steady-state value for the temperature difference ΔT . Table 9.3 contains a list of these values.

9.3. Steady-state dispersion calculations for Goldfish experiments

The first three Goldfish experiments may be simulated using the HFPLUME and HEGADAS-S programs. The 6 minutes release duration for Goldfish 2 and Goldfish 3 was sufficiently long for steady conditions to be obtained in the dispersing cloud (see Figure 9.2 for Goldfish 3). The release time of 125 seconds for Goldfish 1 was perhaps too short for steady conditions to be reached in the far-field, but it is believed that a useful comparison can be made with steady-state predictions nearer to the source (see Figure 9.1).

The flashing of the released liquid HF, the subsequent high-momentum two-phase yet behaviour close to the source, the plume touchdown and the onset of gravity slumping are appropriately simulated in HFPLUME. In the region further downwind the windspeed approaches the ambient windspeed and the heavy-gas type of entrainment is dominant. In this region the program HEGADAS-S can be applied.

In the steady-state simulations of Goldfish 1, Goldfish 2 and Goldfish 3 presented in this section the program HFPLUME is first run to calculate the post-flash data and the dispersion data up to the transition point. The post-flash data and transition data calculated by HFPLUME are then used as input to HEGADAS-S, and HEGADAS-S is run downwind of the transition point; see Section 7.8.3. for further details.

Predictions of flash data by HFPLUME

See Chapter 5 for full details of the flash calculations by HFPLUME. Table 9.5 summarizes the calculated post-flash data, i.e. the temperature, the mass fraction of liquid in the HF, the jet velocity and the jet diameter. The post-flash temperature and liquid HF mass fraction are input to HEGADAS-S.

Predictions of near-source dispersion data by HFPLUME

Tables 9.6a and 9.6b summarize results of the Goldfish 3 run for HFPLUME

up to the transition point. Table 9.6b clearly demonstrates the proportional decrease of jet and gravity-slumping entrainment with increasing downwind distance of the release point, and the proportional increase of heavy-gas entrainment with increasing downwind distance of the release point. Note that the gravity-slumping entrainment is switched off after 79 m, i.e. at the point at which the Richardson number reduces to 10.

HFPLUME predictions for the cloud concentrations and the cloud temperatures are included in Figures 9.6, 9.11, 9.16 and Figures 9.10, 9.15, 9.20 for Goldfish 3, Goldfish 2, Goldfish 1, respectively. Note that the HFPLUME predictions plotted are of sectional-mean concentration and of sectional-mean temperature.

Point of transition between HFPLUME and HEGADAS-S

At the transition between HFPLUME and HEGADAS-S the jet speed u_{jet} must be sufficiently close to the ambient windspeed u_{amb} and the heavy-gas-dispersion entrainment $Entr_{gas}^{heavy}$ must be sufficiently large relative to the jet entrainment $Entr_{jet}$. The transition is chosen at the downwind distance for which the following two conditions are first simultaneously satisfied (see also Section 7.8.3):

- the absolute value of $RU = u_{jet}/u_{amb} - 1$ is smaller than $RULST = 0.20$
- the entrainment ratio $RE = (Entr_{total} - Entr_{gas}^{heavy})/Entr_{total}$ is smaller than $RELST = 0.60$. This rather large value for $RELST$ is chosen to enable a HFPLUME/HEGADAS transition at a downwind distance sufficiently upwind of 300 m. Thus a more proper comparison of the HEGADAS crosswind concentration profile against the experimental data at 300 m can be made. In the Goldfish experiments the HFPLUME/HEGADAS transition is rather late because of low values of the surface roughness and friction velocity. These low values induce a small amount of drag and a proportionally small amount of heavy-gas-entrainment.

The transition points were found to be located at 94, 143, 188 m for the Goldfish 3, Goldfish 2 and Goldfish 1 experiments, respectively.

Corresponding entrainment ratios were $RE = 0.54, 0.60, 0.60$, values of RU were $RU = 0.20, 0.12, 0.11$ and Richardson numbers $Ri_* = 8.8, 22.4, 24.6$, respectively.

HFPLUME/HEGADAS-S analyses were also carried out which adopted the more common and severe transition criteria $RELST = 0.30$, $RULST = 0.1$ (default values). The results of these analyses are not reported in this Chapter, but it is noted that the centre-line groundlevel concentrations predicted by these analyses ($RELST = 0.30$, $RULST = 0.1$) never deviate more than 15% from the results for the analyses reported in this Chapter ($RELST = 0.60$, $RULST = 0.2$).

Predictions of dispersion data by HEGADAS-S

Figures 9.6-9.10, 9.11-9.15 and 9.16-9.20 include results for HEGADAS-S simulations for the Goldfish 3, Goldfish 2 and the Goldfish 1 experiment, respectively. The concentrations predicted by HEGADAS-S are plotted at ground-level ($z = 0$) and at 1 m height ($z = 1$). The temperature predicted by HEGADAS-S corresponds to the mixture temperature at ground-level. Tables 9.7, 9.8 and 9.9 present HEGADAS-S output data for the Goldfish 3, Goldfish 2 and Goldfish 1 experiments, respectively. The HEGADAS-S runs required typically 3 minutes CPU on a IBM-PS2 personal computer, Model 50 and 1 minute on an IBM-PS2, Model 70 [both machines being equipped with a math-coprocessor chip].

From the Figures 9.6-9.20 and the Tables 9.7-9.9 the following conclusions can be drawn.

- At the transition point, the ground-level concentration c_A is matched to the ground-level concentration given by a Gaussian profile in HFPLUME. This matching results in c_A being $2^{1/2}$ times as large than the sectional-mean concentration calculated by HFPLUME (Section 7.8.3). This explains the jump in concentration at the transition point in Figures 9.6, 9.11 and 9.16.
- In the temperature plots, the HFPLUME temperature corresponds to the sectional-mean mixture temperature, while the HEGADAS temperature

corresponds to the mixture temperature at ground level. This explains the jump in temperature at the transition point in Figures 9.10, 9.15 and 9.20.

- For Goldfish 3, Goldfish 2, Goldfish 1 the collapse of gravity spreading (see Section 7.3.2) was found to be approximately located at the downwind distances $x_{CD} = 975, 650$ and 725 m, respectively.
- The predictions of the centreline concentrations replicate the observed experimental data quite well. There may be a tendency to underpredict at 300 m. This does not seem to persist to the measurement locations further downwind.
- The predicted crosswind concentration profiles are in good agreement with the experimental data, with only a slight overprediction of the cloud width (and therefore, because of conservation of mass, an underprediction of the cloud height) downwind of distances at approximately $x = 1000$ m.
- The variation in temperature along the plume is well simulated by HFPLUME and HEGADAS-S, particularly for Goldfish 3. The underprediction of temperature for Goldfish 1 and Goldfish 2 may well be caused by the centre-line of the plume not being aligned with the line on which the temperature measurements were made (temperature was measured along the centre-line of the sensor array).

9.4. Transient dispersion calculations for Goldfish 1 experiment

The release duration $T_{dur} = 125$ seconds for Goldfish 1 was too short for steady conditions to be reached at the further distances of interest. This applies in particular for positions downwind of $x = 1000$ m; see Figure 9.1. For these reasons a time-dependent simulation of the Goldfish 1 experiment by the program HEGADAS-T has been carried out. This simulation is discussed in this section.

Evaluation of HEGADAS-T data at transition point from HFPLUME

As discussed in Section 7.8.4, the near-source model HFPLUME can be automatically interfaced with the time-dependent model HEGADAS-T for a finite-duration release. Breakpoint data are applied at the HFPLUME/HEGADAS-T transition point (breakpoint) $x = x_{br}$ for a period corresponding to the release duration $T_{dur} = 125$ seconds. The position of the breakpoint and the applied breakpoint data correspond with the steady-state HFPLUME/HEGADAS-S transition data. Thus at the breakpoint $x_{br} = 188$ m, the total gas flow $E = 27.1$ kg/s, the ground-level molar HF-fraction $y_{HF} = 0.0503$ and the effective cloud half-width $B_{eff} = 39.1$ m are applied for a period of $T_{dur} = 125$ seconds.

Gas is being released at the release point $x = 0$ during the period $0 < \text{time } t < T_{dur}$. In applying the above transition data at $x = x_{br}$ the travel time T_{br} of the plume between the release point $x = 0$ and the transition point $x = x_{br}$ is taken into account. Thus the transition data are applied for $T_{br} < \text{time } t < T_{br} + T_{dur}$. It was found that $T_{br} = 25.7$ seconds. See Section 7.8.4 for further details of the link from HFPLUME to HEGADAS-T.

Details of HEGADAS-T simulation of Goldfish 1

In the HEGADAS-T simulation the flash data predicted by HFPLUME are adopted, i.e. the post-flash HF temperature 19.55°C and the liquid HF mass-fraction 0.837 are adopted (see Section 9.3 and Table 9.5). The data at the HFPLUME/HEGADAS-T transition point (breakpoint) $x_{br} = 188$ m are specified as a function of the time t with a time step $\Delta t = T_{dur}/25 = 5$ seconds. The following breakpoint data are applied:

- o $T_{br} + \frac{1}{2}\Delta t < t < T_{br} + T_{dur} - \frac{1}{2}\Delta t$ (28.3 < t < 148.3 s):
the transition data described above (gas flow $E = 27.13$ kg/s, ground-level molar HF-fraction $y_{HF} = 0.0503$ and effective cloud half-width $B_{eff} = 39.1$ m)
- o $t < T_{br} - \frac{1}{2}\Delta t$ (=23.3 s) and $t > T_{br} + T_{dur} + \frac{1}{2}\Delta t$ (= 153.3 s):
zero concentration data ($E = 0$ kg/s)
- o $T_{br} - \frac{1}{2}\Delta t < t < T_{br} + \frac{1}{2}\Delta t$ and $T_{br} + T_{dur} - \frac{1}{2}\Delta t < t < T_{br} + T_{dur} + \frac{1}{2}\Delta t$:
concentration data linearly varying between the above given data

Thus, effectively, a constant gas-flow $E = 27.13$ kg/s is applied for $T_{br} < t < T_{br} + T_{dur}$ (25.7 < t < 150.7 s), i.e. the plume arrives at $x = x_{br}$ at $t = T_{br} = 25.7$ s and moves for a period $T_{dur} = 125$ s along $x = x_{br}$. See Section 7.6.3 for further details of the time-dependent breakpoint in HEGADAS-T.

The simulation was carried out using the HEGADAS-T algorithm for automated release of observers described in Section 7.9. Twenty-one observers were found to be required to ensure convergence for the observer concentrations within the specified (default) convergence tolerance $\epsilon_{obs} = 0.05$ (see Table 9.10). Downwind diffusion effects were included using the heavy-gas adaptation of the downwind spreading formulation by Wilson and Chatwin (see Section 7.4). The run required about 13½ minutes CPU-time on an IBM-PS2, Model 70 [machine equipped with a math-coprocessor chip].

HEGADAS-T predictions for Goldfish 1

Table 9.10 and Figures 9.21-9.24 include HEGADAS-T predictions for the

Goldfish 1 experiment. The following is concluded.

1. The graphs in Figures 9.21 and 9.23 include steady-state HEGADAS-S predictions (Section 9.3) and HEGADAS-T predictions at the times $t = 140, 250, 300, 500$ and 700 seconds.

From the centre-line groundlevel concentration versus downwind distance graph (Figure 9.21) it is seen that the downwind edge of the cloud has arrived at time $t = 140$ at about $x = 1000$ m. It is seen that upwind of this distance the time-dependent HEGADAS-T concentration predictions are in good agreement with the steady-state HEGADAS-S predictions.

The cloud shape correction for gravitational spreading in the downwind direction adopted in HEGADAS-T in case of a breakpoint (Section 7.6.3) causes for the smaller times the HEGADAS-T concentration predictions downwind of the breakpoint to be slightly higher than the steady-state HEGADAS-S values; see Figure 9.21. The reduced gravitational spreading in the crosswind direction also results in smaller HEGADAS-T predictions of the effective cloud half-width; see Figure 9.23.

2. Figures 9.21 and 9.23 demonstrate the movement of the gas cloud as a function of time:
 - Whilst the gas cloud passes the transition point $x_{br} = 188$ m ($26 < t < 151$), the gas concentrations build up downwind of x_{br} . The centre-line groundlevel concentration and the effective cloud half-width increase to their steady-state values (for $x < 1000$ m).
 - After the cloud has passed the transition point, the gas cloud moves downwind, spreads somewhat in the downwind direction and dilutes (see Figure 9.21). The cloud width increases with time (see Figure 9.23).
 - Downwind diffusion is taken into account for bulk Richardson number $Ri_* < Ri_*^{cr} = 10$ and affects the outer, low-concentration part of the cloud. In the middle part of the cloud $Ri_* > 10$ applies and we have

zero downwind diffusion. It was found that after $t = 250$ seconds Ri_* had dropped below 10 in the entire cloud.

The effect of downwind diffusion on concentration is only felt at downwind distances near regions with a significant gradient in concentration, i.e. near the outer parts of the gas cloud (rapid decay of concentration). In the middle part of the gas cloud the transient concentration equals the steady-state concentration (Figure 9.21).

Whilst the cloud moves in the downwind direction, the outer parts of the gas cloud get more and more eroded away because of downwind diffusion and the middle part of the cloud (part of cloud touching the steady-state envelope) gradually disappears; see Figure 9.21. Notice that only after the middle part has disappeared entirely, does the peak concentration drop below the steady-state value.

3. HEGADAS-T predictions were output for the times $t = 80, 100, 120, 140, 160, 180, 200, 225, 250, 280, 310, 340, 380, 420, 460, 500, 550, 600, 650$ and 700 seconds. Figures 9.22 and 9.24 contain results for the groundlevel concentrations and effective cloud half-width as a function of these times for the three distances $x = 300$ m, 1000 m and 3000 m. These results can be compared with the experimental data obtained for Goldfish 1 (Figure 9.1):

- According to Figure 9.22 the cloud is "observed" at $x = 300$ m between 35 and 160 seconds, at $x = 1000$ m between 140 and 310 seconds, and at $x = 3000$ m between 440 and 640 seconds. This seems to be in reasonable agreement with the experimental data depicted in Figure 9.1.
- According to Figure 9.24 the (maximum) effective cloud half-width is at $x = 300$ m about 60 m, at $x = 1000$ m about 120 m, and at $x = 3000$ m about 180 m. This seems to be in reasonable agreement with the experimental data depicted in Figure 9.1.

9.5 Discussion and conclusions

For there to be confidence in applying the model beyond the conditions under which it is validated, it is important to compare as many aspects of the observations as possible with the predictions. If there is consistency over a range of comparisons, there is less likelihood that good agreement on centre-line concentration is the result of two errors happening to cancel each other out. For this reason, we have presented other data such as crosswind profiles and temperatures in this chapter.

The data from Goldfish 2 at 1000 m are of particular interest with regard to cloud width. In this case, good crosswind profile observations were obtained, and the predicted gravity-spread transition was sufficiently far upwind (at 700 m) to affect the predictions at this location. Define the observed plume half-width as half the distance between the points at which the concentration drops to 0.46 times its value in the central region of the plume. (This is consistent with the definition of B_{eff} in Appendix 3.) Then the observed B_{eff} at 1000m in Goldfish 2 is 120 m; B_{eff} from the model predictions is 137 m, in reasonable agreement. By contrast, if the old gravity-spread formulation is used, with no transition, then the predicted B_{eff} is 185 m. This provides further evidence that the findings from the wind-tunnel data regarding gravity spreading have general applicability.

Overall the observed plume widths appear to be smaller than predicted, although the discrepancy is much less than the changes in predictions resulting from the allowance for gravity-spread transition (Figure 8.3). Perhaps some of this difference is due to uncertainties in the ambient humidity. The cloud development for HF may also be influenced to some extent by the rapid changes in (negative) buoyancy resulting from its thermodynamic behaviour.

In Table 9.11, the average concentrations derived for the Goldfish experiments (from Table 9.2) are listed, together with the HEGADAS predictions. The predicted concentrations quoted for 300 m in Table 9.11 are values of the concentration at ground level and at 1 m height.

Taking the set of seven observations, the mean ratio of predicted to observed concentration is 0.89 with a standard deviation of 0.29. The periods of data from which the averages are derived were rather short for Goldfish 1 and Goldfish 2, and more confidence can be attached to the values from Goldfish 3. But in fact, taking Goldfish 3 alone, a very similar result is found (mean 0.91, s.d. 0.34). It should be noted that there would be variations amongst a series of experiments performed in the atmosphere under nominally identical conditions of mean wind, stability, etc. Such variations may well be comparable with the standard deviations found here. The ideal data for comparison would be an ensemble average over many nominally identical releases. However, it is not practically possible to obtain such full scale data. It may be possible, however, to gain insight into this variation through the use of wind-tunnel simulations.

In practice, it is often of interest to determine the distance to a given concentration. Examination of these HEGADAS runs shows that at 1000 m and beyond, the ratio of predicted to observed distance to a given concentration is very close to the square root of the ratio of concentrations at a given distance as quoted in Table 9.11. Thus proportionate uncertainties in distance predictions are roughly half of those for concentration.

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Table 9.1. Parameters describing the experiments Goldfish 1 ("GOLD1"), Goldfish 2 ("GOLD2") and Goldfish 3 ("GOLD3"); the parameters are input to one of more of the programs HFPLUME and HEGADAS (indicated shortly by the letters P, H, respectively); the "note" column refers to the notes listed in Section 9.2.

Data	Symbol	GOLD1	GOLD2	GOLD3	unit	input to	note
RESERVOIR:							
- temperature	T_{res}	40.0	37.8	39.4	°C	P	1
- pressure	P_{res}	8.56	8.83	8.96	atm	P	1
PIPE EXIT-PLANE:							
- orifice diameter	D_{exit}	.0419	.0242	.0242	m	P	3
- orifice height	z_{exit}	1.263	1.263	1.263	m	P	4
RELEASE DATA:							
- HF release rate	E	27.13	10.26	10.07	kg/s	P,H	2
- release duration	T_{dur}	125	360	360	sec	HEGADAS-T	1
AMBIENT:							
- temperature	T_a	37.0	36.0	36.5	°C	P,H	1
- pressure	P_a	1.	1.	1.	atm	P	5
- relative humidity	$100r_H$	5.62	12.6	35.	%	P,H	6
- windspeed at z=2m	u_2	5.6	4.2	5.4	m/s	P,H	1
- surface roughness	z_R	.0002	.0002	.0002	m	P,H	7
- stability class	-	D	D	D	-	P,H	1,8
CONCENTRATION MEASUREMENT:							
- averaging time	t_{av}	60	60	60	sec	(H)	9

Table 9.2. Maximum measured downwind concentration, $c_{\max}$ (% molar fraction), and estimated values for steady-state centre-line concentration, c (% molar fraction); data are at 1 m height

downwind distance (m)	Goldfish 1		Goldfish 2		Goldfish 3	
	$c_{\max}$	c_{AV}	$c_{\max}$	c_{AV}	$c_{\max}$	c_{AV}
300	2.65	2.1	2.00	1.7	1.84	1.6
1000	0.32	0.32	0.27	0.2	0.23	0.23
3000	0.043	?*	?**	?**	0.024	0.02

* steady-state value never achieved

** missing good-quality experimental data

Table 9.3. Estimated values for steady-state temperature difference from ambient ($^{\circ}\text{C}$)

downwind distance (m)	Goldfish 1	Goldfish 2	Goldfish 3
20	-57	-46	-37
40	-54	-30	-16
60	-49	-19	-11
100	-17	-8	-7
200	-8.5	-5	-4
1000	-2	-1	-1

Table 9.4. Comparison of predictions for crosswind dispersion coefficient σ_y (in meters) by Pasquill's formula $\sigma_y = \sigma_\theta f(x) x$ (with $\sigma_\theta = 4^\circ$), the original HEGADAS power-law $\sigma_y = \delta x^\beta = 0.081 x^{0.905}$ and HEGADAS Briggs formula $\sigma_y = \delta x / (1 + \beta x)^{0.5} = 0.05x / (1 + 0.0001x)^{0.5}$ (both corresponding to stability class D, averaging time = 1 minute) and the law $\sigma_y = 0.17 x^{0.79}$ (from fit with Pasquill's formula between $x=400$ and $x=4000$)

x	f(x)	σ_y Pasquill	σ_y HEGADAS	σ_y BRIGGS	$0.17 x^{0.79}$
100	0.8	5.6	5.2	5.0	6.5
200	0.7	9.8	9.8	10.0	11.2
400	0.65	18.1	18.3	19.8	19.3
1000	0.6	41.9	42.0	48.1	39.9
2000	0.5	69.8	78.7	92.1	68.9
4000	0.4	112	147	170.7	119

Table 9.5. HFPLUME predictions of post-flash data

data	Goldfish 1	Goldfish 2	Goldfish 3
temperature (Celsius)	19.55	19.55	19.55
jet velocity (m/s)	47.01	44.75	45.84
jet diameter (m)	0.21	0.12	0.13
liquid HF mass fraction	0.837	0.855	0.842

Table 9.6A. GOLDFISH3. HFPLUME PREDICTIONS (part of .HPR file)

Interpretation:

x: horizontal displacement (m);
 z: plume-axis height (m);
 D: plume effective diameter (m);
 u: mean plume velocity (m/s);
 phi: plume axis inclination (degrees);
 T: mean plume temperature (C);

beta: "volumetric" concentration HF(%);
 r: jet mean density (kg/m³);
 c: HF mass-concentration (kg/m³);
 x: mass-fraction vapour-phase (-);
 alpha: plume mixture void fraction (-);
 dm/dt: total plume mass-flux (kg/s);
 xx hf: total mass-fraction HF (-).

x	z	D	u	phi	T	beta	r	c	x	alpha	dm/dt	xx HF
1.0	1.3	0.32	39.	-0.254	-1.05	87.	4.05	3.34	0.540	1.00	12.	0.82
2.0	1.3	0.49	32.	-0.533	-8.42	73.	2.62	1.72	0.774	1.00	15.	0.65
3.0	1.2	0.66	26.	-0.849	-11.4	61.	2.11	1.11	0.892	1.00	19.	0.52
4.0	1.2	0.84	23.	-1.21	-11.6	52.	1.87	0.799	0.922	1.00	24.	0.43
5.0	1.2	1.0	20.	-1.62	-11.2	44.	1.73	0.614	0.931	1.00	28.	0.36
6.0	1.2	1.2	17.	-2.06	-10.6	38.	1.63	0.491	0.935	1.00	33.	0.30
7.0	1.1	1.4	16.	-2.55	-10.0	33.	1.56	0.403	0.938	1.00	39.	0.26
8.0	1.1	1.6	14.	-3.08	-9.34	29.	1.51	0.338	0.940	1.00	45.	0.22
9.0	1.0	1.8	13.	-3.63	-8.59	26.	1.47	0.287	0.942	1.00	52.	0.20
10.0	0.95	2.1	12.	-3.91	-7.84	23.	1.44	0.250	0.943	1.00	58.	0.17
11.	0.89	2.3	12.	-3.11	-7.27	22.	1.42	0.229	0.944	1.00	63.	0.16
12.	0.84	2.6	11.	-2.15	-6.77	20.	1.41	0.213	0.945	1.00	66.	0.15
13.	0.81	3.0	11.	-1.40	-6.30	20.	1.40	0.202	0.946	1.00	70.	0.14
14.	0.79	3.3	11.	-0.912	-5.86	19.	1.39	0.192	0.947	1.00	73.	0.14
15.	0.78	3.7	10.	-0.606	-5.42	18.	1.38	0.183	0.947	1.00	76.	0.13
16.	0.77	4.0	10.	-0.596	-4.94	17.	1.37	0.176	0.948	1.00	79.	0.13
17.	0.76	4.3	9.9	-0.580	-4.45	17.	1.37	0.169	0.949	1.00	82.	0.12
18.	0.75	4.6	9.7	-0.545	-3.93	16.	1.36	0.162	0.949	1.00	85.	0.12
19.	0.74	4.9	9.6	-0.502	-3.38	16.	1.35	0.156	0.950	1.00	87.	0.12
20.	0.73	5.3	9.4	-0.456	-2.77	15.	1.35	0.150	0.951	1.00	90.	0.11
25.	0.70	7.0	8.7	-0.228	1.07	13.	1.32	0.126	0.955	1.00	1.05E+02	0.095
30.	0.69	9.0	8.1	-4.760E-02	6.14	12.	1.29	0.108	0.959	1.00	1.20E+02	0.083
35.	0.69	11.	7.7	6.356E-02	11.4	10.	1.26	9.339E-02	0.963	1.00	1.36E+02	0.074
40.	0.70	13.	7.4	0.122	16.1	9.3	1.24	8.197E-02	0.966	1.00	1.52E+02	0.066
45.	0.71	15.	7.1	0.147	19.9	8.4	1.22	7.295E-02	0.969	1.00	1.69E+02	0.059
50.	0.73	17.	6.8	0.153	22.9	7.7	1.21	6.574E-02	0.971	1.00	1.85E+02	0.054
55.	0.74	19.	6.6	0.149	25.1	7.1	1.20	5.989E-02	0.973	1.00	2.02E+02	0.050
60.	0.75	20.	6.5	0.140	26.8	6.5	1.19	5.508E-02	0.974	1.00	2.18E+02	0.046
65.	0.76	22.	6.3	0.129	28.0	6.1	1.18	5.105E-02	0.976	1.00	2.34E+02	0.043
70.	0.77	24.	6.2	0.117	29.0	5.7	1.18	4.763E-02	0.977	1.00	2.49E+02	0.040
75.	0.78	25.	6.1	0.106	29.7	5.4	1.18	4.470E-02	0.979	1.00	2.65E+02	0.038
76.	0.79	26.	6.1	0.103	29.8	5.3	1.18	4.417E-02	0.979	1.00	2.68E+02	0.037
77.	0.79	26.	6.1	0.101	29.9	5.3	1.17	4.365E-02	0.979	1.00	2.71E+02	0.037
78.	0.79	26.	6.1	9.890E-02	30.0	5.2	1.17	4.314E-02	0.979	1.00	2.74E+02	0.036
79.	0.79	27.	6.0	9.674E-02	30.1	5.2	1.17	4.264E-02	0.980	1.00	2.77E+02	0.036
80.	0.79	27.	6.0	8.706E-02	30.2	5.1	1.17	4.217E-02	0.980	1.00	2.80E+02	0.035
85.	0.80	29.	6.0	7.309E-02	30.6	4.9	1.17	4.000E-02	0.981	1.00	2.95E+02	0.034
86.	0.80	29.	5.9	7.152E-02	30.7	4.8	1.17	3.960E-02	0.981	1.00	2.98E+02	0.033
87.	0.80	29.	5.9	6.996E-02	30.8	4.8	1.17	3.920E-02	0.981	1.00	3.01E+02	0.033
88.	0.80	30.	5.9	6.842E-02	30.8	4.7	1.17	3.882E-02	0.981	1.00	3.03E+02	0.033
89.	0.80	30.	5.9	6.689E-02	30.9	4.7	1.17	3.844E-02	0.982	1.00	3.06E+02	0.032
90.	0.81	30.	5.9	6.538E-02	31.0	4.6	1.17	3.808E-02	0.982	1.00	3.09E+02	0.032
91.	0.81	30.	5.9	6.388E-02	31.0	4.6	1.17	3.772E-02	0.982	1.00	3.12E+02	0.032
92.	0.81	31.	5.9	6.240E-02	31.1	4.6	1.17	3.737E-02	0.982	1.00	3.15E+02	0.032
93.	0.81	31.	5.9	6.094E-02	31.1	4.5	1.17	3.702E-02	0.982	1.00	3.18E+02	0.031
94.	0.81	31.	5.8	5.981E-02	31.2	4.5	1.17	3.676E-02	0.982	1.00	3.20E+02	0.031
94.	0.81	31.	5.8	5.981E-02	31.2	4.5	1.17	3.676E-02	0.982	1.00	3.20E+02	0.031

Table 9.68. GOLDFISH3. CONTRIBUTIONS TO VOLUMETRIC ENTRAINMENT DURING VARIOUS STAGES OF "HFPLUME" PLUME (part of .HP2 file)

Interpretation:								Interpretation:		
dx: plume centroid displacement (m);								aspect: plume cross-section aspect-ratio (-);		
entr: total entrainment/unit axis length (kg/s/m);								u/u_atm: ratio of plume to ambient speed		
jet: proportion jet entrainment (-);								stage: stage (geometry) of plume development (-);		
pass: proportion passive entrainment (-);										
cross: proportion cross-wind entrainment (-);										
slump: gravity-slumping entrainment part (-);										
heavy: heavy-gas advection entrainment (-)										
Ri: heavy-gas (bulk) Richardson number (-).										
dx	entr	jet	pass	cross	slump	heavy	Ri	u/u_atm	aspect	stage
1.0	2.7	0.93	0.07	0.00	0.00	0.00	0.000E-01	7.54	1.0	airborne
2.0	3.6	0.90	0.09	0.01	0.00	0.00	0.000E-01	6.20	1.0	airborne
3.0	4.1	0.87	0.12	0.01	0.00	0.00	0.000E-01	5.17	1.0	airborne
4.0	4.6	0.83	0.15	0.02	0.00	0.00	0.000E-01	4.41	1.0	airborne
5.0	5.0	0.78	0.18	0.03	0.00	0.00	0.000E-01	3.85	1.0	airborne
6.0	5.4	0.74	0.21	0.05	0.00	0.00	0.000E-01	3.42	1.0	airborne
7.0	5.8	0.69	0.24	0.07	0.00	0.00	0.000E-01	3.09	1.0	airborne
8.0	6.3	0.64	0.27	0.09	0.00	0.00	0.000E-01	2.82	1.0	airborne
9.0	6.7	0.59	0.29	0.12	0.00	0.00	0.000E-01	2.61	1.0	airborne
10.0	5.1	0.67	0.32	0.00	0.00	0.00	89.0	2.45	0.95	touchdown <-- touchdown
11.	4.2	0.72	0.25	0.00	0.01	0.01	78.3	2.36	0.83	touchdown
12.	3.6	0.79	0.17	0.00	0.02	0.02	71.1	2.29	0.72	touchdown
13.	3.2	0.86	0.09	0.00	0.03	0.02	66.1	2.23	0.63	touchdown
14.	2.9	0.92	0.03	0.00	0.03	0.03	62.4	2.18	0.56	touchdown
15.	2.9	0.91	0.00	0.00	0.06	0.03	59.8	2.14	0.50	touchdown
16.	2.9	0.92	0.00	0.00	0.05	0.04	57.1	2.09	0.46	slumped <-- slumping
17.	2.9	0.91	0.00	0.00	0.05	0.04	54.7	2.05	0.42	slumped
18.	2.9	0.91	0.00	0.00	0.05	0.04	52.6	2.02	0.38	slumped
19.	2.9	0.91	0.00	0.00	0.05	0.05	50.5	1.99	0.35	slumped
20.	2.9	0.90	0.00	0.00	0.05	0.05	48.6	1.95	0.33	slumped
25.	3.0	0.88	0.00	0.00	0.04	0.07	40.2	1.82	0.24	slumped
30.	3.1	0.86	0.00	0.00	0.04	0.10	33.3	1.70	0.18	slumped
35.	3.2	0.83	0.00	0.00	0.04	0.13	27.6	1.61	0.15	slumped
40.	3.3	0.80	0.00	0.00	0.03	0.16	23.1	1.54	0.13	slumped
45.	3.3	0.77	0.00	0.00	0.03	0.20	19.7	1.47	0.11	slumped
50.	3.3	0.73	0.00	0.00	0.03	0.24	17.0	1.42	0.10	slumped
55.	3.3	0.69	0.00	0.00	0.03	0.28	15.0	1.38	9.41E-02	slumped
60.	3.2	0.66	0.00	0.00	0.03	0.31	13.5	1.34	8.73E-02	slumped
65.	3.2	0.64	0.00	0.00	0.03	0.33	12.3	1.31	8.17E-02	slumped
70.	3.1	0.62	0.00	0.00	0.03	0.35	11.3	1.28	7.69E-02	slumped
75.	3.1	0.59	0.00	0.00	0.03	0.38	10.6	1.26	7.28E-02	slumped
76.	3.1	0.59	0.00	0.00	0.03	0.38	10.4	1.26	7.21E-02	slumped
77.	3.1	0.59	0.00	0.00	0.03	0.39	10.3	1.25	7.13E-02	slumped
78.	3.0	0.58	0.00	0.00	0.03	0.39	10.2	1.25	7.06E-02	slumped
79.	3.0	0.58	0.00	0.00	0.03	0.39	10.1	1.25	6.99E-02	slumped <-- RI = 10 switch off gravity-slumping entrainment
80.	2.9	0.59	0.00	0.00	0.00	0.41	9.97	1.24	6.92E-02	slumped <-- RE = 0.60 = RELST
81.	2.9	0.59	0.00	0.00	0.00	0.41	9.85	1.24	6.85E-02	slumped
82.	2.9	0.58	0.00	0.00	0.00	0.42	9.74	1.23	6.79E-02	slumped
83.	2.9	0.58	0.00	0.00	0.00	0.42	9.64	1.23	6.72E-02	slumped
84.	2.9	0.57	0.00	0.00	0.00	0.43	9.55	1.23	6.66E-02	slumped
85.	2.9	0.57	0.00	0.00	0.00	0.43	9.45	1.22	6.59E-02	slumped
86.	2.9	0.57	0.00	0.00	0.00	0.43	9.36	1.22	6.53E-02	slumped
87.	2.9	0.56	0.00	0.00	0.00	0.44	9.27	1.22	6.47E-02	slumped
88.	2.9	0.56	0.00	0.00	0.00	0.44	9.19	1.22	6.42E-02	slumped
89.	2.9	0.56	0.00	0.00	0.00	0.44	9.10	1.21	6.36E-02	slumped
90.	2.8	0.55	0.00	0.00	0.00	0.45	9.03	1.21	6.30E-02	slumped
91.	2.8	0.55	0.00	0.00	0.00	0.45	8.95	1.21	6.25E-02	slumped
92.	2.8	0.54	0.00	0.00	0.00	0.46	8.87	1.20	6.19E-02	slumped
93.	2.8	0.54	0.00	0.00	0.00	0.46	8.80	1.20	6.14E-02	slumped
94.	2.8	0.54	0.00	0.00	0.00	0.46	8.75	1.20	6.10E-02	slumped
94.	2.8	0.54	0.00	0.00	0.00	0.46	8.75	1.20	6.10E-02	slumped <-- RU = 1.20 = RULST

Table 9.7A. GOLDFISH3. PREDICTIONS BY HEGADAS-S BASED ON HFPLUME LINK
=====[part of .HSR file; see HEGADAS user's guide (Appendix
8.D in User's Manual) for precise meaning of data]

DISTANCE (M)	CONC (% VOL.)	SZ (M)	SY (M)	MIDP (M)	YCU (M)	ZCU (M)	YCL (M)	ZCL (M)	RIB	TMP (DEG.C)	CA (KG/M3)	
- breakpoint at DISTS = 93.8 m												
93.8	6.34	1.58	0.000E-01	13.0	13.0	8.71	13.0	11.2	12.3	27.4	5.14E-02	VISIBLE
100.	6.16	1.50	3.71	10.9	20.7	8.25	22.2	10.6	11.2	27.9	4.99E-02	VISIBLE
200.	3.14	1.47	18.2	13.3	58.8	7.37	66.6	9.74	5.07	32.7	2.50E-02	VISIBLE
300.	1.64	1.94	28.0	16.8	82.9	8.82	95.3	12.0	4.54	33.1	1.31E-02	VISIBLE
400.	1.02	2.37	36.6	21.3	104.	9.96	121.	13.8	5.36	32.4	8.10E-03	VISIBLE
500.	0.701	2.71	44.8	27.1	124.	10.7	146.	15.2	6.45	31.7	5.61E-03	VISIBLE
600.	0.517	3.00	52.7	34.1	145.	11.1	171.	16.1	7.15	31.4	4.14E-03	
700.	0.392	3.36	60.4	40.6	163.	11.8	194.	17.4	5.97	32.7	3.12E-03	
800.	0.302	3.81	67.9	46.0	180.	12.6	215.	19.0	5.14	33.6	2.40E-03	
900.	0.238	4.32	75.2	50.7	194.	13.5	234.	20.8	4.52	34.2	1.89E-03	
1.000E+03	0.191	4.95	82.3	52.3	204.	14.6	249.	23.1	4.11	34.7	1.51E-03	
1.100E+03	0.159	5.83	88.9	46.6	206.	16.4	256.	26.4	3.97	35.0	1.26E-03	
1.200E+03	0.135	6.70	95.1	41.4	208.	18.0	262.	29.5	3.84	35.2	1.07E-03	
1.300E+03	0.118	7.56	101.	36.5	209.	19.5	267.	32.6	3.73	35.4	9.32E-04	
1.400E+03	0.104	8.42	106.	31.9	210.	20.9	272.	35.5	3.63	35.5	8.23E-04	
1.500E+03	9.326E-02	9.27	112.	27.6	211.	22.2	277.	38.3	3.54	35.6	7.37E-04	
1.600E+03	8.430E-02	10.1	117.	23.5	211.	23.4	282.	41.1	3.46	35.7	6.66E-04	
1.700E+03	7.683E-02	11.0	121.	19.6	211.	24.6	286.	43.7	3.38	35.8	6.07E-04	
1.800E+03	7.052E-02	11.8	126.	15.8	212.	25.6	290.	46.3	3.31	35.9	5.57E-04	
1.900E+03	6.512E-02	12.6	131.	12.2	212.	26.6	293.	48.9	3.24	35.9	5.14E-04	
2.000E+03	6.044E-02	13.4	135.	8.68	211.	27.6	297.	51.3	3.18	35.9	4.77E-04	
2.100E+03	5.635E-02	14.3	139.	5.32	211.	28.5	300.	53.7	3.11	36.0	4.45E-04	
2.200E+03	5.274E-02	15.1	143.	2.06	211.	29.3	303.	56.1	3.05	36.0	4.16E-04	
2.265E+03	5.062E-02	15.6	146.	0.000E-01	210.	29.8	305.	57.6	3.02	36.0	3.99E-04	
2.300E+03	4.908E-02	15.9	147.	0.000E-01	211.	30.0	307.	58.3	2.96	36.1	3.87E-04	
2.400E+03	4.501E-02	16.8	151.	0.000E-01	212.	30.4	312.	60.4	2.82	36.1	3.55E-04	
2.500E+03	4.142E-02	17.7	155.	0.000E-01	213.	30.8	317.	62.4	2.68	36.1	3.27E-04	
2.600E+03	3.824E-02	18.5	159.	0.000E-01	213.	31.1	322.	64.5	2.55	36.2	3.01E-04	
2.700E+03	3.539E-02	19.4	163.	0.000E-01	214.	31.4	327.	66.4	2.43	36.2	2.79E-04	
2.800E+03	3.285E-02	20.3	167.	0.000E-01	214.	31.6	331.	68.4	2.31	36.2	2.59E-04	
2.900E+03	3.056E-02	21.3	171.	0.000E-01	214.	31.7	336.	70.3	2.20	36.2	2.41E-04	
3.000E+03	2.849E-02	22.2	174.	0.000E-01	214.	31.8	340.	72.1	2.10	36.2	2.25E-04	
3.100E+03	2.662E-02	23.1	178.	0.000E-01	213.	31.8	345.	74.0	2.00	36.3	2.10E-04	
3.200E+03	2.492E-02	24.0	182.	0.000E-01	213.	31.7	349.	75.8	1.90	36.3	1.96E-04	
3.300E+03	2.338E-02	25.0	186.	0.000E-01	212.	31.6	353.	77.5	1.80	36.3	1.84E-04	
3.400E+03	2.196E-02	25.9	189.	0.000E-01	211.	31.4	357.	79.3	1.71	36.3	1.73E-04	
3.500E+03	2.067E-02	26.9	193.	0.000E-01	210.	31.2	361.	81.0	1.63	36.3	1.63E-04	
3.600E+03	1.948E-02	27.9	197.	0.000E-01	208.	30.9	364.	82.7	1.54	36.3	1.54E-04	
3.700E+03	1.839E-02	28.9	201.	0.000E-01	207.	30.5	368.	84.3	1.46	36.3	1.45E-04	
3.800E+03	1.738E-02	29.9	204.	0.000E-01	205.	30.1	371.	85.9	1.38	36.4	1.37E-04	
3.900E+03	1.645E-02	30.9	208.	0.000E-01	203.	29.6	375.	87.5	1.31	36.4	1.30E-04	
4.000E+03	1.559E-02	31.9	211.	0.000E-01	200.	29.0	378.	89.1	1.23	36.4	1.23E-04	

Table 9.7B. GOLDFISH3. PREDICTIONS BY HEGADAS-S BASED ON HFPLUME LINK; HF-DATA

[part of .HSF file; see HEGADAS user's guide
(Appendix 8.D in User's Manual) for precise
meaning of data]

DISTANCE (M)	FRAMOL	Y11 (monomer)	Y12 (dimer)	Y16 (hexamer)	Y18 (octomer)	YC (complex)	Y2 (water)	YA (air)	TMP (Celsius)	XL (HF-fog)	LFOG (fog moles)	FOG
93.8	6.336E-02	4.504E-02	1.296E-04	1.362E-08	2.714E-11	4.755E-05	2.676E-03	0.952	27.4	0.535	3.683E-02	VISIBLE
100.	6.156E-02	4.384E-02	1.185E-04	1.029E-08	1.899E-11	5.042E-05	2.967E-03	0.953	27.9	0.530	3.591E-02	VISIBLE
200.	3.135E-02	2.343E-02	2.411E-05	7.880E-11	3.341E-14	7.985E-05	1.039E-02	0.966	32.7	0.448	1.840E-02	VISIBLE
300.	1.643E-02	1.310E-02	7.315E-06	2.183E-12	2.838E-16	6.586E-05	1.555E-02	0.971	33.1	0.390	8.646E-03	VISIBLE
400.	1.015E-02	8.716E-03	3.404E-06	2.231E-13	1.326E-17	5.295E-05	1.833E-02	0.973	32.4	0.355	3.985E-03	VISIBLE
500.	7.009E-03	6.505E-03	1.994E-06	4.549E-14	1.556E-18	4.417E-05	1.999E-02	0.973	31.7	0.331	1.408E-03	VISIBLE
600.	5.174E-03	5.136E-03	1.268E-06	1.174E-14	2.535E-19	3.690E-05	2.095E-02	0.974	31.4	-	-	-
700.	3.916E-03	3.889E-03	6.653E-07	1.657E-15	1.937E-20	2.680E-05	2.099E-02	0.975	32.7	-	-	-
800.	3.019E-03	2.998E-03	3.718E-07	2.842E-16	1.899E-21	2.007E-05	2.101E-02	0.976	33.6	-	-	-
900.	2.377E-03	2.361E-03	2.208E-07	5.882E-17	2.371E-22	1.549E-05	2.103E-02	0.977	34.2	-	-	-
1.000E+03	1.912E-03	1.900E-03	1.386E-07	1.440E-17	3.683E-23	1.228E-05	2.104E-02	0.977	34.7	-	-	-
1.100E+03	1.588E-03	1.577E-03	9.350E-08	4.399E-18	7.650E-24	1.009E-05	2.105E-02	0.977	35.0	-	-	-
1.200E+03	1.354E-03	1.346E-03	6.702E-08	1.613E-18	2.022E-24	8.550E-06	2.106E-02	0.978	35.2	-	-	-
1.300E+03	1.179E-03	1.171E-03	5.020E-08	6.756E-19	6.369E-25	7.403E-06	2.106E-02	0.978	35.4	-	-	-
1.400E+03	1.042E-03	1.036E-03	3.888E-08	3.131E-19	2.294E-25	6.517E-06	2.107E-02	0.978	35.5	-	-	-
1.500E+03	9.326E-04	9.267E-04	3.092E-08	1.572E-19	9.180E-26	5.813E-06	2.107E-02	0.978	35.6	-	-	-
1.600E+03	8.430E-04	8.377E-04	2.512E-08	8.415E-20	4.001E-26	5.240E-06	2.107E-02	0.978	35.7	-	-	-
1.700E+03	7.683E-04	7.636E-04	2.077E-08	4.750E-20	1.871E-26	4.765E-06	2.107E-02	0.978	35.8	-	-	-
1.800E+03	7.052E-04	7.008E-04	1.743E-08	2.803E-20	9.276E-27	4.366E-06	2.108E-02	0.978	35.9	-	-	-
1.900E+03	6.512E-04	6.471E-04	1.481E-08	1.718E-20	4.836E-27	4.025E-06	2.108E-02	0.978	35.9	-	-	-
2.000E+03	6.044E-04	6.006E-04	1.272E-08	1.088E-20	2.632E-27	3.730E-06	2.108E-02	0.978	35.9	-	-	-
2.100E+03	5.635E-04	5.600E-04	1.103E-08	7.082E-21	1.488E-27	3.474E-06	2.108E-02	0.978	36.0	-	-	-
2.200E+03	5.274E-04	5.242E-04	9.640E-09	4.727E-21	8.688E-28	3.248E-06	2.108E-02	0.978	36.0	-	-	-
2.265E+03	5.062E-04	5.031E-04	8.869E-09	3.680E-21	6.225E-28	3.115E-06	2.108E-02	0.978	36.0	-	-	-
2.300E+03	4.908E-04	4.877E-04	8.327E-09	3.045E-21	4.837E-28	3.019E-06	2.108E-02	0.978	36.1	-	-	-
2.400E+03	4.501E-04	4.473E-04	6.986E-09	1.797E-21	2.397E-28	2.765E-06	2.108E-02	0.978	36.1	-	-	-
2.500E+03	4.142E-04	4.117E-04	5.903E-09	1.083E-21	1.222E-28	2.542E-06	2.108E-02	0.979	36.1	-	-	-
2.600E+03	3.824E-04	3.800E-04	5.019E-09	6.657E-22	6.391E-29	2.344E-06	2.108E-02	0.979	36.2	-	-	-
2.700E+03	3.539E-04	3.518E-04	4.293E-09	4.163E-22	3.421E-29	2.168E-06	2.109E-02	0.979	36.2	-	-	-
2.800E+03	3.285E-04	3.265E-04	3.692E-09	2.646E-22	1.871E-29	2.011E-06	2.109E-02	0.979	36.2	-	-	-
2.900E+03	3.056E-04	3.037E-04	3.191E-09	1.707E-22	1.044E-29	1.869E-06	2.109E-02	0.979	36.2	-	-	-
3.000E+03	2.849E-04	2.832E-04	2.770E-09	1.117E-22	5.933E-30	1.742E-06	2.109E-02	0.979	36.2	-	-	-
3.100E+03	2.662E-04	2.646E-04	2.416E-09	7.405E-23	3.431E-30	1.627E-06	2.109E-02	0.979	36.3	-	-	-
3.200E+03	2.492E-04	2.477E-04	2.115E-09	4.969E-23	2.016E-30	1.522E-06	2.109E-02	0.979	36.3	-	-	-
3.300E+03	2.338E-04	2.323E-04	1.859E-09	3.372E-23	1.203E-30	1.427E-06	2.109E-02	0.979	36.3	-	-	-
3.400E+03	2.196E-04	2.183E-04	1.640E-09	2.313E-23	7.281E-31	1.340E-06	2.109E-02	0.979	36.3	-	-	-
3.500E+03	2.067E-04	2.054E-04	1.451E-09	1.603E-23	4.465E-31	1.261E-06	2.109E-02	0.979	36.3	-	-	-
3.600E+03	1.948E-04	1.936E-04	1.288E-09	1.121E-23	2.773E-31	1.188E-06	2.109E-02	0.979	36.3	-	-	-
3.700E+03	1.839E-04	1.828E-04	1.147E-09	7.908E-24	1.742E-31	1.121E-06	2.109E-02	0.979	36.3	-	-	-
3.800E+03	1.738E-04	1.727E-04	1.024E-09	5.626E-24	1.107E-31	1.059E-06	2.109E-02	0.979	36.4	-	-	-
3.900E+03	1.645E-04	1.635E-04	9.164E-10	4.035E-24	7.107E-32	1.002E-06	2.109E-02	0.979	36.4	-	-	-
4.000E+03	1.559E-04	1.549E-04	8.223E-10	2.915E-24	4.608E-32	9.493E-07	2.109E-02	0.979	36.4	-	-	-

Table 9.8. GOLDFISH2. PREDICTIONS BY HEGADAS-S BASED ON HFPLUME LINK
=====[part of .HSR file; see HEGADAS user's guide (Appendix
8.D in User's Manual) for precise meaning of data]

DISTANCE (M)	CONC (% VOL.)	SZ (M)	SY (M)	MIDP (M)	YCU (M)	ZCU (M)	YCL (M)	ZCL (M)	RIB	TMP (DEG.C)	CA (KG/M3)	
- breakpoint at DIST = 143. m												
143.	3.91	1.45	0.000E-01	30.1	30.1	7.54	30.1	9.86	25.0	17.1	3.28E-02	VISIBLE
200.	3.06	1.28	18.0	29.1	74.0	6.42	81.6	8.47	17.4	20.8	2.54E-02	VISIBLE
300.	1.86	1.40	33.0	38.7	118.	6.52	132.	8.78	14.6	23.5	1.53E-02	VISIBLE
400.	1.19	1.63	45.4	49.5	154.	7.07	174.	9.73	14.6	24.6	9.76E-03	VISIBLE
500.	0.805	1.94	56.8	59.8	185.	7.86	212.	11.1	11.7	28.3	6.52E-03	
600.	0.566	2.34	67.4	68.3	211.	8.84	244.	12.7	9.63	30.6	4.54E-03	
700.	0.417	2.92	77.3	67.0	225.	10.4	264.	15.3	8.70	32.1	3.33E-03	
800.	0.328	3.62	86.2	59.5	231.	12.2	275.	18.3	8.31	33.0	2.61E-03	
900.	0.269	4.30	94.2	52.9	235.	13.8	285.	21.1	8.00	33.5	2.14E-03	
1.000E+03	0.227	4.98	102.	46.8	239.	15.4	293.	23.8	7.74	33.9	1.81E-03	
1.100E+03	0.196	5.65	109.	41.1	243.	16.8	301.	26.4	7.51	34.2	1.56E-03	
1.200E+03	0.173	6.32	115.	35.9	245.	18.2	309.	29.0	7.30	34.4	1.37E-03	
1.300E+03	0.154	6.98	121.	31.0	248.	19.4	315.	31.4	7.11	34.6	1.22E-03	
1.400E+03	0.138	7.64	127.	26.3	250.	20.7	322.	33.8	6.94	34.8	1.09E-03	
1.500E+03	0.125	8.29	133.	21.9	252.	21.8	328.	36.1	6.77	34.9	9.93E-04	
1.600E+03	0.115	8.93	138.	17.7	253.	22.9	333.	38.3	6.62	35.0	9.08E-04	
1.700E+03	0.106	9.58	144.	13.7	255.	23.9	339.	40.5	6.48	35.1	8.35E-04	
1.800E+03	9.760E-02	10.2	149.	9.90	256.	24.9	344.	42.6	6.35	35.1	7.72E-04	
1.900E+03	9.071E-02	10.9	154.	6.20	257.	25.8	349.	44.7	6.22	35.2	7.17E-04	
2.000E+03	8.466E-02	11.5	159.	2.65	258.	26.7	354.	46.7	6.10	35.3	6.69E-04	
2.077E+03	8.049E-02	12.0	162.	0.000E-01	259.	27.3	357.	48.2	6.00	35.3	6.36E-04	
2.100E+03	7.877E-02	12.1	163.	0.000E-01	259.	27.5	359.	48.7	5.93	35.3	6.23E-04	
2.200E+03	7.195E-02	12.8	168.	0.000E-01	262.	28.1	365.	50.6	5.64	35.4	5.69E-04	
2.300E+03	6.595E-02	13.5	173.	0.000E-01	264.	28.7	372.	52.5	5.37	35.4	5.21E-04	
2.400E+03	6.064E-02	14.2	177.	0.000E-01	266.	29.2	378.	54.4	5.11	35.5	4.79E-04	
2.500E+03	5.593E-02	15.0	182.	0.000E-01	268.	29.7	384.	56.2	4.87	35.5	4.42E-04	
2.600E+03	5.172E-02	15.7	186.	0.000E-01	270.	30.2	391.	58.0	4.64	35.6	4.09E-04	
2.700E+03	4.795E-02	16.4	191.	0.000E-01	271.	30.6	396.	59.8	4.42	35.6	3.79E-04	
2.800E+03	4.456E-02	17.2	195.	0.000E-01	272.	31.0	402.	61.6	4.21	35.6	3.52E-04	
2.900E+03	4.150E-02	17.9	199.	0.000E-01	274.	31.3	408.	63.4	4.02	35.7	3.28E-04	
3.000E+03	3.873E-02	18.7	204.	0.000E-01	274.	31.6	413.	65.1	3.83	35.7	3.06E-04	
3.100E+03	3.622E-02	19.5	208.	0.000E-01	275.	31.8	419.	66.8	3.65	35.7	2.86E-04	
3.200E+03	3.393E-02	20.2	213.	0.000E-01	275.	32.0	424.	68.5	3.48	35.7	2.68E-04	
3.300E+03	3.184E-02	21.0	217.	0.000E-01	276.	32.1	429.	70.2	3.32	35.7	2.51E-04	
3.400E+03	2.992E-02	21.8	221.	0.000E-01	276.	32.2	434.	71.9	3.16	35.8	2.36E-04	
3.500E+03	2.816E-02	22.7	225.	0.000E-01	275.	32.3	439.	73.5	3.00	35.8	2.22E-04	
3.600E+03	2.655E-02	23.5	230.	0.000E-01	275.	32.3	444.	75.2	2.86	35.8	2.10E-04	
3.700E+03	2.506E-02	24.3	234.	0.000E-01	274.	32.2	449.	76.8	2.71	35.8	1.98E-04	
3.800E+03	2.368E-02	25.2	238.	0.000E-01	274.	32.1	453.	78.4	2.58	35.8	1.87E-04	
3.900E+03	2.240E-02	26.0	242.	0.000E-01	272.	32.0	458.	79.9	2.44	35.8	1.77E-04	
4.000E+03	2.122E-02	26.9	247.	0.000E-01	271.	31.8	462.	81.5	2.31	35.8	1.68E-04	

Table 9.9. GOLDFISH1. PREDICTIONS BY HEGADAS-S BASED ON HFPLUME LINK
=====[part of .HSR file; see HEGADAS user's guide (Appendix
8.D in User's Manual) for precise meaning of data]

DISTANCE (M)	CONC (% VOL.)	SZ (M)	SY (M)	MIDP (M)	YCU (M)	ZCU (M)	YCL (M)	ZCL (M)	RIB	TMP (DEG.C)	CA (KG/M3)
- breakpoint at DIST = 188. m											
188.	5.03	1.60	0.000E-01	39.1	39.1	8.68	39.1	11.2	28.6	1.15	4.47E-02 VISIBLE
200.	4.86	1.54	8.24	35.3	56.7	8.29	60.1	10.7	26.4	2.43	4.30E-02 VISIBLE
300.	3.35	1.46	27.9	43.3	114.	7.48	125.	9.84	16.6	13.5	2.85E-02 VISIBLE
400.	2.22	1.68	41.2	53.2	153.	8.08	171.	10.8	13.8	19.2	1.85E-02 VISIBLE
500.	1.54	1.96	52.9	63.4	188.	8.88	211.	12.1	12.9	22.2	1.27E-02
600.	1.11	2.32	63.6	72.6	217.	9.92	247.	13.7	10.6	26.6	9.00E-03
700.	0.819	2.73	73.6	80.5	243.	11.1	278.	15.6	9.05	29.4	6.60E-03
800.	0.635	3.40	82.9	74.3	253.	13.1	292.	18.8	8.55	31.2	5.09E-03
900.	0.516	4.08	91.3	67.3	259.	15.1	304.	21.9	8.23	32.3	4.12E-03
1.000E+03	0.434	4.76	98.9	60.9	265.	17.0	314.	25.0	7.95	33.1	3.45E-03
1.100E+03	0.373	5.43	106.	55.1	269.	18.8	323.	27.9	7.72	33.6	2.96E-03
1.200E+03	0.326	6.10	113.	49.7	274.	20.5	332.	30.7	7.52	34.1	2.59E-03
1.300E+03	0.290	6.76	119.	44.6	278.	22.1	339.	33.5	7.33	34.4	2.30E-03
1.400E+03	0.260	7.41	125.	39.8	281.	23.6	347.	36.2	7.16	34.7	2.06E-03
1.500E+03	0.236	8.06	131.	35.3	284.	25.1	354.	38.8	7.01	34.9	1.87E-03
1.600E+03	0.215	8.71	136.	31.0	287.	26.5	361.	41.3	6.87	35.1	1.70E-03
1.700E+03	0.198	9.35	142.	26.9	290.	27.9	367.	43.8	6.73	35.3	1.57E-03
1.800E+03	0.183	9.98	147.	23.0	293.	29.2	373.	46.2	6.61	35.4	1.45E-03
1.900E+03	0.170	10.6	152.	19.2	295.	30.4	379.	48.6	6.49	35.5	1.34E-03
2.000E+03	0.159	11.2	157.	15.6	297.	31.6	384.	50.9	6.37	35.6	1.25E-03
2.100E+03	0.149	11.9	162.	12.1	299.	32.8	390.	53.1	6.27	35.7	1.17E-03
2.200E+03	0.140	12.5	166.	8.73	301.	33.9	395.	55.4	6.16	35.8	1.10E-03
2.300E+03	0.132	13.1	171.	5.47	303.	34.9	400.	57.5	6.06	35.9	1.04E-03
2.400E+03	0.124	13.7	175.	2.30	304.	36.0	405.	59.7	5.97	35.9	9.81E-04
2.475E+03	0.119	14.2	178.	0.000E-01	306.	36.7	408.	61.3	5.90	36.0	9.42E-04
2.500E+03	0.117	14.4	179.	0.000E-01	306.	37.0	410.	61.8	5.84	36.0	9.24E-04
2.600E+03	0.109	15.0	184.	0.000E-01	310.	37.8	416.	63.9	5.60	36.1	8.56E-04
2.700E+03	0.101	15.7	188.	0.000E-01	313.	38.6	423.	66.0	5.38	36.1	7.96E-04
2.800E+03	9.402E-02	16.4	192.	0.000E-01	315.	39.4	429.	68.0	5.17	36.2	7.41E-04
2.900E+03	8.777E-02	17.1	196.	0.000E-01	318.	40.2	436.	70.1	4.97	36.3	6.92E-04
3.000E+03	8.211E-02	17.8	200.	0.000E-01	321.	40.9	442.	72.1	4.78	36.3	6.47E-04
3.100E+03	7.696E-02	18.6	205.	0.000E-01	323.	41.6	448.	74.1	4.60	36.4	6.06E-04
3.200E+03	7.226E-02	19.3	209.	0.000E-01	325.	42.2	454.	76.1	4.43	36.4	5.69E-04
3.300E+03	6.796E-02	20.0	213.	0.000E-01	328.	42.9	460.	78.0	4.26	36.4	5.35E-04
3.400E+03	6.401E-02	20.7	217.	0.000E-01	330.	43.4	466.	80.0	4.11	36.5	5.04E-04
3.500E+03	6.039E-02	21.5	221.	0.000E-01	332.	44.0	472.	81.9	3.96	36.5	4.76E-04
3.600E+03	5.705E-02	22.2	225.	0.000E-01	333.	44.5	477.	83.8	3.81	36.5	4.49E-04
3.700E+03	5.397E-02	23.0	229.	0.000E-01	335.	45.0	483.	85.8	3.68	36.6	4.25E-04
3.800E+03	5.112E-02	23.7	233.	0.000E-01	336.	45.4	488.	87.6	3.54	36.6	4.03E-04
3.900E+03	4.848E-02	24.5	237.	0.000E-01	338.	45.9	493.	89.5	3.41	36.6	3.82E-04
4.000E+03	4.603E-02	25.3	241.	0.000E-01	339.	46.3	499.	91.4	3.29	36.6	3.62E-04

Table 9.10. GOLDFISH1. PREDICTIONS BY HEGADAS-T BASED ON HFPLUME LINK [data from .HTR file; see HEGADAS user's guide (Appendix 8.D in User's Manual) for precise meaning of data]
 [Dispersion data at times 100,120,180,225,280,310,380,420,460,500,550,600,650,700 are not printed for reasons of brevity]

HTMAIN
DATE 07/11/90

HEGADAS-T PROGRAM (VERSION NOV90)
STANDARD REPORT FILE

PAGE 0
TIME 09:32

<<< Transient simulation of Goldfish 1 experiment >>>

=====

HEGADAS-T INPUT DATA

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-----> CONTROL data block: control parameters
OUTPUT CODE          ICNT =      0      (no output of cumulative cloud data)
SURFACE-TRANSFER CODE ISURF =     3      (only heat transfer, no water vapour)
GAS-BLANKET FORMULATION BLMODEL =    1      (new, non-oscillatory formulation)
CLOUD-SHAPE CORRECTION CODE ICSCOR =    1      (correction included)

-----> AMBIENT data block: ambient data
AIR TEMP. AT HEIGHT ZAIRTEMP AIRTEMP = 37.000 CELSIUS
REF. HEIGHT FOR AIR TEMP. ZAIRTEMP = 0.89800 M
RELATIVE HUMIDITY RHPERC = 5.6200 %
WIND VELOCITY AT HEIGHT ZO UO = 5.6000 M/S
REFERENCE HEIGHT FOR WIND VEL. ZO = 2.0000 M
EARTH-S SURFACE TEMPERATURE TGROUND = TAP (see below for value of TAP)

-----> DISP data block: dispersion data
SURFACE ROUGHNESS PARAMETER ZR = 2.00000E-04 M
PASQUILL STABILITY CLASS POSTAB = 0
MONIN - OBUKHOV LENGTH OBUKL = 1.00000E+05 M
TYPE OF FORMULA FOR SIGMA_Y MODSY = 1 (power-law)
      with parameters: DELTA = 0.21000 M**(1-BETA)
                      BETA = 0.79000
CONST. IN GRAV. SPREADING LAW CE = 1.1500
CONST. IN GRAV. SPREADING LAW CD = 5.0000
TYPE OF FORMULA FOR SIGMA_X MODSX = 3 (Chatwin/Wilson)
      with parameters: ASIGX = 10.000
                      BSIGX = 0.10000

-----> GASDATA data block: gas data
TEMPERATURE OF EMITTED GAS TEMPGAS = 19.500 CELSIUS
SPECIFIC HEAT OF EMITTED GAS CPGAS = 29.100 J/MOLE/CELSIUS
MOLECULAR WEIGHT OF EM. GAS MWGAS = 20.000 KG/KMOLE
PICKED-UP WATER BY EM. GAS WATGAS = 0.00000E-01 (MOLAR FRACTION)
HEAT GROUP IN HEAT FLUX QH HEATGR = 24.000
THERMODYNAMIC MODEL THERMOO = 2 (hydrogen fluoride)
INITIAL LIQUID IN HF HFLIQFR = 0.83700 (MASS FRACTION)

-----> TIMEDATA data block: source/breakpoint data
TIME-DEPENDENT RECORD DATA: ITPBR = 2 (breakpoint data: B_eff, CONC, GSFLOW)
- skip increment for reading INCRT = 0
- start time for data TSTPOOL = 23.200 S
- time step between read records DT = 5.0000 S
- number of records read NTYD = 25 (see list of breakpoint data below for record data read)

-----> CLOUD data block: control of cloud output
OUTPUT STEP LENGTH XSTEP = 50.000 M
CA AT WHICH CALC. IS STOPPED CAMIN = 5.00000E-06 KG/M3
UPPER CONCENTRATION LIMIT CU = 5.00000E-05 KG/M3
LOWER CONCENTRATION LIMIT CL = 5.00000E-06 KG/M3

-----> CALC data block: control of output times
PNTS. OF TIME FOR CLOUD CALC. TSTAR = 80.000 SEC 100.00 SEC
                                      120.00 SEC 140.00 SEC
                                      160.00 SEC 180.00 SEC
                                      200.00 SEC 225.00 SEC
                                      250.00 SEC 280.00 SEC
                                      310.00 SEC 340.00 SEC
                                      380.00 SEC 420.00 SEC
                                      460.00 SEC 500.00 SEC
                                      550.00 SEC 600.00 SEC
                                      650.00 SEC 700.00 SEC

-----> TRANSIT data block(s): breakpoint data
FULL BREAKPOINT AT DIST = 188.00 M

=====
WIND PROFILE EXPONENT ALPHA = 0.13265
FRICTION VELOCITY USTAR = 0.24928 M/S
AIR TEMP. AT GROUND LEVEL TAP = 37.000 CELSIUS
  
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Table 9.10. GOLDFISH1. PREDICTIONS BY HEGADAS-T BASED ON HFPLUME LINK (continued)
=====HTMAIN
DATE 07/11/90HEGADAS-T PROGRAM (VERSION NOV90)
STANDARD REPORT FILEPAGE 1
TIME 09:32

<<<< Transient simulation of Goldfish 1 experiment >>>>

=====

TIME-DEPENDENT DATA AT FULL BREAKPOINT X = 188. M

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TIME - TSTPOOL (S)	CONC (% VOL.)	CLOUD HALF-WIDTH (M)	CLOUD HEIGHT (M)	GAS FLOW (KG/S)	SZ (M)	RIB	TMP (C)	CA (KG/M3)
0.802	0.808	6.28	8.44	4.35	8.82	31.0	28.8	6.524E-03
7.22	5.03	39.1	1.54	27.1	1.61	28.8	1.16	4.474E-02
13.6	5.03	39.1	1.54	27.1	1.61	28.8	1.16	4.474E-02
20.1	5.03	39.1	1.54	27.1	1.61	28.8	1.16	4.474E-02
26.5	5.03	39.1	1.54	27.1	1.61	28.8	1.16	4.474E-02
32.9	5.03	39.1	1.54	27.1	1.61	28.8	1.16	4.474E-02
39.3	5.03	39.1	1.54	27.1	1.61	28.8	1.16	4.474E-02
45.7	5.03	39.1	1.54	27.1	1.61	28.8	1.16	4.474E-02
52.2	5.03	39.1	1.54	27.1	1.61	28.8	1.16	4.474E-02
58.6	5.03	39.1	1.54	27.1	1.61	28.8	1.16	4.474E-02
65.0	5.03	39.1	1.54	27.1	1.61	28.8	1.16	4.474E-02
71.4	5.03	39.1	1.54	27.1	1.61	28.8	1.16	4.474E-02
77.8	5.03	39.1	1.54	27.1	1.61	28.8	1.16	4.474E-02
84.3	5.03	39.1	1.54	27.1	1.61	28.8	1.16	4.474E-02
90.7	5.03	39.1	1.54	27.1	1.61	28.8	1.16	4.474E-02
97.1	5.03	39.1	1.54	27.1	1.61	28.8	1.16	4.474E-02
104.	5.03	39.1	1.54	27.1	1.61	28.8	1.16	4.474E-02
110.	5.03	39.1	1.54	27.1	1.61	28.8	1.16	4.474E-02
116.	5.03	39.1	1.54	27.1	1.61	28.8	1.16	4.474E-02
123.	5.03	39.1	1.54	27.1	1.61	28.8	1.16	4.474E-02
129.	0.808	6.28	8.44	4.35	8.82	31.0	28.8	6.524E-03

Observer-dispersion data set at breakpoint; total CPU = 21 seconds

Table 9.10. GOLDFISH1. PREDICTIONS BY HEGADAS-T BASED ON HFPLUME LINK (continued)

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DISPERSION DATA AT TIME = 160.0 SEC									
DISTANCE (M)	CONC (% VOL.)	SZ (M)	SY (M)	MIDP (M)	YCU (M)	ZCU (M)	YCL (M)	ZCL (M)	CA (KG/M3)
200.	0.000E-01	3.85	5.31	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01
250.	2.95	2.34	16.6	27.6	68.9	11.8	76.0	15.5	2.535E-02
300.	3.42	1.47	25.6	40.3	105.	7.51	116.	9.87	2.914E-02
350.	2.83	1.55	30.9	43.6	120.	7.71	134.	10.2	2.387E-02
400.	2.36	1.65	35.6	46.8	134.	8.00	149.	10.7	1.970E-02
450.	1.98	1.77	39.8	50.0	146.	8.34	163.	11.2	1.652E-02
500.	1.70	1.89	43.5	53.1	156.	8.68	176.	11.7	1.408E-02
550.	1.46	2.02	47.0	56.0	166.	9.07	187.	12.4	1.205E-02
600.	1.27	2.17	50.3	58.6	175.	9.50	198.	13.0	1.038E-02
650.	1.11	2.32	53.3	61.0	183.	9.95	207.	13.8	9.018E-03
700.	0.886	2.49	56.2	63.1	188.	10.2	215.	14.3	7.181E-03
750.	0.866	2.66	59.0	65.1	196.	10.9	224.	15.3	6.989E-03
800.	0.774	2.87	61.8	65.5	201.	11.5	230.	16.3	6.233E-03
850.	0.697	3.15	64.9	63.1	204.	12.4	235.	17.6	5.595E-03
900.	0.633	3.43	67.8	60.6	206.	13.2	239.	18.9	5.071E-03
950.	0.582	3.70	70.6	58.2	209.	14.1	243.	20.2	4.655E-03
1.000E+03	0.544	3.98	73.3	55.9	211.	14.9	247.	21.5	4.346E-03
1.050E+03	0.175	5.42	51.9	24.3	119.	15.7	148.	24.9	1.395E-03
1.100E+03	3.676E-02	6.23	43.6	0.000E-01	57.8	10.3	87.8	21.5	2.912E-04
1.150E+03	4.199E-03	6.48	46.7	0.000E-01	0.000E-01	0.000E-01	64.1	11.3	3.299E-05
1.200E+03	2.299E-04	6.73	49.7	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	1.785E-06

DISPERSION DATA AT TIME = 200.0 SEC									
DISTANCE (M)	CONC (% VOL.)	SZ (M)	SY (M)	MIDP (M)	YCU (M)	ZCU (M)	YCL (M)	ZCL (M)	CA (KG/M3)
400.	7.898E-21	2.55	19.9	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	6.459E-23
450.	0.977	2.44	29.9	26.3	93.8	10.2	108.	14.2	7.983E-03
500.	1.60	1.94	45.1	54.5	161.	8.83	181.	12.0	1.324E-02
550.	1.38	2.08	48.5	57.3	170.	9.23	192.	12.6	1.134E-02
600.	1.20	2.23	51.7	59.9	179.	9.67	202.	13.3	9.798E-03
650.	1.05	2.39	54.8	62.1	186.	10.1	212.	14.1	8.541E-03
700.	0.929	2.56	57.6	64.2	193.	10.6	220.	14.8	7.520E-03
750.	0.829	2.74	60.4	65.9	200.	11.1	228.	15.6	6.682E-03
800.	0.740	2.98	63.4	64.9	203.	11.9	234.	16.8	5.949E-03
850.	0.668	3.26	66.4	62.3	206.	12.7	238.	18.1	5.360E-03
900.	0.609	3.55	69.3	59.8	208.	13.6	242.	19.5	4.874E-03
950.	0.559	3.82	72.1	57.5	210.	14.4	245.	20.8	4.466E-03
1.000E+03	0.516	4.10	74.8	55.1	212.	15.2	249.	22.1	4.122E-03
1.050E+03	0.479	4.38	77.4	53.0	214.	16.0	252.	23.3	3.821E-03
1.100E+03	0.447	4.65	79.9	50.9	216.	16.8	256.	24.5	3.561E-03
1.150E+03	0.419	4.93	82.3	48.9	218.	17.5	259.	25.7	3.335E-03
1.200E+03	0.399	5.20	84.7	47.0	219.	18.3	262.	27.0	3.172E-03
1.250E+03	0.359	5.47	87.0	45.1	220.	18.8	264.	28.0	2.854E-03
1.300E+03	0.184	6.90	70.8	25.4	155.	20.2	194.	32.0	1.464E-03
1.350E+03	5.557E-02	8.57	51.0	0.000E-01	75.3	17.0	108.	32.2	4.403E-04
1.400E+03	1.267E-02	8.85	54.0	0.000E-01	45.0	6.41	93.5	23.3	1.001E-04
1.450E+03	1.946E-03	9.13	56.9	0.000E-01	0.000E-01	0.000E-01	60.2	10.1	1.532E-05
1.500E+03	1.893E-04	9.40	59.8	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	1.483E-06

Table 9.10. GOLDFISH1. PREDICTIONS BY HEGADAS-T BASED ON HFPLUME LINK (continued)

DISPERSION DATA AT TIME = 250.0 SEC									
DISTANCE (M)	CONC (% VOL.)	SZ (M)	SY (M)	MIDP (M)	YCU (M)	ZCU (M)	YCL (M)	ZCL (M)	CA (KG/M3)
600.	7.979E-07	3.54	26.5	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	6.368E-09
650.	4.806E-03	3.80	30.0	0.000E-01	0.000E-01	0.000E-01	42.6	7.04	3.741E-05
700.	8.565E-02	4.05	33.4	1.77	55.7	9.46	75.8	16.5	6.803E-04
750.	0.657	3.14	60.7	59.1	190.	12.2	219.	17.4	5.276E-03
800.	0.666	3.27	66.9	62.5	207.	12.8	239.	18.2	5.345E-03
850.	0.606	3.55	69.8	60.2	209.	13.6	243.	19.5	4.854E-03
900.	0.557	3.84	72.6	57.6	211.	14.4	247.	20.8	4.451E-03
950.	0.514	4.12	75.3	55.3	213.	15.2	250.	22.1	4.106E-03
1.000E+03	0.477	4.39	77.9	53.2	215.	16.0	254.	23.4	3.807E-03
1.050E+03	0.445	4.67	80.4	51.1	217.	16.8	257.	24.6	3.547E-03
1.100E+03	0.417	4.94	82.8	49.0	219.	17.5	260.	25.8	3.319E-03
1.150E+03	0.392	5.22	85.2	47.0	220.	18.3	263.	27.0	3.119E-03
1.200E+03	0.370	5.49	87.5	45.1	222.	19.0	266.	28.2	2.939E-03
1.250E+03	0.350	5.76	89.8	43.3	223.	19.7	269.	29.4	2.779E-03
1.300E+03	0.332	6.04	92.0	41.3	224.	20.4	272.	30.5	2.635E-03
1.350E+03	0.315	6.30	94.1	39.7	226.	21.0	274.	31.6	2.503E-03
1.400E+03	0.301	6.57	96.2	38.0	227.	21.7	277.	32.8	2.384E-03
1.450E+03	0.288	6.84	98.2	36.4	228.	22.3	279.	33.9	2.280E-03
1.500E+03	0.272	7.11	100.	34.8	229.	22.9	282.	34.9	2.154E-03
1.550E+03	0.225	7.37	102.	33.2	226.	22.7	281.	35.2	1.781E-03
1.600E+03	0.129	9.41	102.	17.3	195.	24.9	253.	41.2	1.021E-03
1.650E+03	4.519E-02	11.8	102.	0.000E-01	143.	21.4	211.	42.4	3.577E-04
1.700E+03	1.084E-02	12.1	105.	0.000E-01	76.8	7.00	176.	30.4	8.572E-05
1.750E+03	2.127E-03	12.4	107.	0.000E-01	0.000E-01	0.000E-01	118.	14.7	1.680E-05
1.800E+03	3.406E-04	12.7	109.	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	2.685E-06
DISPERSION DATA AT TIME = 340.0 SEC									
DISTANCE (M)	CONC (% VOL.)	SZ (M)	SY (M)	MIDP (M)	YCU (M)	ZCU (M)	YCL (M)	ZCL (M)	CA (KG/M3)
1.050E+03	1.096E-04	7.97	42.3	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	8.603E-07
1.100E+03	1.131E-03	8.31	45.4	0.000E-01	0.000E-01	0.000E-01	34.5	5.12	8.913E-06
1.150E+03	7.801E-03	8.64	48.5	0.000E-01	22.2	2.17	76.8	19.5	6.162E-05
1.200E+03	3.998E-02	8.97	51.5	0.000E-01	69.9	15.4	105.	31.5	3.165E-04
1.250E+03	0.142	8.17	70.0	15.4	139.	22.3	178.	36.3	1.125E-03
1.300E+03	0.263	6.66	97.4	37.7	226.	21.3	277.	32.6	2.086E-03
1.350E+03	0.286	6.93	99.5	36.2	230.	22.6	282.	34.3	2.266E-03
1.400E+03	0.271	7.20	102.	34.5	231.	23.2	284.	35.3	2.148E-03
1.450E+03	0.259	7.47	103.	32.8	232.	23.8	287.	36.4	2.053E-03
1.500E+03	0.249	7.73	105.	31.3	233.	24.4	289.	37.5	1.970E-03
1.550E+03	0.239	8.00	107.	29.8	234.	25.0	291.	38.5	1.892E-03
1.600E+03	0.230	8.26	109.	28.3	235.	25.6	293.	39.6	1.820E-03
1.650E+03	0.222	8.53	111.	26.8	236.	26.1	295.	40.6	1.754E-03
1.700E+03	0.214	8.79	113.	25.4	237.	26.7	298.	41.7	1.692E-03
1.750E+03	0.207	9.05	115.	24.0	238.	27.3	300.	42.7	1.634E-03
1.800E+03	0.200	9.31	116.	22.6	239.	27.8	302.	43.7	1.579E-03
1.850E+03	0.193	9.57	118.	21.2	239.	28.4	303.	44.7	1.528E-03
1.900E+03	0.187	9.84	120.	20.0	240.	28.9	305.	45.7	1.480E-03
1.950E+03	0.181	10.1	121.	18.7	241.	29.4	307.	46.6	1.430E-03
2.000E+03	0.172	10.4	123.	17.4	241.	29.7	309.	47.4	1.362E-03
2.050E+03	0.156	10.6	125.	16.2	239.	29.7	309.	47.9	1.236E-03
2.100E+03	0.128	10.9	126.	14.9	234.	28.7	306.	47.5	1.013E-03
2.150E+03	8.940E-02	12.6	127.	10.7	218.	29.9	294.	51.9	7.062E-04
2.200E+03	5.076E-02	17.9	128.	0.000E-01	185.	34.2	269.	65.9	4.010E-04
2.250E+03	2.304E-02	18.2	131.	0.000E-01	148.	22.9	248.	56.4	1.819E-04
2.300E+03	8.418E-03	18.6	133.	0.000E-01	71.0	6.13	214.	43.1	6.647E-05
2.350E+03	2.553E-03	19.0	135.	0.000E-01	0.000E-01	0.000E-01	160.	25.4	2.015E-05
2.400E+03	6.666E-04	19.3	138.	0.000E-01	0.000E-01	0.000E-01	31.0	1.39	5.260E-06
2.450E+03	1.533E-04	19.7	140.	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	1.209E-06

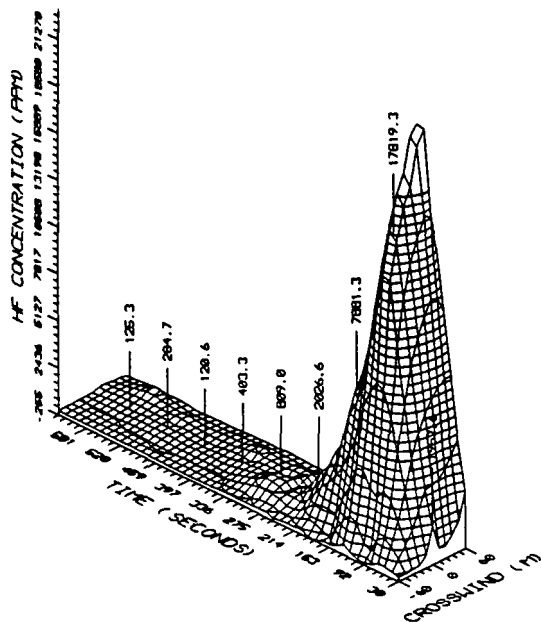
Cloud data set; total CPU = 810 seconds

- simulation of GOLDFISH experiments -

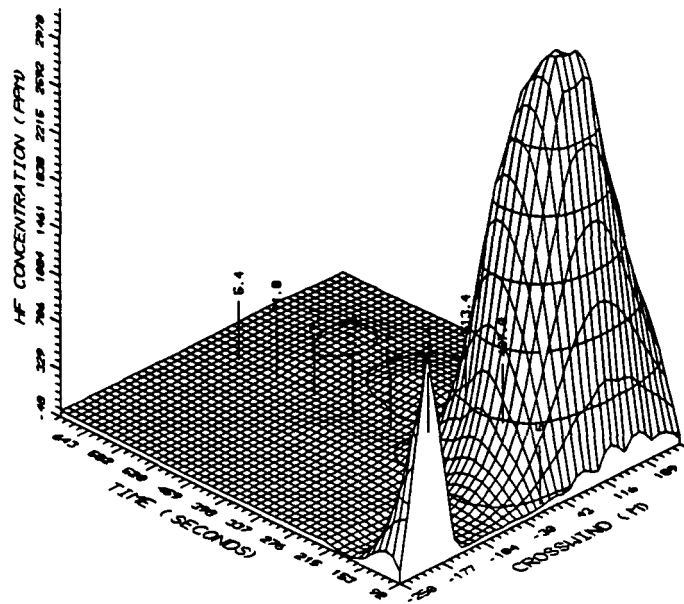
Table 9.11. Observed and predicted mean center-line concentrations (% molar fraction) for the Goldfish experiments. The predicted data are given both at ground level ($z=0$) and at the height at which the data are measured ($z=1$).

Goldfish test no.	downwind distance (m)	concentr. observed at $z=1$	concentr. predicted at $z=0$	concentr. predicted at $z=1$	ratio of pred. to obs. concentr. ($z=1$)
1	300	2.1	3.35	1.75	0.83
	1000	0.32	0.43	0.37	1.14
	3000	-	0.082	0.079	-
2	300	1.7	1.86	0.94	0.55
	1000	0.2	0.23	0.19	0.97
	3000	-	0.039	0.037	-
3	300	1.6	1.64	1.02	0.64
	1000	0.23	0.19	0.16	0.71
	3000	0.02	0.0285	0.0277	1.39

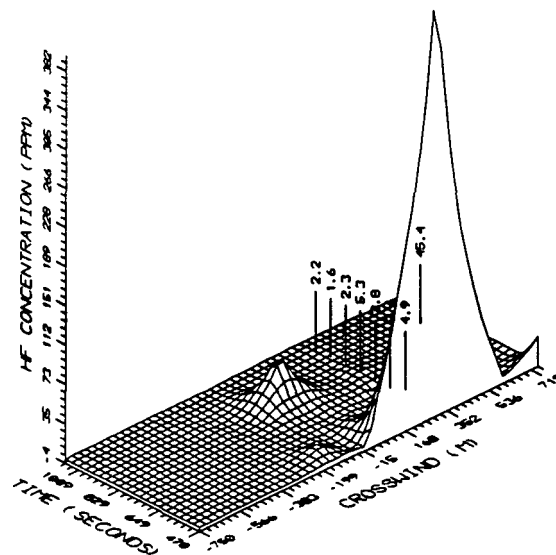
Mean: 0.89
Standard deviation: 0.29



(a)



(b)



(c)

Fig. 9.1. HF concentrations observed in Goldfish 1 experiment (sensor height $z = 1$ m);
 (a) downwind distance $x = 300$ m
 (b) downwind distance $x = 1000$ m
 (c) downwind distance $x = 3000$ m

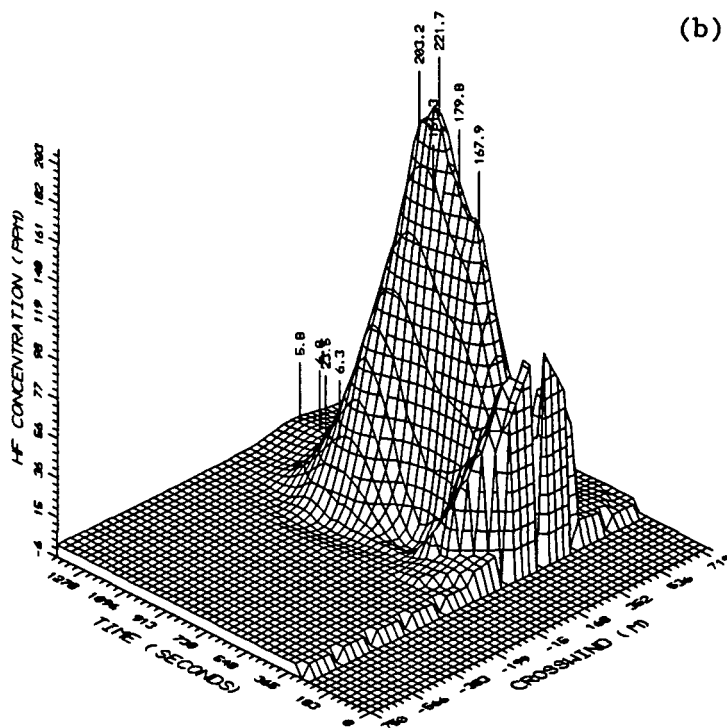
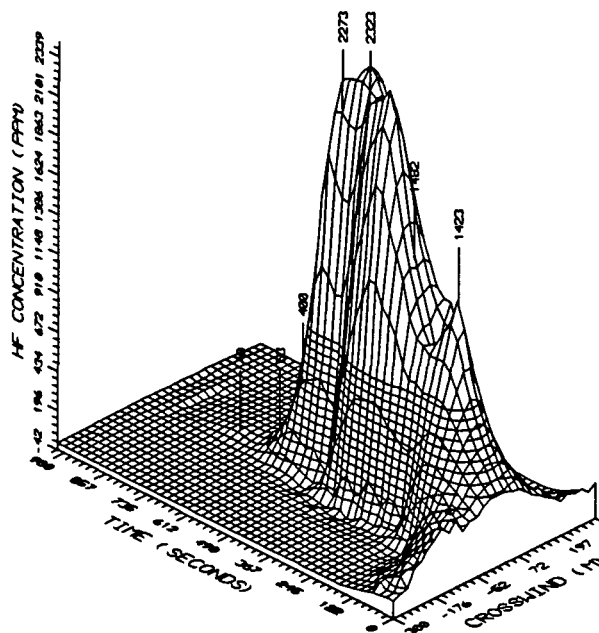
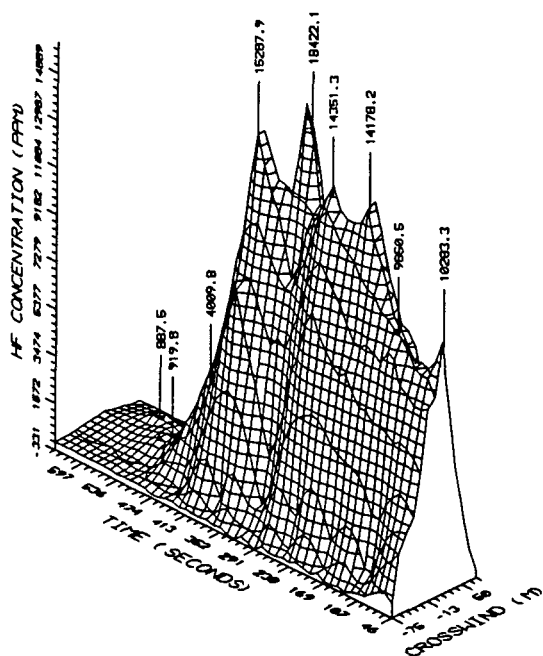


Fig. 9.2. HF concentrations observed in Goldfish 3 experiment (sensor height $z = 1$ m);
 (a) downwind distance $x = 300$ m
 (b) downwind distance $x = 1000$ m
 (c) downwind distance $x = 3000$ m

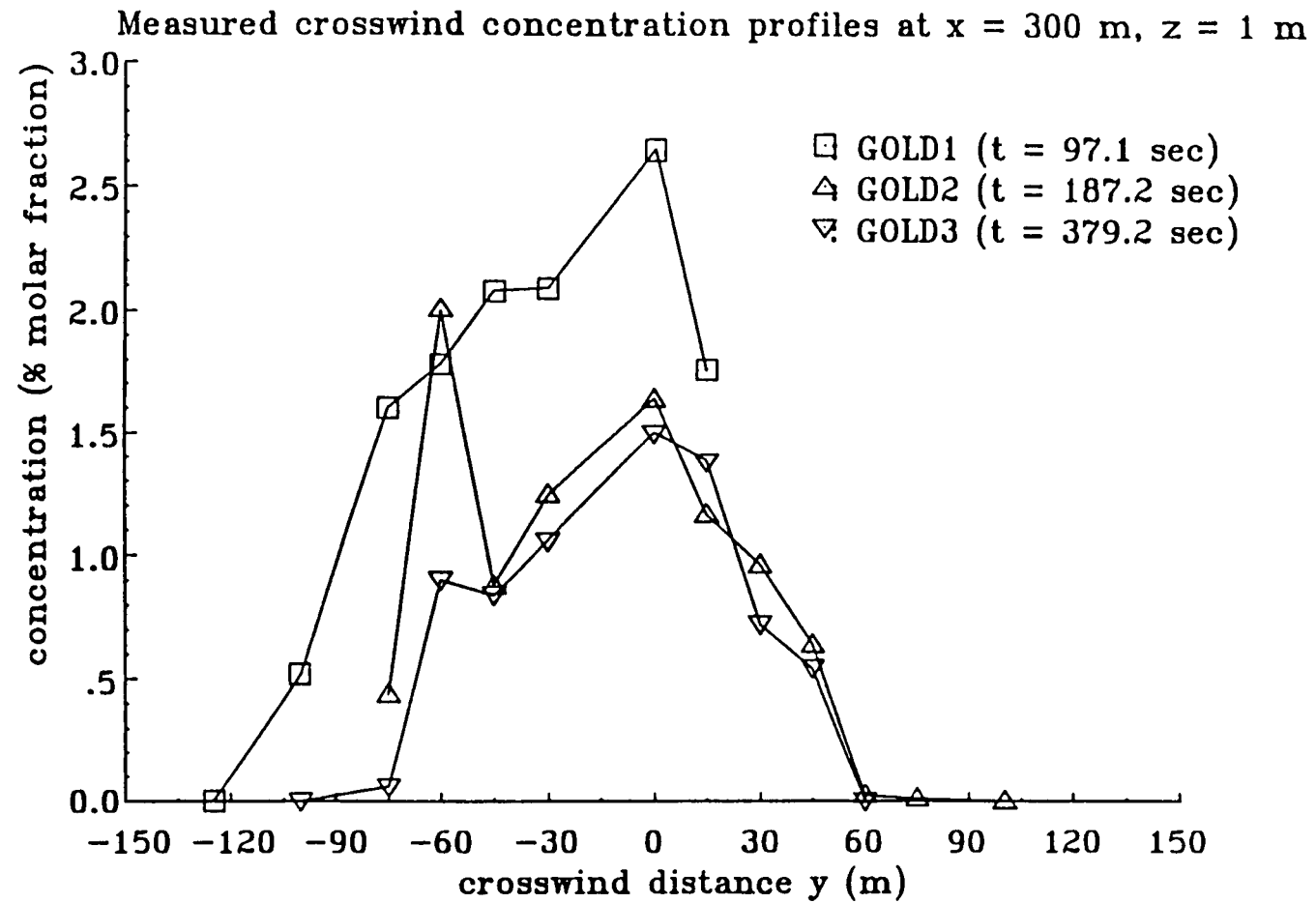


Fig. 9.3. Crosswind concentration profiles observed in Goldfish experiments at time during which steady-state seems to be most closely achieved; $x = 300$ m, $z = 1$ m

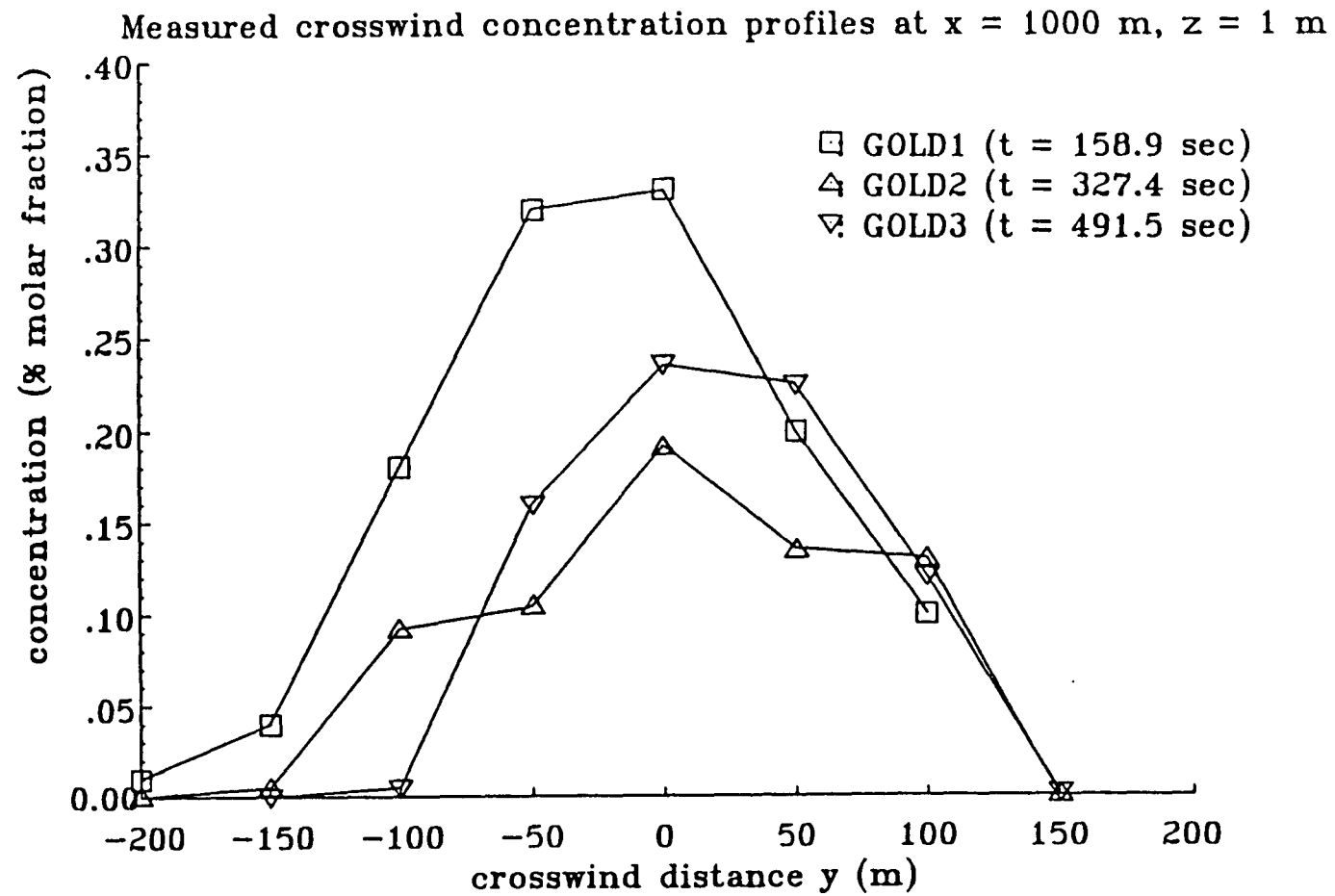


Fig. 9.4. Crosswind concentration profiles observed in Goldfish experiments at time during which steady-state seems to be most closely achieved; $x = 1000$ m, $z = 1$ m

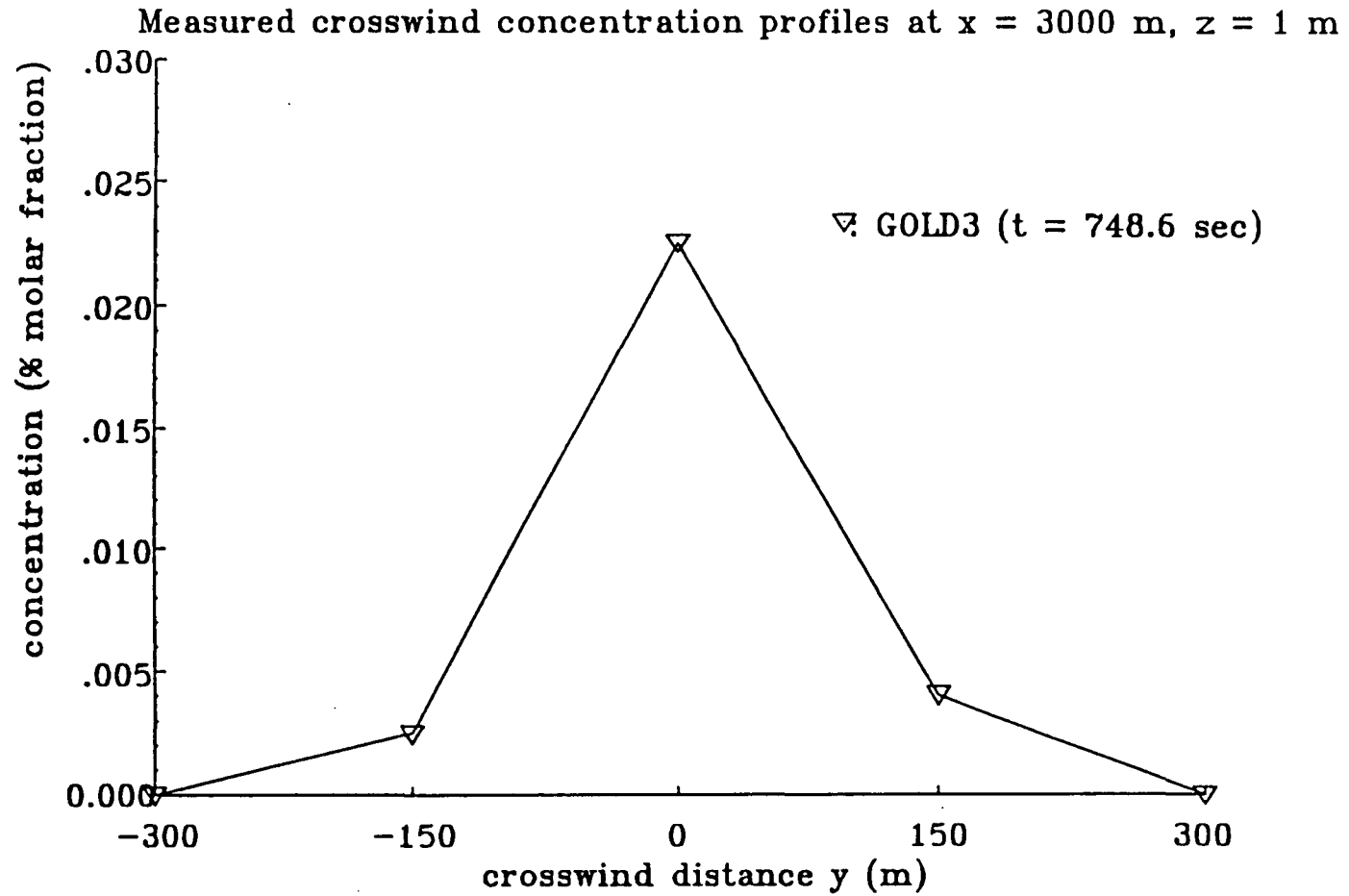


Fig. 9.5. Crosswind concentration profile observed in Goldfish 3 experiment at time during which steady-state seems to be most closely achieved; $x = 3000$ m, $z = 1$ m

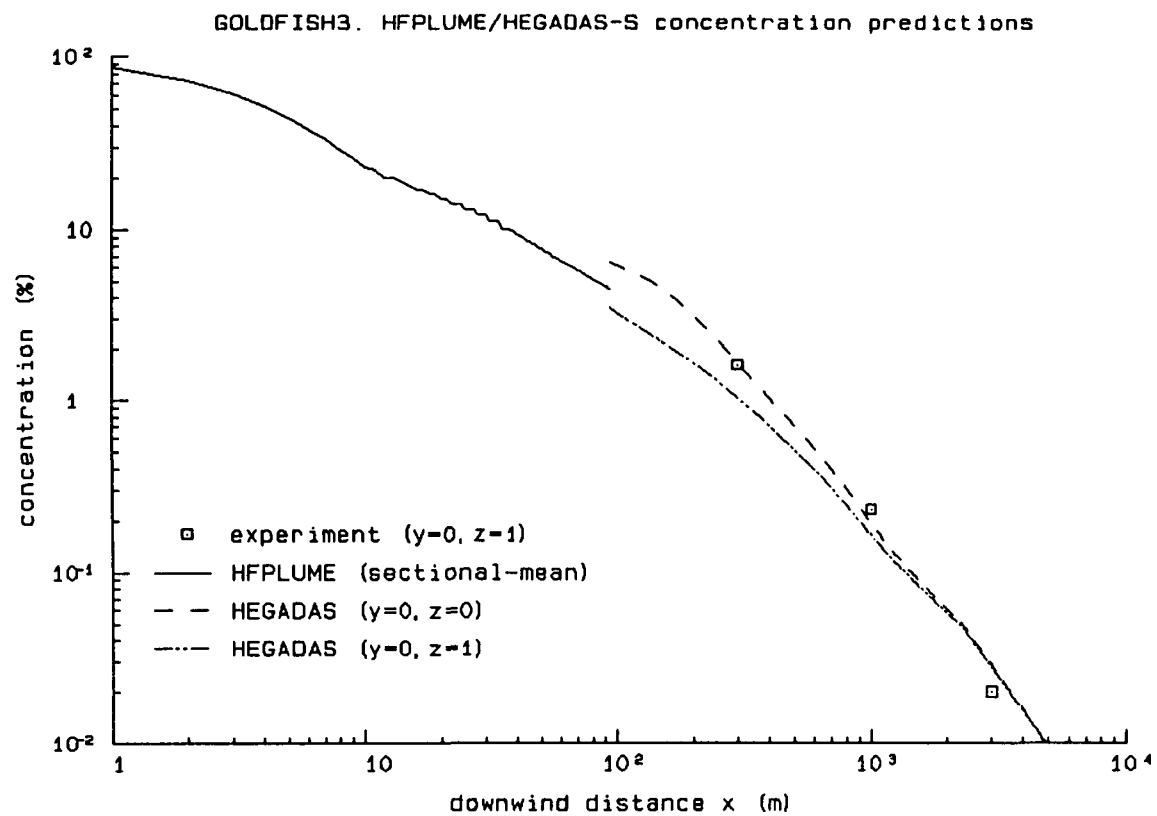


Fig. 9.6. Goldfish 3 predictions of centre-line concentration (% molar fraction) by HFPLUME (sectional-mean) and HEGADAS-S at ground level and 1m.

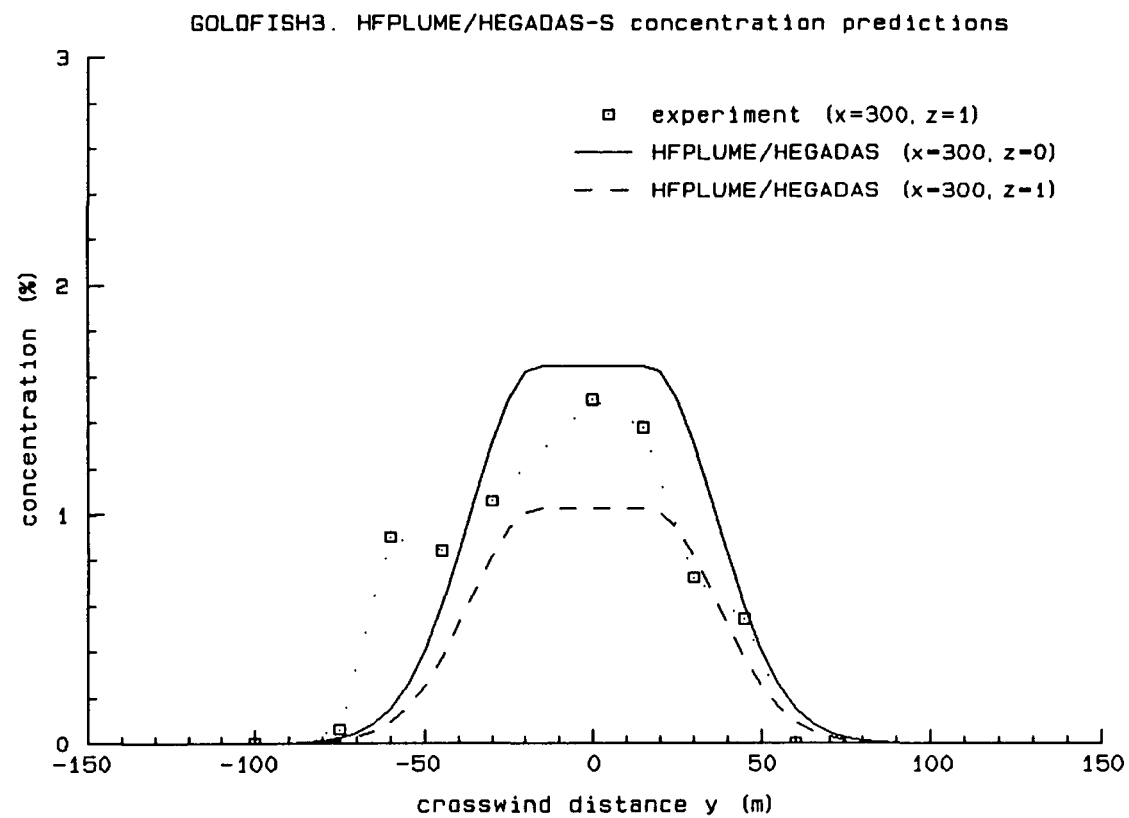


Fig. 9.7. Goldfish 3 predictions of crosswind concentration profile by HEGADAS-S at ground level and 1m; x = 300 m

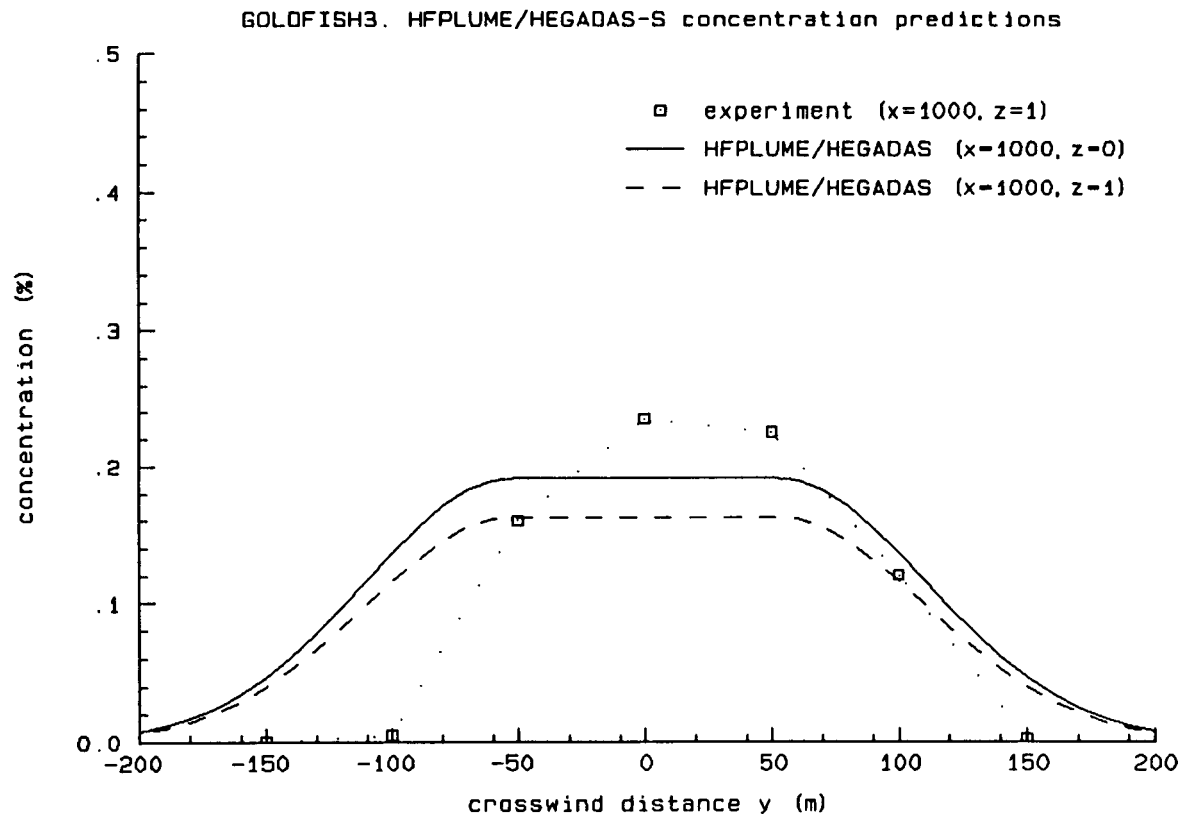


Fig. 9.8. Goldfish 3 predictions of crosswind concentration profile by HEGADAS-S at ground level and 1m; x = 1000 m

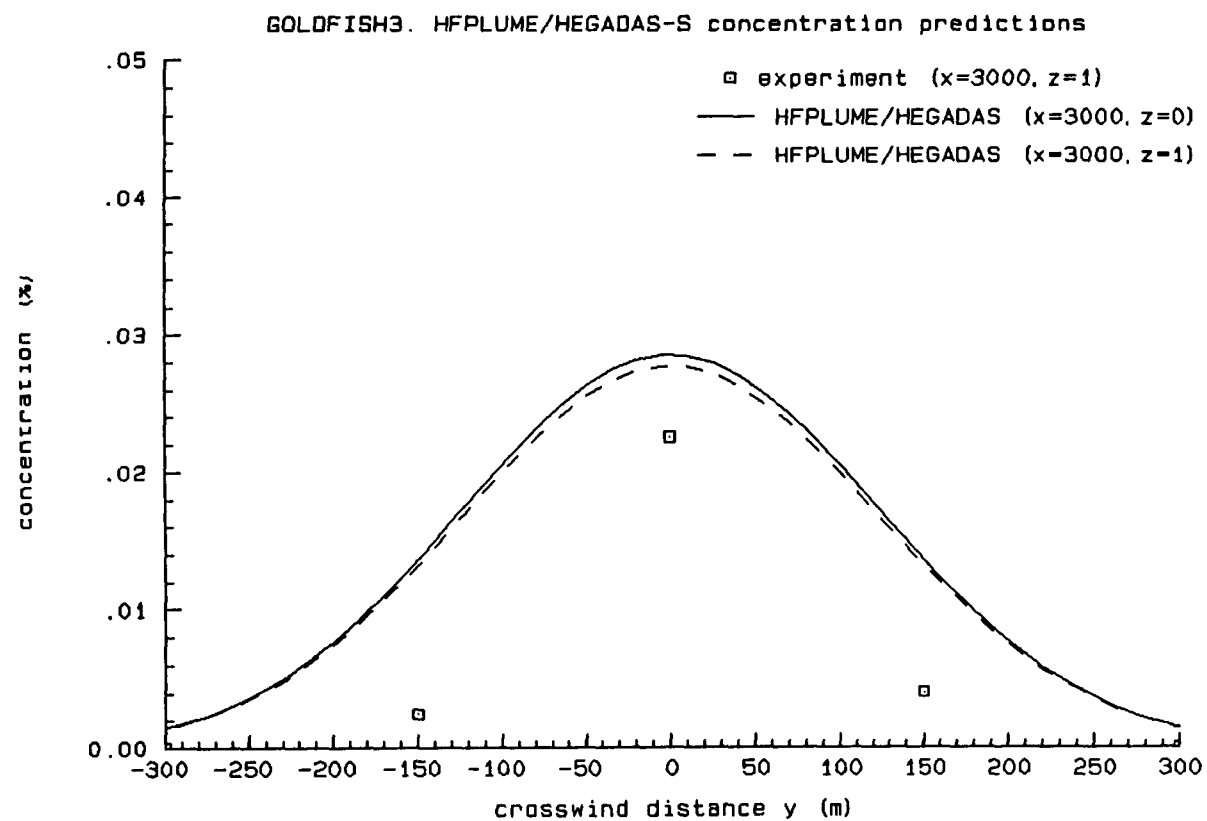


Fig. 9.9. Goldfish 3 predictions of crosswind concentration profile by HEGADAS-S at ground level and 1m; x = 3000 m

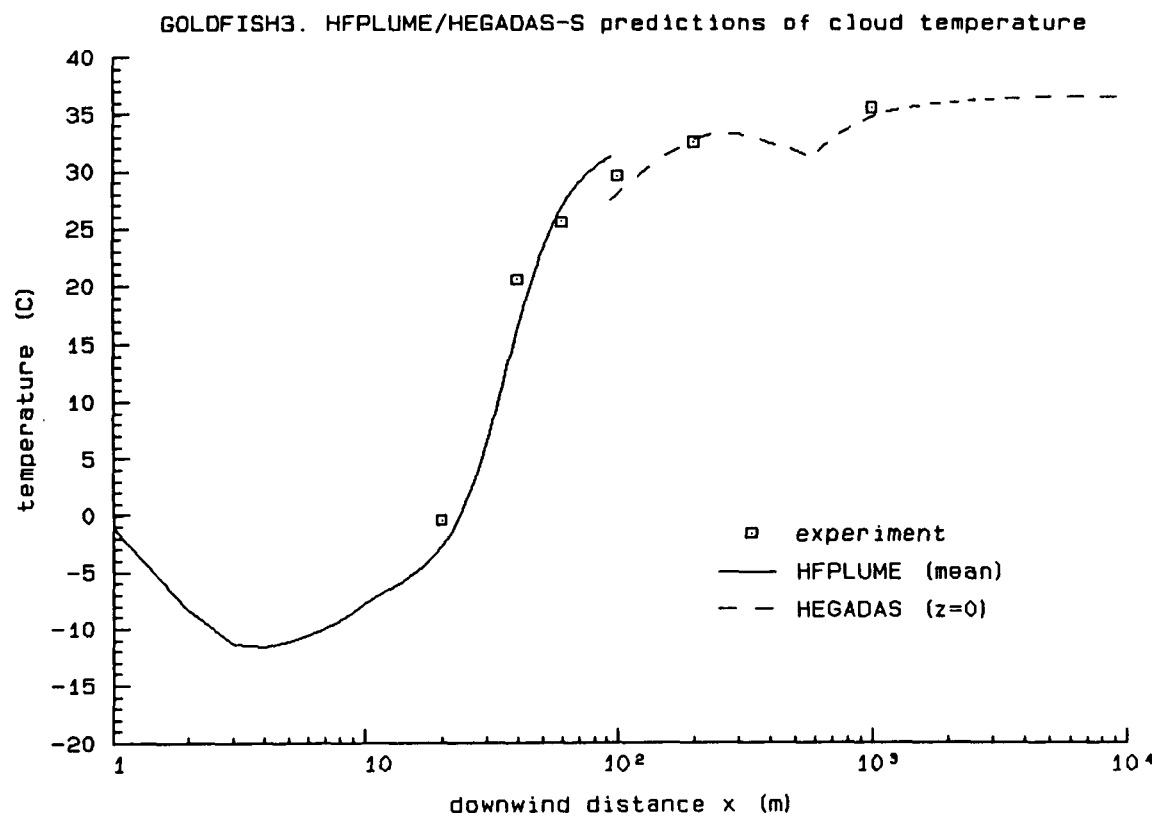


Fig. 9.10. Goldfish 3 predictions of temperature by HFPLUME/HEGADAS-S

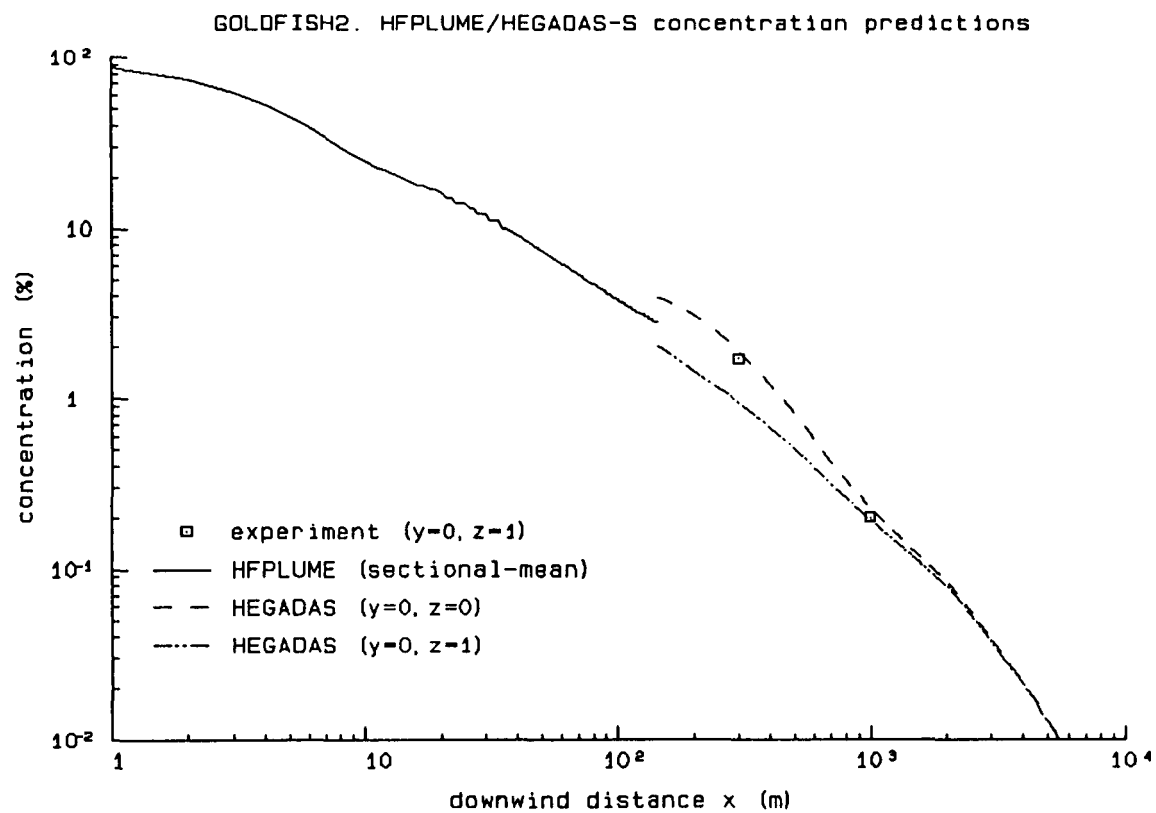


Fig. 9.11. Goldfish 2 predictions of centre-line concentration (% molar fraction) by HFPLUME (sectional-mean) and HEGADAS-S at ground level and 1m.

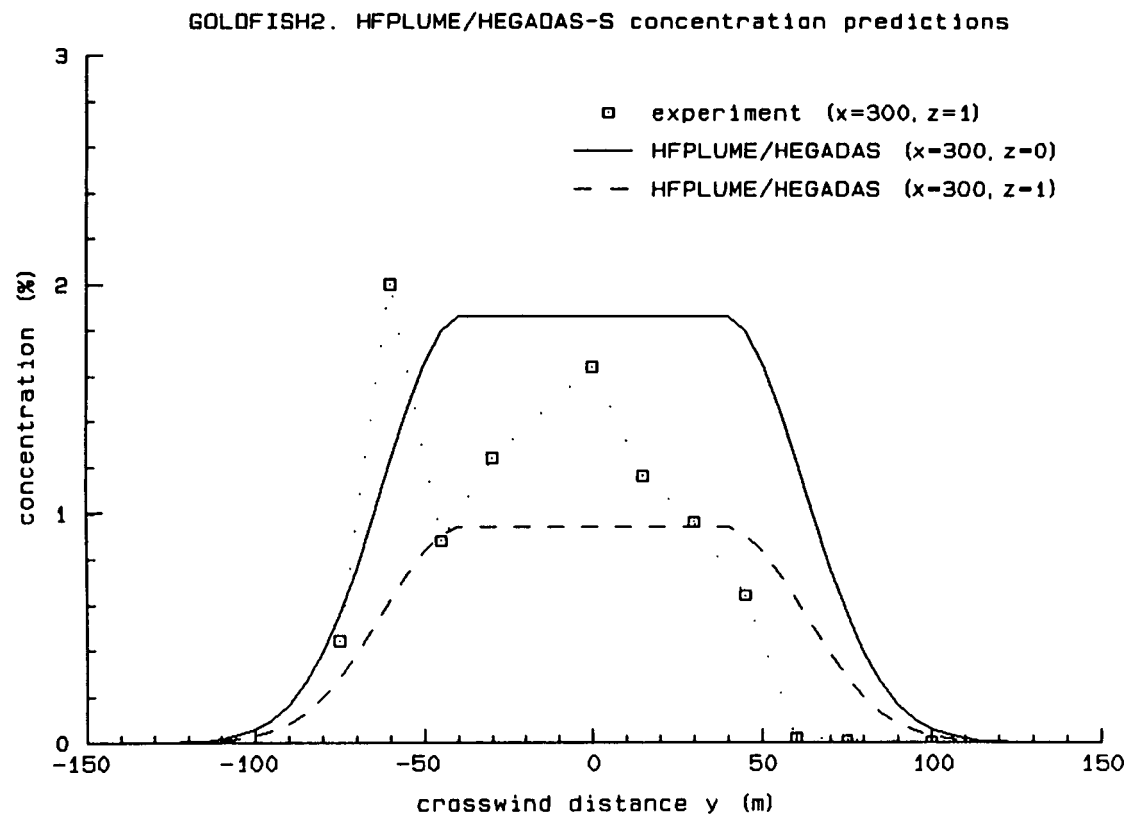


Fig. 9.12. Goldfish 2 predictions of crosswind concentration profile by HEGADAS-S at ground level and 1m; $x = 300$ m

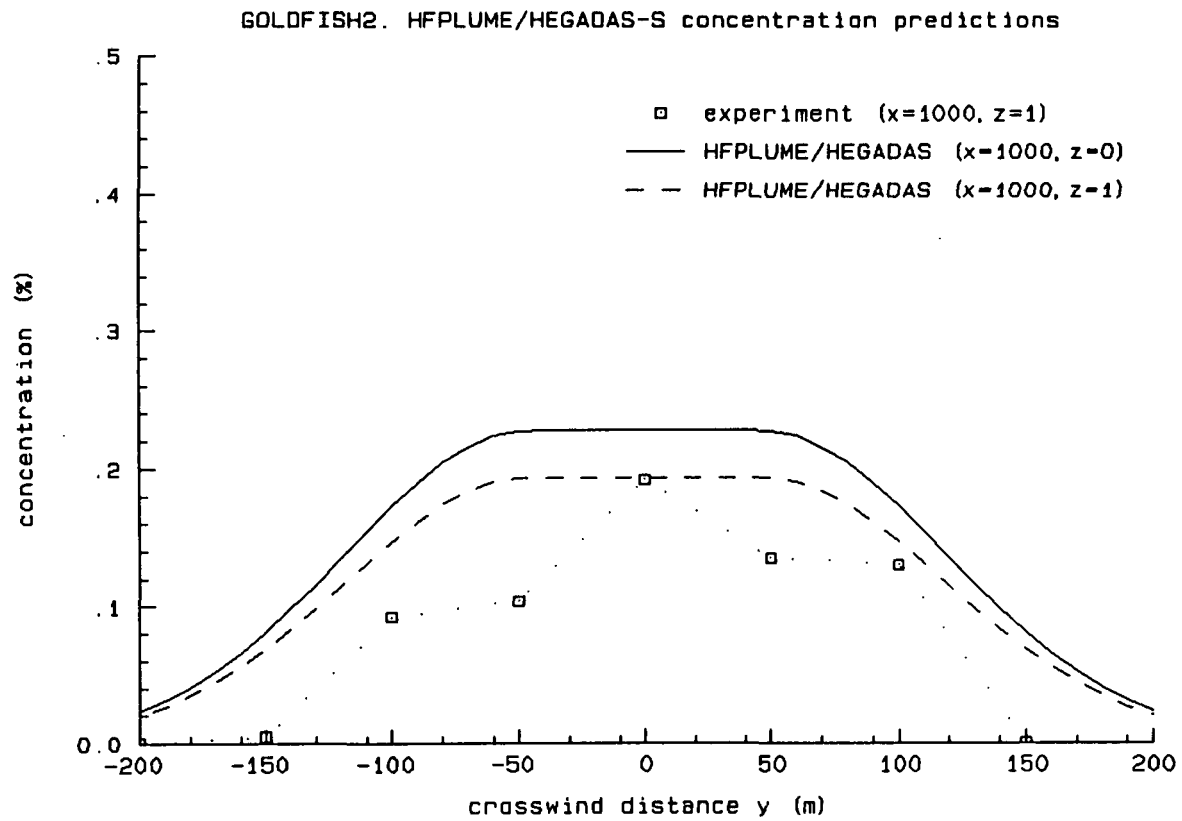


Fig. 9.13. Goldfish 2 predictions of crosswind concentration profile by HEGADAS-S at ground level and 1m; x = 1000 m

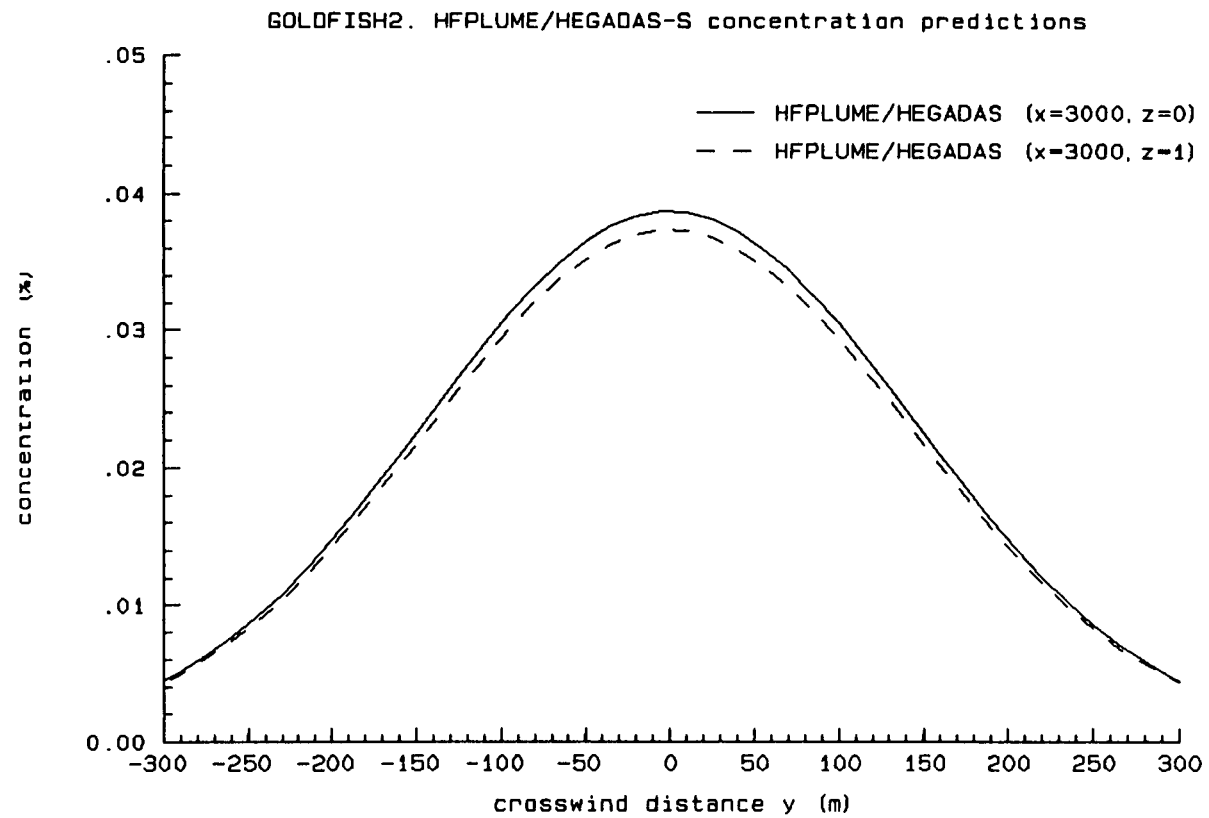


Fig. 9.14. Goldfish 2 predictions of crosswind concentration profile by HEGADAS-S at ground level and 1m; x = 3000 m

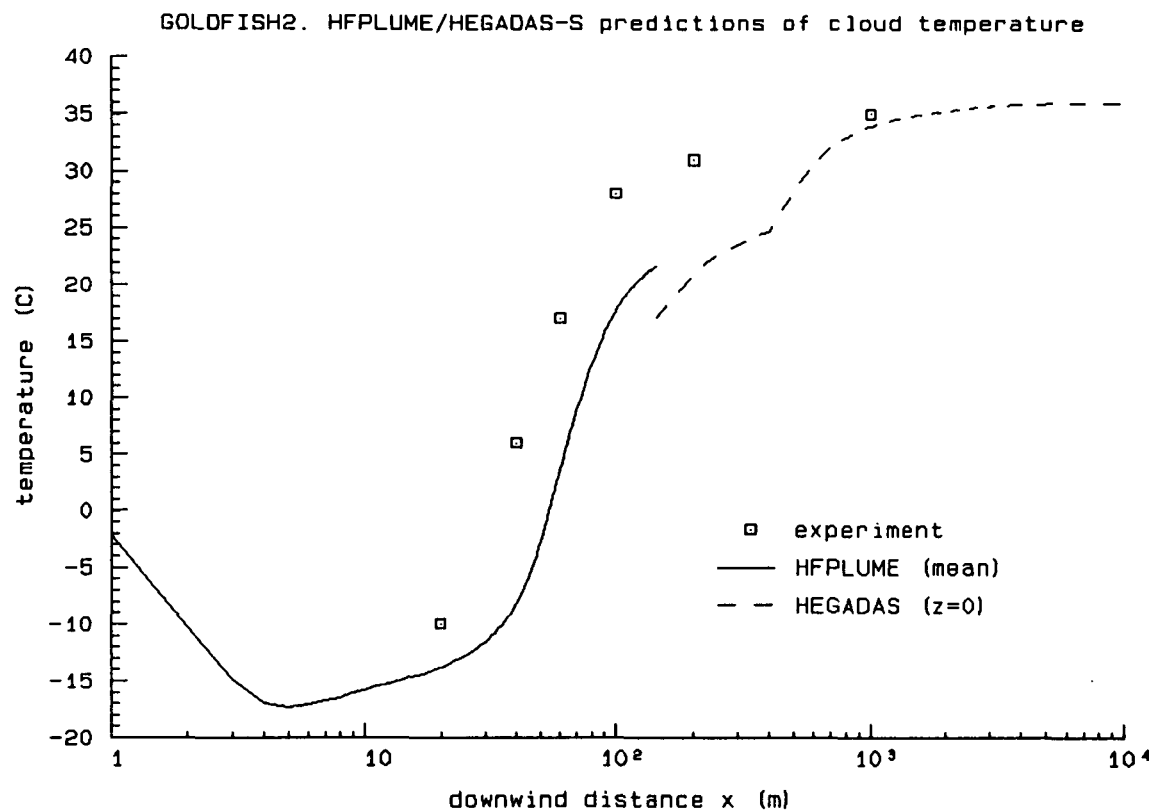


Fig. 9.15. Goldfish 2 predictions of temperature by HFPLUME/HEGADAS-S
[experimental data are too high, since the centre-line of the
plume was not aligned with the line on which the temperature
measurements were made]

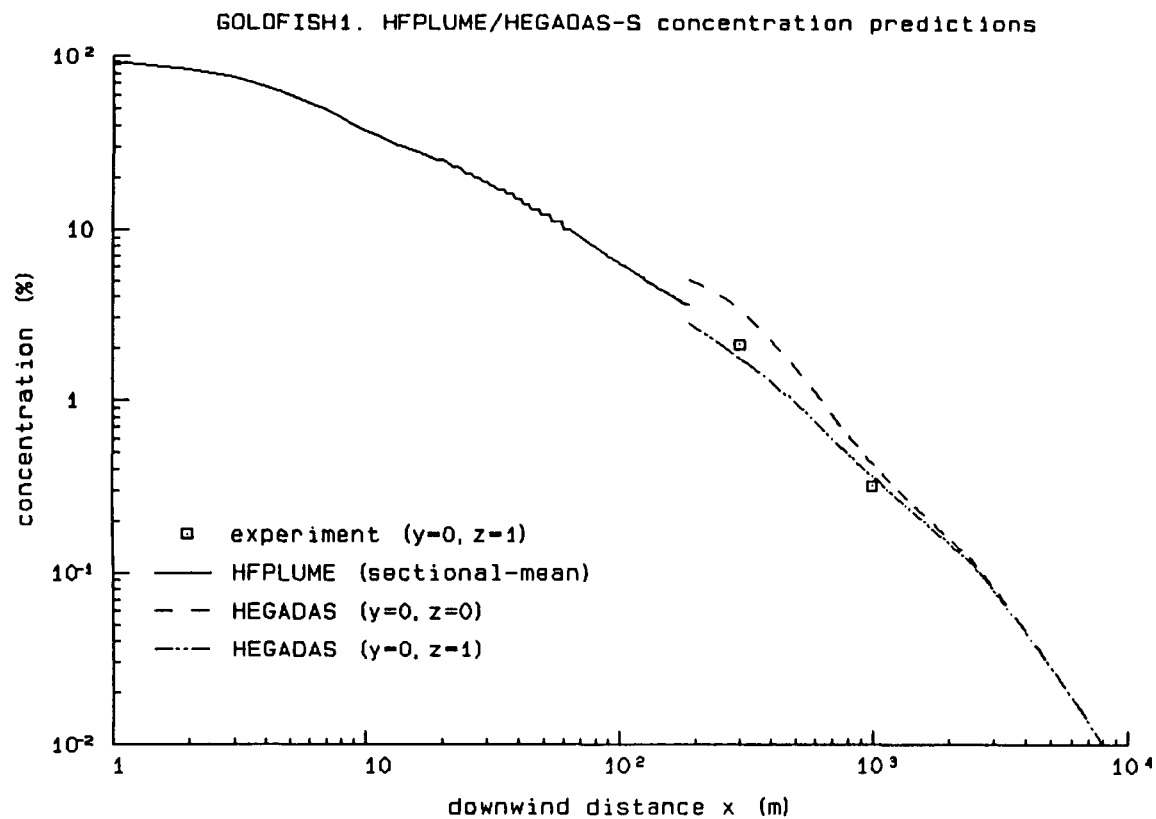


Fig. 9.16. Goldfish 1 predictions of centre-line concentration (% molar fraction) by HFPLUME (sectional mean) and HEGADAS-S at ground level and 1m

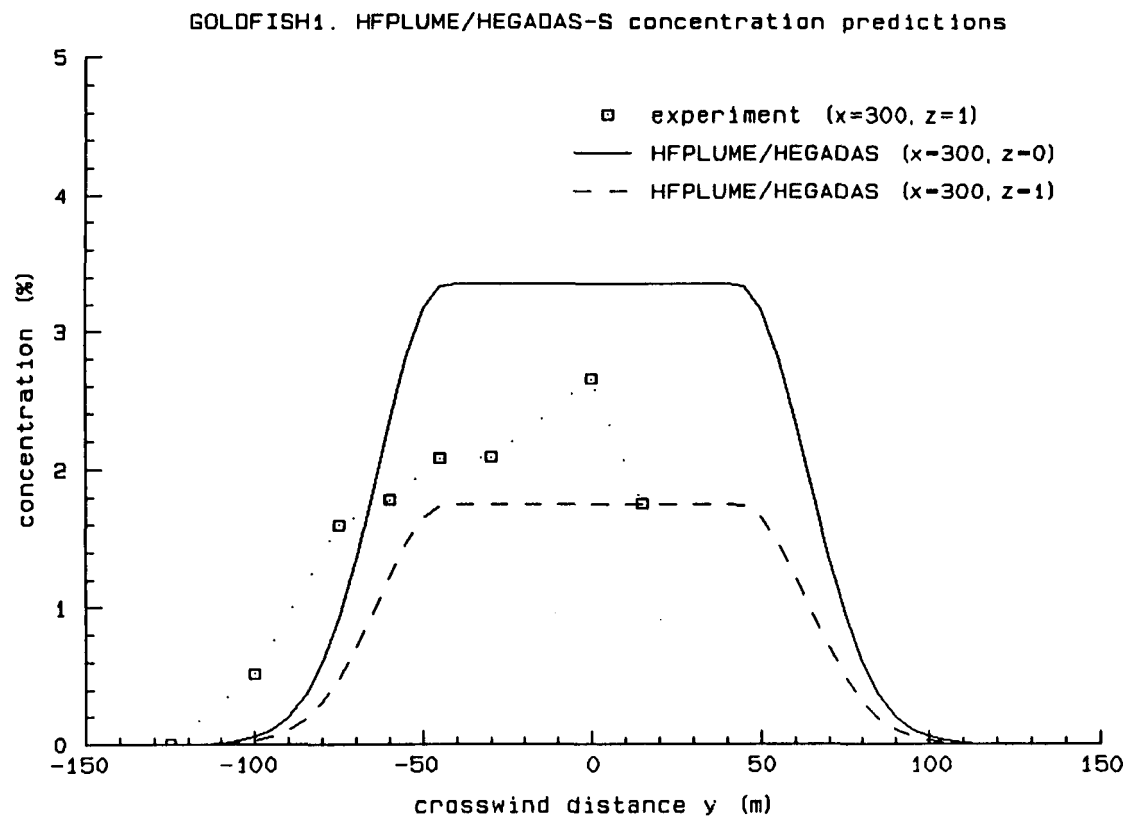


Fig. 9.17. Goldfish 1 predictions of crosswind concentration profile by HEGADAS-S at ground level and 1m; x = 300 m

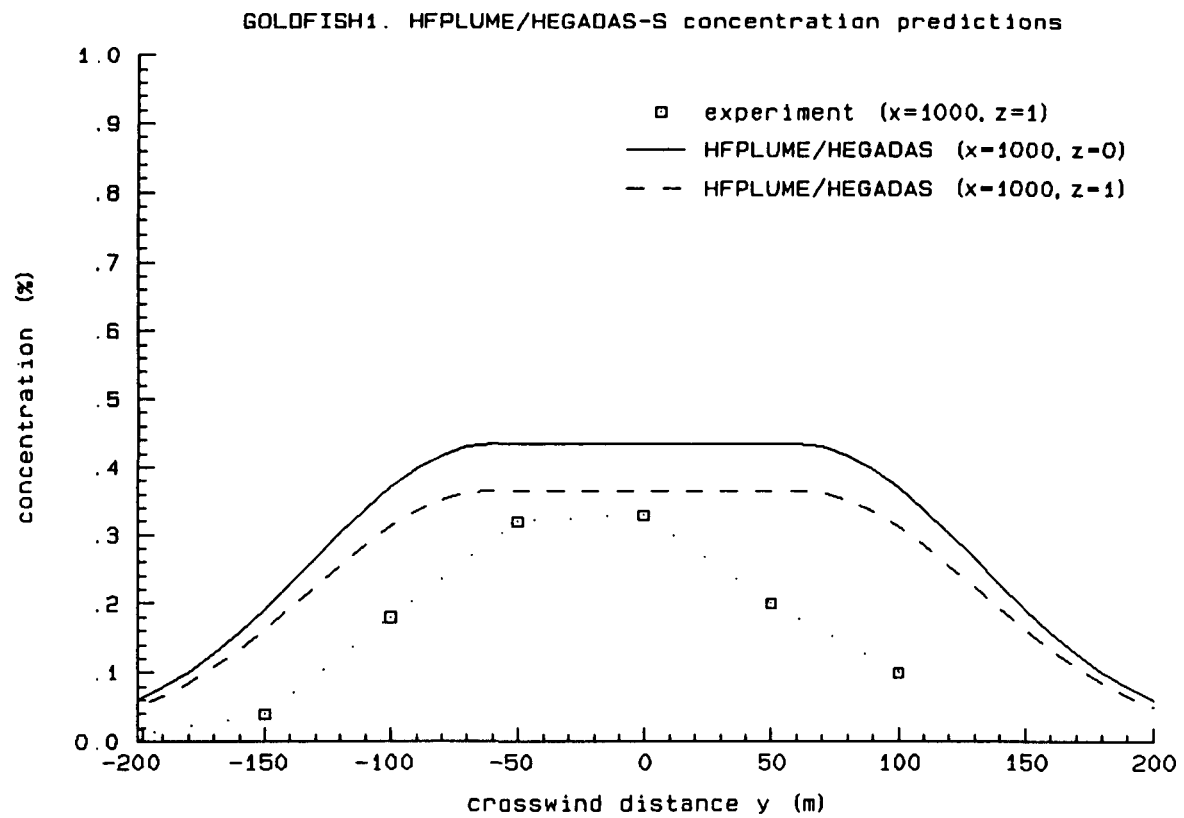


Fig. 9.18. Goldfish 1 predictions of crosswind concentration profile by HEGADAS-S at ground level and 1m; x = 1000 m

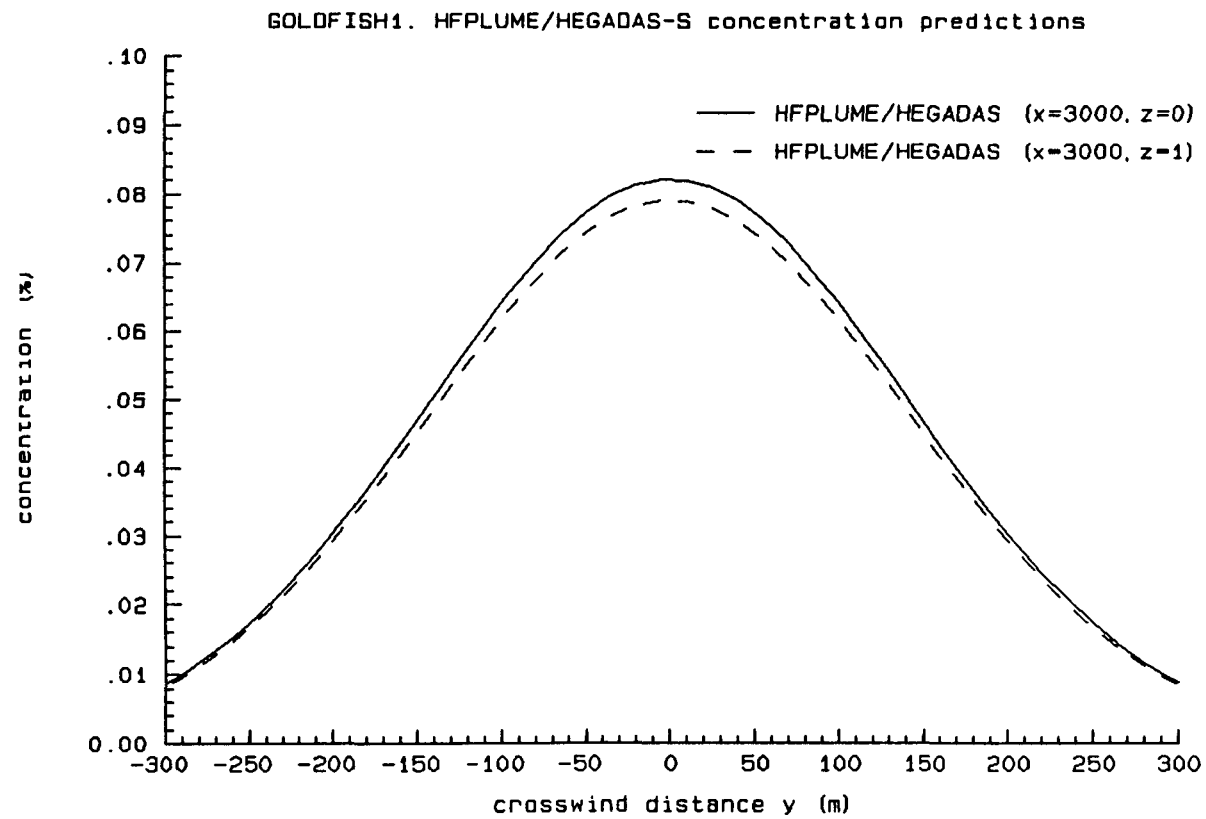


Fig. 9.19. Goldfish 1 predictions of crosswind concentration profile by HEGADAS-S at ground level and 1m; x = 3000 m

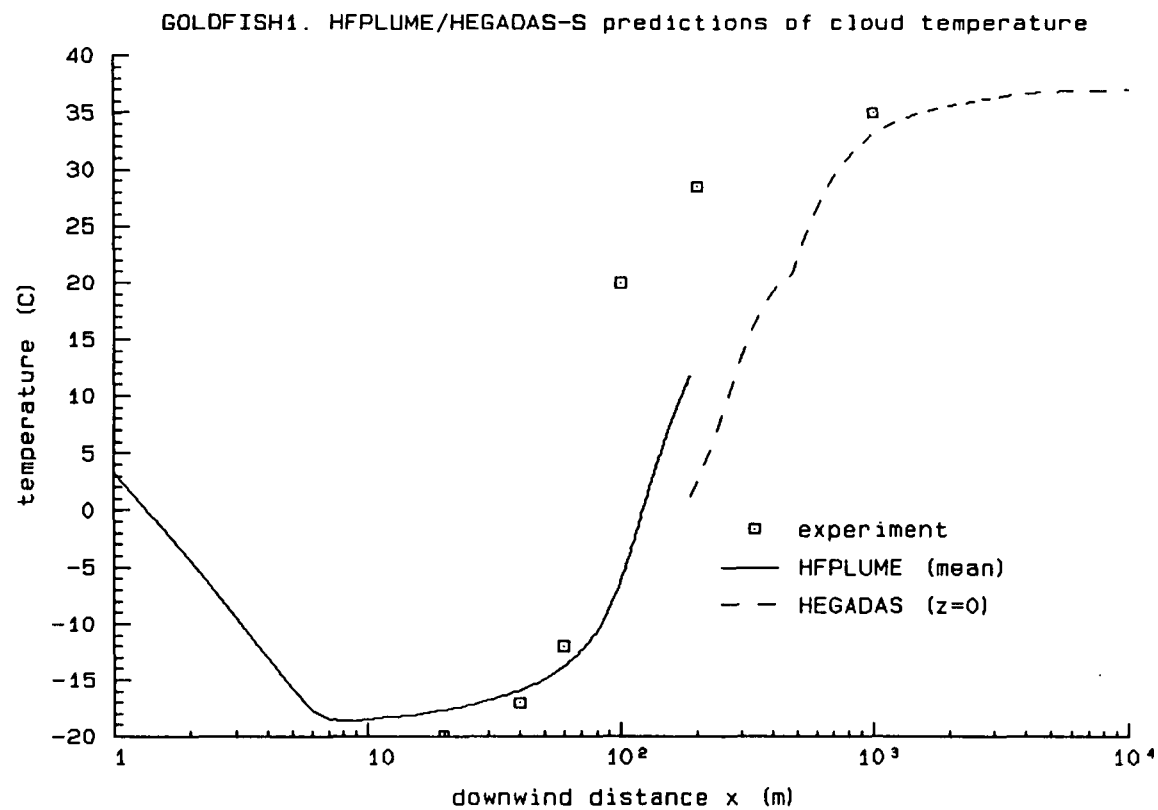


Fig. 9.20. Goldfish 1 predictions of temperature by HFPLUME/HEGADAS-S
[experimental data are too high, since the centre-line of the
plume was not aligned with the line on which the temperature
measurements were made]

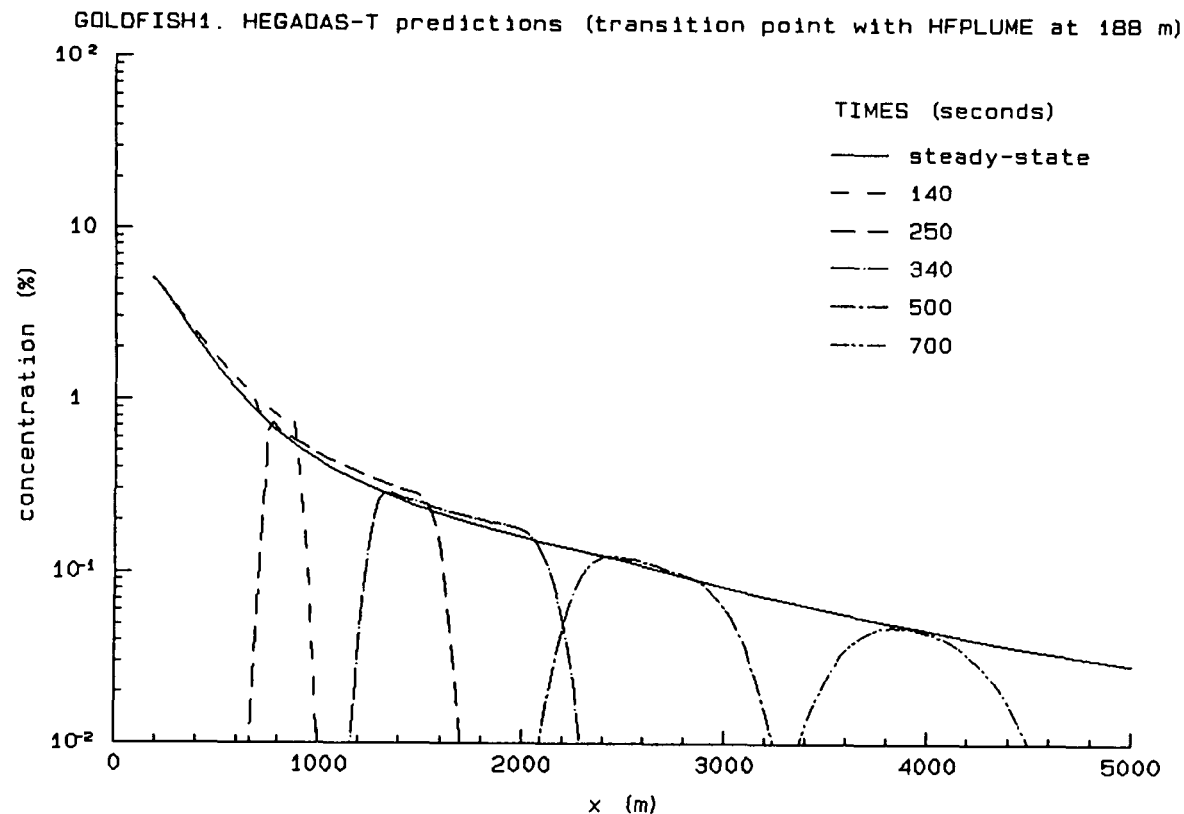


Fig. 9.21. Goldfish 1 centre-line groundlevel concentration (% molar fraction) as a function of the downwind distance x from the release point; predictions by HEGADAS-S (steady-state) and HEGADAS-T (transient, at times $t = 140, 250, 340, 500$ and 700 seconds) with both programs being based on HFPLUME transition data at 188 m

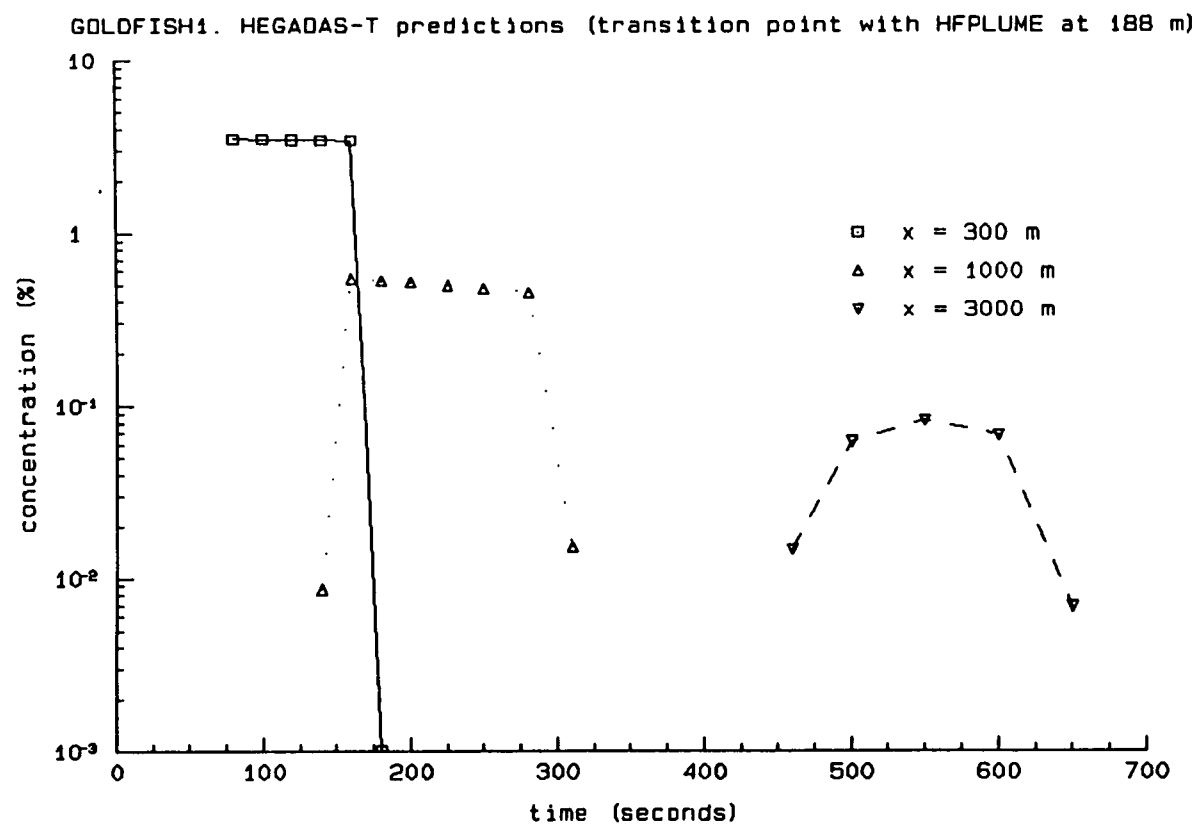


Fig. 9.22. Goldfish 1 predictions by HEGADAS-T of the centre-line groundlevel concentration as a function of the time; downwind distances $x = 300, 1000, 3000$ m

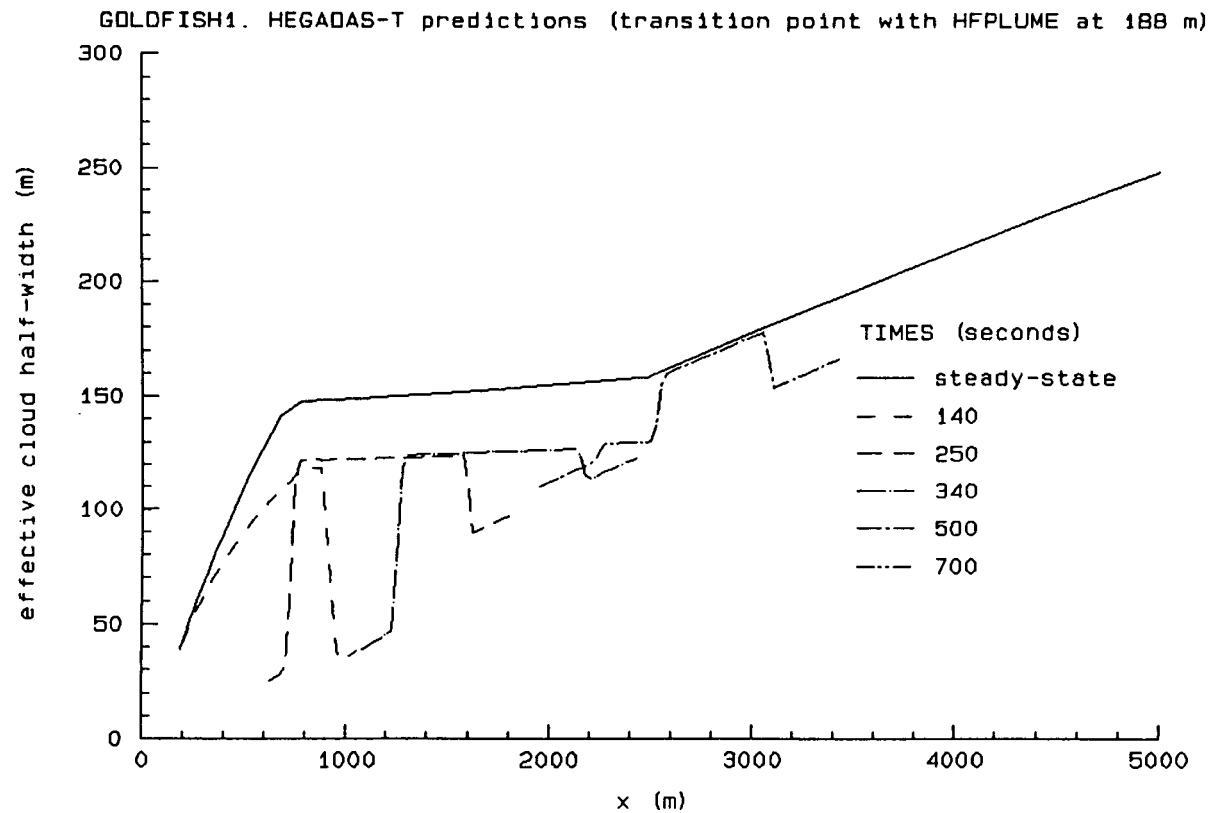


Fig. 9.23. Goldfish 1 effective cloud half-width (% molar fraction) as a function of the downwind distance x from the release point; predictions by HEGADAS-S (steady-state) and HEGADAS-T (transient, at times $t = 140, 250, 340, 500$ and 700 seconds) with both programs being based on HFPLUME transition data at 188 m

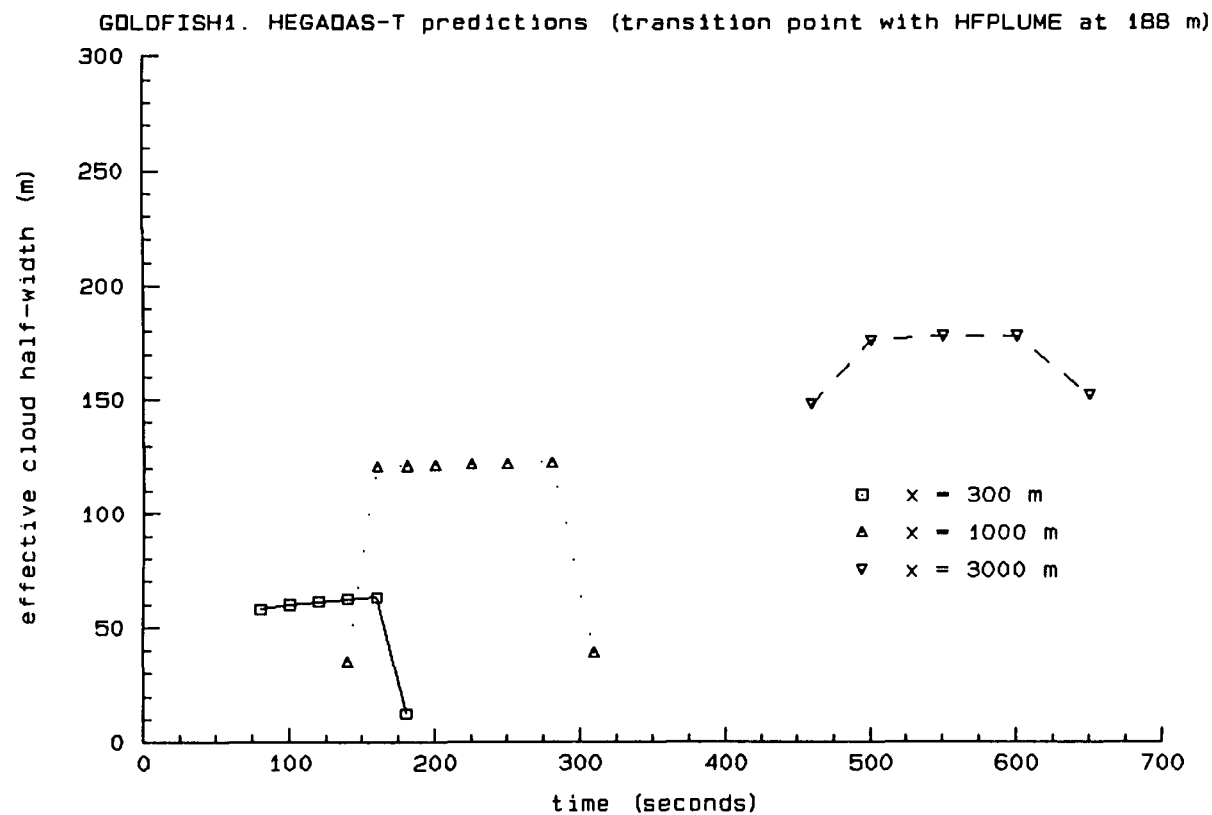


Fig. 9.24. Goldfish 1 predictions by HEGADAS-T of the effective cloud half-width as a function of the time; downwind distances $x = 300$, 1000, 3000 m

10. SENSITIVITY ANALYSIS

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10.1. INTRODUCTION

This chapter presents the results of the sensitivity analyses which were conducted as part of the development of the HGSYSTEM models. These analyses are an important part of the development and testing of the models contained within HGSYSTEM.

Historically models are verified by comparison with experimental data to model predictions. These experiments typically are designed to replicate the application for which the model will ultimately be used. The intended application of HGSYSTEM is to simulate accidental releases of HF in an industrial setting. However, there is no one set of experimental data against which all aspects of the model can be tested in its entirety. In verifying the models sensitivity analyses are the only method of testing the interaction of all components of the models and the validity of the several model assumptions. From these analyses it can be ensured that the results are physically reasonable.

Many experimental data were used in developing and validating the HGSYSTEM models:

- The empirical entrainment relations in HEGADAS and HFPLUME are based on a large number of wind tunnel experiments. See Chapter 5 for the entrainment relations in HFPLUME. See Section 3 in Appendix 3 for the entrainment relations in HEGADAS
- In the crosswind spreading formulation in HEGADAS the initial crosswind spreading (C_E formulation) is based on experiments by Van Ulden (1984); see Section 4.1 in Appendix 3. The subsequent collapse of gravity spreading (C_D formulation) is based on experiments by Linden and Simpson (1988); see Section 7.3.2. The far-field crosswind spreading is based on empirical formulas for the non-dense crosswind dispersion coefficient σ_y ; see Section 7.3.1.

- The HF-thermodynamics formulation in HEGADAS and HFPLUME is based on experimental data by Schotte (1987,1988); see Chapter 2, Section 7.2 and Appendix 5.

A further validation and verification of the thus developed models was carried out by simulation of wind tunnel experiments and large-scale field experiments. The near-source plume model HFPLUME was validated against wind tunnel experiments, experimental propane releases (see Chapter 5) and the Goldfish experiments (see Chapter 9). HEGADAS was validated against a large number of experiments, e.g. the Maplin Sands and Thorney Island field experiments, the HTAG wind tunnel data (see Chapter 8) and the Goldfish experiments (see Chapter 9).

The sensitivity analysis in this chapter is split up into the following two parts.

- In Section 10.2 the sensitivity to the input variables (meteorological data, source data, etc.) for a HFPLUME/HEGADAS-S analysis is investigated. Two base cases are considered, one case with conditions similar to the Goldfish 2 experiment (high temperature, low surface roughness and humidity) and one with more typical rural conditions. First the important variables are altered individually. Secondly for those parameters which have an interactive relationship several variables were altered simultaneously.
- In Section 10.3 the sensitivity of a number of basic model assumptions in a HFPLUME/HEGADAS-S analysis is studied, i.e. the type of HFPLUME/HEGADAS-S transition criterion (values of RULST, RELST), the effect of the modified gravity spreading formulation (parameter C_D), and the type of σ_y crosswind-spreading law (power-law or Briggs formula).

10.2. SENSITIVITY OF INPUT VARIABLES (HFPLUME/HEGADAS-S ANALYSIS)

10.2.1. Base cases

The input data to the HFPLUME and HEGADAS-S programs are described in detail in the HFPLUME and HEGADAS user's guides (Chapters 5 and 8 in the User's Manual). See also Table 9.1 for a short list of these input data. In the Sections 10.2.2 and 10.2.3 the effect of variations in the input variables on the HFPLUME/HEGADAS-S predictions are investigated. In Section 10.2.2 the important variables are altered individually, and in Section 10.2.3 for those parameters which have an interactive relationship several variables are altered simultaneously.

The above variable variations are carried out assuming two different base cases A and B. The input data and the results of the HFPLUME/HEGADAS-S runs for these base cases are discussed in the present section.

Input data to base bases

The two different base cases A and B are chosen as follows.

A. The conditions for base case A are similar to those of the Goldfish 2 experiment (see Table 9.1: high temperature, low surface roughness and humidity), but the release rate is somewhat lower. The input variables for this base case are as follows:

- ambient data: temperature $T_a = 35^\circ\text{C}$, relative humidity $r_H = 10\%$, wind speed u_0 at 10m = 5 m/s, Pasquill Stability Class PQSTAB = D (with default values for δ, β in σ_y power-law), surface roughness $z_R = .0003\text{m}$
- averaging time: 60 seconds
- release rate: GSFLOW = 5 kg/s = 85 gal/min
- release angle: 0 degrees
- reservoir data: temperature = 36°C , pressure = 9 atm
- pipe exit-plane data: pressure = 8.5 atm, orifice diameter = .025 m, orifice height = 1.25 m

- B. The release data for base case B are the same as those mentioned above for base case A, now occurring under typical rural conditions, i.e. a lower ambient temperature $T_a = 15^\circ\text{C}$, a higher relative humidity $r_H = 70\%$ and a higher surface roughness $z_R = 0.03 \text{ m}$

HFPLUME/HEGADAS-S predictions for base cases and transition points

Figures 10.1 and 10.2 as well as Tables 10.1 and 10.2 present HFPLUME/HEGADAS-S predictions for the base cases A and B respectively. These figures include results of following data.

- o The centre-line concentration (equivalent molar fraction of HF, with all HF based on HF monomer). This concentration is taken to be the sectional-mean concentration (c^{p1} ; value at plume centroid) in the HFPLUME region, and the centre-line ground-level concentration (c_A) in the HEGADAS region. At the HFPLUME/HEGADAS-S transition c_A is $2^{1/2}$ times as large than c^{p1} (see eq. (7.73)), which explains the discontinuity in concentration at the transition point shown in Figures 10.1 and 10.2.
- o The "effective" cloud half-width, B_{eff} , used in the HEGADAS equations (see Section 3.1 in Appendix 3; for use in e.g. the crosswind gravitational spreading law). In the HFPLUME region the plotted value equals $[3 \pi D^{p1}]/[16 \cdot 2^{1/2}]$, with D^{p1} being the HFPLUME plume "diameter". This value equals the HEGADAS effective cloud half-width at the transition point (cf. eq. (7.74)).
- o The cloud half-width, W_h , given by the frequently adopted definition

$$W_h^2 = \frac{\int_{-\infty}^{\infty} y^2 c(x,y,z) dy}{\int_{-\infty}^{\infty} c(x,y,z) dy}$$

For HEGADAS, W_h is set by insertion of the HEGADAS concentration profile in the above formula. For HFPLUME, the plotted value of W_h equals

$[3 \pi D^{p1}]/[16*6^*]$, with D^{p1} being the HFPLUME plume "diameter". This value can be shown to equal the HEGADAS value of the cloud half-width W_h at the transition point (cf. eq. (7.74)).

- o The half-width of the middle part of the HEGADAS-S crosswind concentration profile (see Section 7.1.2), b.
- o The bulk Richardson number, Ri_* . In the HFPLUME region the bulk Richardson number $Ri_* = Ri_*(c^{p1})$ is based on the sectional-mean concentration c^{p1} , and in the HEGADAS region $Ri_* = Ri_*(c_A)$ is based on the (higher) concentration c_A . This explains the discontinuous increase in Richardson number at the transition point in Figures 10.1 and 10.2.

The value of the entrainment ratio $(Entr_{total} - Entr_{gas}^{heavy})/(Entr_{total})$ defines the relative drop of entrainment at x_{tr}^{HP} , caused by neglect in HEGADAS-S of the jet entrainment $Entr_{jet}$. This induces a discontinuous decrease in slope of the concentration. It should also be noted that the HFPLUME and HEGADAS heavy-gas entrainments are calculated somewhat differently. The HFPLUME entrainment (Section 5.8) is formulated in terms of $Ri_* = Ri_*(c^{p1})$, whereas the HEGADAS entrainment (Section 3 in Appendix 3 to this Technical Reference Manual) is based on the larger Richardson number $Ri_* = Ri_*(c_A)$.

In the figures and the tables the following transitions are indicated.

- The HFPLUME/HEGADAS transition at the downwind position $x = x_{tr}^{HP}$.

For the runs presented in this chapter the transition parameters $RELST = 0.3$ and $RULST = 0.1$ (default values) are chosen, i.e. the transition from HFPLUME to HEGADAS-S takes place at the downwind position, at which first the conditions $RE = (Entr_{total} - Entr_{gas}^{heavy})/(Entr_{total}) < RELST$ and $RU = |u^{p1}/u^{amb} - 1| < RULST$ are simultaneously satisfied. Here $Entr_{total}$ is the total HFPLUME entrainment, $Entr_{gas}^{heavy}$ is the proportion of heavy-gas entrainment, u^{p1} the HFPLUME plume speed, and u^{amb} the ambient velocity at the plume centroid. See Section 7.8.3 for full details.

- The transition in HEGADAS-S or HFPLUME between the C_E and C_D crosswind spreading formulation at the downwind position $x = x_{tr}^{CD}$. At this point turbulent collapse takes place and crosswind gravity spreading (i.e. increase of effective cloud half-width B_{eff}) is considerably diminished; see Section 7.3.2 for full details.
- The downwind position $x = x_{tr}^b$ at which the middle part of the HEGADAS-S crosswind concentration profile vanishes, i.e. at which b becomes 0. Downwind of this position the crosswind concentration profile is assumed to be purely Gaussian, with further development of the crosswind dispersion coefficient S_y determined from the σ_y formula valid for passive flow; see Section 7.3.1 for full details.
- The downwind position $x = x_{tr}^{Ri}$ in HFPLUME or HEGADAS-S at which the flow becomes neutral, i.e. the position at which the mixture density equals the ambient density. This position is close to the position at which the bulk Richardson number Ri_* becomes negative. It is noted that in case of $x_{tr}^{Ri} < x_{tr}^b$ no gravity spreading is assumed for $x_{tr}^{Ri} < x < x_{tr}^b$. From the collapse criterion (7.27), it follows that x_{tr}^{Ri} is always downwind of the point of turbulent collapse x_{tr}^{CD} .

The above transitions were found to be located at x_{tr}^{PH} , x_{tr}^{CD} , x_{tr}^b , x_{tr}^{Ri} = 224, 550, 1454, 3550 and 75, 68, 189, 70 m for the base cases A and B, respectively (cf. Figures 10.1 and 10.2). Thus for the low-humidity base case A the subsequent phases in the downwind direction are

- heavy-gas flow, transition from HFPLUME to HEGADAS-S
- heavy-gas " C_E " gravity spreading, turbulent collapse
- reduced heavy-gas " C_D " gravity spreading
- passive type of crosswind spreading and transition to neutral flow

For the high-humidity base case B the phases are

- heavy-gas flow, turbulent collapse

- no crosswind spreading; during this phase first the transition to neutral flow occurs and then the transition from HFPLUME to HEGADAS-S
- passive type of crosswind spreading.

At the transition point x_{tr}^{HP} the transition data are as follows (Tables 10.1a, 10.2a):

- base case A: $RE = 0.30$, $RU = 0.05$, $Ri_{*} = 13.2$
- base case B: $RE = 0.15$, $RU = 0.10$, $Ri_{*} = -0.32$

10.2.2. Effect of single parameter variations

In this section results of HFPLUME/HEGADAS-S analyses are discussed in which a single parameter in the base cases A and B is varied.

Types of single parameter variations

The variations of the parameters are chosen as follows.

- ambient temperature: $T_a = 5, 15, 25, 35$ °C
- ambient relative humidity: $r_H = 10, 30, 50, 70, 90$ %
- surface roughness: $z_R = .0001, .0003, .001, .003, .01, .1, .5$ m
- wind speed: $u_0 = 2, 3.5, 5, 10$ m/s
- Pasquill Stability Class PQSTAB = B, D, E or F in combination with low wind speed $u_0 = 2$ m/s
- averaging time: 10, 30, 120, 300, 600, 900 seconds
- release rate: $E = 2.5, 5, 10, 20$ kg/s (= 43, 85, 171, 342 gal/min)
- release angle: $\phi = 30, 60, 90$ degrees

Note that the HFPLUME-specific reservoir data and pipe exit-plane data are not varied.

HFPLUME/HEGADAS-S predictions

Figures 10.3-10.19 summarise results of the above HFPLUME/HEGADAS-S analyses. Figure 10.3 includes temperature plots for the case of variation of the ambient temperature. Figures 10.4-10.19 depict the predictions for the concentration and the effective cloud half-width (B_{eff}). The following remarks and conclusions are given.

In most analyses the HFPLUME calculations were carried out, a transition was made to HEGADAS, and the HEGADAS calculations were performed (up to a user-specified maximum downwind distance or minimum concentration). In a relatively small proportion of the analyses the HFPLUME/HEGADAS run was not completed in the usual manner. In the figures these analyses are briefly

indicated by the annotations P1 or PE. These annotations stand for the following:

- P1: analyses in which HFPLUME is terminated prematurely because the (change in) shape of the plume cannot any more be properly be modelled by HFPLUME (see Chapter 5 and HFPLUME User's Guide for further details). There is no increase of cloud plume diameter, i.e. $dD/dx=0$, signalled by HFPLUME as "unexpected plume lift-off following plume slumping". The case of a plume which first touches down and subsequently becomes buoyant enough to lift off cannot be dealt with by HFPLUME.

This type of termination of the HFPLUME run occurred for the 100% humidity variation of base case A (Figure 10.6) and the low (2 m/s) wind-speed variation of base case B (Figures 10.11 and 10.13).

- PE: HFPLUME is terminated because neither HFPLUME/HEGADAS interface criteria or HFPLUME/PGPLUME criteria are satisfied at the user-specified maximum distance of XLST = 1000 m.

This type of termination of the HFPLUME run occurred for the low (2 m/s) wind-speed and stable (classes E,F) stability-class variations of base case A (Figure 10.12).

In HEGADAS-S a passive dispersion formula is used for the calculation of the effective cloud half-width B_{eff} after the middle part of the HEGADAS concentration profile has vanished; see Section 7.3.1. For large downwind distances $B_{eff} = \pi^{1/2} S_y(x)/2$ converges to the passive limit $(\pi/2)^{1/2} \sigma_y(x) = (\pi/2)^{1/2} \delta x^\beta$, with δ, β dependent on the averaging time AVTIMC and the stability class PQSTAB only (see Tables 7.1 and 7.2). It is clearly illustrated by Figures 10.4b, ..., 10.19b that B_{eff} always converges to the same passive limit for $x \rightarrow \infty$, apart from Figures 12b, 13b, 18b and 19b, in which PQSTAB and AVTIMC are varied.

From the figures the following remarks and conclusions can be given concerning the effect of single parameter variations:

1. AMBIENT TEMPERATURE (Figures 10.3, 10.4 and 10.5)

Variation of the ambient temperature T_a hardly affects the concentrations for low humidity (base case A; see Figure 10.4). In the case of high humidity, the centre-line ground-level concentration c_A increases and the effective cloud half-width B_{eff} decreases with increasing temperature (see Figure 10.5).

2. RELATIVE HUMIDITY (Figures 10.6 and 10.7)

The effect of humidity is particularly important in HF dispersion. Variations in humidity have a strong effect on the density of an HF-air mixture (Chapter 2, Figure 2.1), and the density variations are important in the dispersion, affecting both the gravity-spreading and the vertical mixing. It should be noted that once the fog droplets have evaporated, the density is almost independent of humidity. But, the higher the humidity, the longer the fog persists.

The resulting predicted effect on concentration as a function of distance (Figure 10.6a) appears complex, but can be explained. At 10% humidity, there is little effect of heat generated by HF-H₂O reaction. In contrast, as the humidity is increased to 30% and 50%, the cloud is less dense in the early stages of dispersion. There is thus less gravity-spreading and the plume is narrower. The narrower plume has a smaller top surface through which mixing can take place, and so subsequent dilution is slower. It can be seen that concentrations are higher than for 10% humidity beyond about 200 m from the source.

At 70% and 90% humidity, the thermodynamic effects persist long enough to increase the rate of vertical mixing over an extended distance downwind. While the fog persists, the lower density results in a much more rapid dilution, despite the narrowness of the plume. The result is lower concentrations than for 10% humidity.

Similar behaviour is predicted for base case B (Figure 10.7).

3. SURFACE ROUGHNESS (Figures 10.8 and 10.9)

The heavy gas entrainment is proportional to the friction velocity u_* , and hence increases with the surface roughness z_R (at fixed u_0). Therefore the concentration c_A decreases with increasing surface roughness z_R (see Figures 10.8a and 10.9a).

Prior to the collapse of crosswind spreading the cloud width increases with increasing z_R (see Figures 10.8b and 10.9b). The several mechanisms of collapses of crosswind spreading were shortly reviewed in Section 10.2.1. Concerning surface roughness effects the following is now noted.

- For the low-humidity base case A crosswind spreading collapses at the transition point x_{tr}^{CD} between the C_E - and C_D -formulation. From the transition criterion described in Section 7.3.2 it can be shown that x_{tr}^{CD} is located further upwind for increasing friction velocity u_* . Thus, since u_* increases with z_R , crosswind spreading stops earlier for larger values of z_R . This phenomenon is clearly illustrated by Figure 10.8b.
- For the high-humidity base case B crosswind spreading collapses already in HFPLUME ($x_{tr}^{CD} < x_{tr}^{HP}$). From Figure 10.9b it is seen that the transition criterion is satisfied at a value of the effective cloud half-width $[B_{eff} = 3 \pi D^{p1}/(16*2^k)]$, which is independent of the surface roughness.

4. AMBIENT WIND SPEED (Figures 10.10 and 10.11)

The heavy-gas entrainment adopted in HEGADAS is proportional to the friction velocity u_* , and hence increases with the wind speed u_0 (at fixed z_R). Thus sufficiently downwind of the transition x_{tr}^{HP} with HFPLUME (which also takes into account the jet entrainment), the concentration c_A decreases with increasing u_0 (see Figures 10.10a, 10.11a).

For increasing wind speed, the cloud is more quickly convected away and spreads less in the crosswind direction. This is illustrated by the smaller cloud widths in Figures 10.10b and 10.11b.

5. ATMOSPHERIC STABILITY (Figures 10.12 and 10.13)

For more stably stratified flow, the heavy-gas entrainment of air into the gas cloud is less. Therefore the concentration c_A is higher downwind of the region in which jet entrainment is important; see Figures 10.12a and 10.13a.

The following can be noted for the two cases.

- For the low-humidity (high density) case the cloud remains long non-buoyant. Thus spreading occurs due to gravity spreading. At given fixed velocity u_0 at 10 m, the velocity at lower heights will be lower for more stably stratified flows. Therefore the cloud is less quickly convected away and spreads more in the crosswind direction. Thus for more stably stratified flow the cloud width increases (see Figure 10.12b).

It is noted that for stability class B (most unstable class with largest amount of air entrainment) the cloud is found to become extremely buoyant in HEGADAS-S (very negative Richardson number) after about 500 m. This results in very low values for the concentration c_A (see Figure 10.12a).

For the stable cases E and F (low entrainment of air; high Richardson numbers) the entrainment criterion $RE < RELST$ was not satisfied after 1000 m. The HFPLUME was terminated at this distance and a transition to HEGADAS was not made.

- For the high-humidity (low-density) case the cloud becomes quickly buoyant in HFPLUME (for $x < x_{tr}^{HP}$).

For all stability classes (B,D,E,F) the HFPLUME run was terminated prematurely at about $x = 90$ m because of $dD/dx = 0$. The case of a plume which first touches down and subsequently becomes buoyant enough to lift off cannot be dealt with by HFPLUME; see Figures 10.13a and 10.13b.

6. RELEASE RATE (Figures 10.14 and 10.15)

The concentration and the cloud width increase with increasing release rate E corresponding to a bigger, more dense cloud; see Figures 10.14 and 10.15.

7. RELEASE ANGLE (Figures 10.16 and 10.17)

For a larger release angle ϕ , the downwind component u_x^{p1} of the jet/plume velocity will be less near the source. The airborne plume will be convected away less quickly and the crosswind entrainment $Entr_{wind}^{cross}$ (see Chapter 5) increases. Hence more dilution and crosswind spreading occurs near the source, i.e. the HFPLUME concentration (c^{p1}) decreases and the cloud width increases for increasing ϕ ; see Figures 10.16 and 10.17.

Further downwind (but prior to the moment of touchdown) the difference in the values of u_x^{p1} for the different release angles gradually diminishes. Therefore the proportional difference in concentration and cloud width decreases; see Figures 10.16 and 10.17.

As the plume touches down to move along the ground the crosswind entrainment is set to zero and heavy-gas entrainment is first taken into account. For the positive release angles $\phi = 30, 60, 90$ degrees, the point of touchdown is at a considerable downwind distance, i.e. for the low-humidity, high-density case A at 38, 52, 49 m and for the high-humidity, low-density case B at about 69, 160 and 168 m, respectively. The sudden loss of $Entr_{wind}^{cross}$ induces a considerable reduction in overall entrainment, and hence a sudden discontinuous decrease in slope of the concentration; see Figures 10.16a and 10.17a.

For the high-humidity case the HFPLUME/HEGADAS-S transition criterion was satisfied immediately after touchdown.

The predictions of the concentration and the cloud width for the different release angles all converge to the same passive limit in the far field; see Figures 10.16 and 10.17.

8. AVERAGING TIME (Figures 10.18 and 10.19)

At the transition point x_{tr}^b the middle part of the HEGADAS concentration profile vanishes. Upwind of this point the averaging time AVTIMC for measuring the calculations appears (through the formula for δ) in the differential equation for the crosswind dispersion coefficient S_y only; see Section 7.3.1 and Tables 7.1 and 7.2. Thus the predictions for c_A and B_{eff} are independent of AVTIMC upwind of x_{tr}^b ; see Figures 10.18 and 10.19. Essentially, meandering of the uniform concentration of the core of the plume does not affect the concentration out the centre.

For increasing AVTIMC, δ increases (see Tables 7.1 and 7.2). From the differential equation for S_y (see eqs. (7.13) and (7.17)), it now easily follows that $\pi^{1/2}S_y/2$ more rapidly increases from 0 (assumed at x_{tr}^{HP} ; see Section 7.8.3) to B_{eff} (at x_{tr}^b) for increasing AVTIMC. Thus x_{tr}^b is located more upwind for increasing AVTIMC. From the power-law for S_y (see eqs. (7.14) and (7.16)), it follows that downwind of x_{tr}^b the slope of the $\log(c_A) - \log(x)$ curve equals β ($= -0.907$ for stability class D), which is independent of averaging time; see Figures 10.18b and 10.19b. Therefore downwind of x_{tr}^b the cloud width is larger for increasing averaging time. This is accompanied with a smaller centre-line ground-level concentration c_A (see Figures 10.18a and 10.19a), i.e. we have a wider and less dense cloud downwind of x_{tr}^b for smaller averaging times. This conclusion is in agreement with the observations made in Section 7.3.1.3.

10.2.3. Effect of multiple parameter variations

In this section results of HFPLUME/HEGADAS-S analyses are discussed in which more than one parameter is varied. Here base case B is only considered. The combined effect of the variation of humidity (r_H), release rate (E) and stability class (PQSTAB) is studied both for typical rural conditions and for typical urban conditions. The following three types of analyses are performed.

- A. Typical rural conditions (surface roughness $z_R = .03$ m) with horizontal jet; relative humidity $r_H = 10, 30, 50, 70$ or 90% ; release rate $E = 5$ or 2.5 kg/s; Pasquill stability class/wind speed $PQSTAB-u_0 = D-5$ (base-case value) or $F-2$. The results of these runs are depicted in Figures 10.7, 10.20-10.22.
- B. Typical urban conditions ($z_R = 0.5$ m) with horizontal jet; $r_H = 10, 30, 50, 70$ or 90% ; $E = 5$ or 2.5 kg/s; $PQSTAB-u_0 = D-5$ (base-case value) or $E-2$. The results of these runs are depicted in Figures 10.23-10.26.
- C. Typical urban conditions ($z_R = 0.5$ m) with vertical jet at 10 m exit height; $r_H = 10, 30, 50, 70$ or 90% ; $E = 5$ or 2.5 kg/s; $PQSTAB-u_0 = D-5$ (base-case value) or $E-2$. The results of these runs are depicted in Figures 10.27-10.30.

In most analyses the HFPLUME calculations were carried out, a transition was made to HEGADAS, and the HEGADAS calculations were performed (up to a user-specified maximum downwind distance or minimum concentration). In the other analyses the HFPLUME/HEGADAS run was not completed in the usual manner. In the figures these analyses are briefly indicated by the annotations PG, P1, P2, P3 or EP. These annotations stand for the following:

- PG: analyses in which a transition from HFPLUME is made not to the heavy-gas dispersion program HEGADAS but to the passive-gas dispersion program PGPLUME (see Chapter 6). See the end of this section for further details.

- P1,P2,P3: analyses in which HFPLUME is terminated prematurely because the (change in) shape of the plume cannot any more be properly be modelled by HFPLUME (see Chapter 5 and HFPLUME User's Guide for further details):

- o P1: no increase of cloud plume diameter, i.e. $dD/dx=0$, signalled by HFPLUME as "unexpected plume lift-off following plume slumping"; the case of a plume which first touches down and subsequently becomes buoyant enough to lift off cannot be dealt with by HFPLUME.

This type of termination of the HFPLUME run occurred under rural conditions (type A) for the high-humidity (70% and 90%) and stability-class F2 variations (Figures 10.21 and 10.22). It also occurred under urban conditions for class E2, 70% humidity and 2.5 kg/s release rate (Figure 10.26).

- o P2: buoyancy induced distortion of "slumped" plume suggests that plume lift-off is imminent.

This type of termination of the HFPLUME run occurred for the 2.5 kg/s release rate, 90% relative-humidity variations for stability class D5 (type A; Figure 10.20) or E2 (type B; Figure 10.26).

- o P3: the entrainment rate inferred from the curvature-limited model decreases more rapidly than the associated empirically determined entrainment rate for the same plume description.

This type of termination of the HFPLUME run occurred for the 5 kg/s release rate, stable-stability class and 10% (types of analyses A, B and C) or 30% (type A) relative-humidity variations; see Figures 10.21, 10.25 and 10.29.

- EP: analysis in which HFPLUME is terminated because of failure to converge for iterative solution to HF thermodynamic equations.

This type of termination occurred in the case of a vertical release (type C) for the stability-class E2, 2.5 kg/s release rate and high-humidity (50, 70 and 90 %) variations (Figure 10.30).

For the effects of relative humidity, stability class and release rate the reader is referred to the previous section. It is again seen from Figures 10.7, 10.20-10.26 that for the non-vertical releases the effective cloud width decreases as a function of humidity, the concentration increases with more stably stratified flow, and the cloud is more dense and wide for a larger release rate.

A transition from HFPLUME to PGPLUME was made for the vertical-jet runs with stability class D5 and the 10, 30, 50 and 70 % relative humidities (Figures 10.27 and 10.28). In Figures 10.27 and 10.28 the plotted PGPLUME concentration corresponds to the centre-line ground-level concentration and the plotted cloud half-width to $(\pi/2)^{1/2} \sigma_y$, with σ_y being the passive crosswind-dispersion coefficient.

The concentration predictions depicted in Figures 10.27a and 10.28a can be explained as follows.

- o The jet flow and near-field dispersion are modelled by HFPLUME. The transition from HFPLUME to PGPLUME is made while the plume is still "airborne". Thus at this transition the peak concentration is assumed above ground level and the PGPLUME centre-line ground-level concentration (c_A) is lower than the HFPLUME sectional-mean concentration (c^{p1}). It should be noted that the HFPLUME concentration is considered to be an instantaneous concentration, while the (lower) PGPLUME concentration is based on an averaging time of 60 seconds.
- o The height at which the peak concentration is assumed, reduces to zero while the plume travels further downwind of the transition point. This results in an initial increase in c_A downwind of the transition point. Further downwind c_A decreases.

- o The HFPLUME/PGPLUME transition point x_{tr}^{HP} is located further downwind for increasing humidity. For higher humidity ($< 90\%$) the plume is closer to touchdown at x_{tr}^{HP} , resulting in less increase in c_A downwind of x_{tr}^{HP} . For 90% humidity a transition from HFPLUME to PGPLUME is not made, while the plume is "airborne". Instead, a transition is made to HEGADAS-S immediately after "touchdown".

The runs depicted in Figures 10.27 and 10.28 are carried out under urban conditions involving a high surface roughness ($z_R = 0.5$ m). The PGPLUME predictions for $r_H = 10, 30, 50$ and 70% all converge to the same asymptotic far-field limit.

The HEGADAS cloud-width prediction for $r_H = 90\%$ (Figures 10.27b, 10.28b) converges to the same asymptotic limit in the far-field as PGPLUME, since HEGADAS and PGPLUME use comparable empirical formulae for the crosswind dispersion coefficient σ_y in the far-field (see Sections 7.3.1.1 and 6.2).

The HEGADAS center-line ground-level prediction for $r_H = 90\%$ (Figures 10.27a, 10.28a) converges to a asymptotic limit in the far-field, which is significantly lower than that for the PGPLUME runs. This difference may be attributed to the formula for the vertical dispersion coefficient σ_z used in PGPLUME. The uncertainty of this formula is reflected in the different σ_z -formulae used by Briggs (1973) for rural and urban conditions. Briggs recommends much higher σ_z values for urban conditions. This results in much lower concentration values, which might explain the difference in HEGADAS and PGPLUME concentrations shown in Figures 10.27a and 10.28a.

10.3. SENSITIVITY OF MODEL ASSUMPTIONS (HFPLUME/HEGADAS-S ANALYSIS)

In this section results of HFPLUME/HEGADAS-S analyses are discussed in which basic model parameters are varied for the base cases A and B. Thus the sensitivity of a number of basic model assumptions in HFPLUME/HEGADAS-S is studied, i.e. the HFPLUME/HEGADAS-S transition criterion, the type of gravity-spreading law and the type of formula for the crosswind dispersion coefficient σ_y .

HFPLUME/HEGADAS-S transition criterion

The HFPLUME/HEGADAS-S transition criterion has been discussed in detail in Section 7.8.3. In this criterion the downwind position $x = x_{tr}^{hp}$ of the transition point is determined by the HFPLUME input parameters RULST, RELST (eq. (7.64)). The HFPLUME/HEGADAS-S transition is made if the proportion of heavy-gas entrainment in the total entrainment is larger than $(1-RELST)*100\%$ and the difference in plume speed and ambient speed is less than $RULST*100\%$.

The sensitivity of the HFPLUME/HEGADAS predictions to the choice of the transition criteria is studied by varying RELST, RULST. The parameter values $(RELST, RULST) = (0.9, 0.5), (0.6, 0.25), (0.3, 0.1), (0.2, 0.05)$ are chosen. Figures 10.31 and 10.32 include predictions of the concentration and the effective cloud half-width for the base cases A and B, respectively. The following is noted.

- The effect of the choice of the transition criterion on the predictions is visible near the transition point only. Upwind of the transition points the results are, of course, identical. At distances sufficiently far downwind of the transition points results are virtually the same.
- At the HFPLUME/HEGADAS transition point $x = x_{tr}^{hp}$ the HEGADAS centre-line, ground-level concentration equals $2^{1/2}$ times the HFPLUME sectional-mean concentration (eq. (7.73)). At x_{tr}^{hp} a proportion RELST of the total entrainment (the proportion of jet entrainment) is neglected. This drop in entrainment leads to a discontinuous concentration slope at x_{tr}^{hp} (Figures 10.31a and 10.32a). The discontinuity is particularly

significant for larger values of RELST ($\text{RELST} > 0.6$). Values of RELST below 0.3 lead to HFPLUME (sectional-mean) concentration curves, which are almost "parallel" at the transition point to the HEGADAS (centre-line, ground-level) concentration curves.

- The predictions for the concentration and the cloud width are almost unaffected by the precise position of the transition point if RELST and RULST are chosen sufficiently small ($\text{RELST} \leq 0.3$, $\text{RULST} \leq 0.2$).

At the transition point a uniform crosswind concentration profile is adopted (see Section 8.6.3; profile without Gaussian flanks, i.e. $S_y = 0$). Thus if the HFPLUME/HEGADAS transition is chosen very far downwind, the crosswind concentration profile cannot be well predicted by HEGADAS. Therefore the default values for RELST, RULST are chosen to be $\text{RELST} = 0.3$, $\text{RULST} = 0.2$. These values lead to relatively smooth transitions of the concentration and the cloud width, while at the same time the transition point is located not too far downwind.

If the user wishes to compare HFPLUME/HEGADAS predictions for a crosswind concentration profile relatively close to the release point, he might consider to carry out an additional run with increased values for RELST and RULST.

Crosswind gravity-spreading law

The new crosswind gravity-spreading formulation in HEGADAS has been discussed in detail in Section 7.3.2. In the gravity-spreading process the subsequent phases are

- initial crosswind spreading defined by the gravity-spreading law by van Ulden (" C_E -formulation"; see Section 4.1 in Appendix 3)
- collapse of gravity at the downwind position defined by criterion given by eq. (7.27)

- considerably reduced amount of spreading defined by adjustable parameter C_D ("C_D-formulation"; see eq. (7.25))

HFPLUME/HEGADAS analyses are carried out with ($C_D > 0$; new HEGADAS-5 model) and without (flagged by $C_D = 0$; old HEGADAS-4 model) the inclusion of collapse of gravity spreading. For the new model three different values of the adjustable parameter C_D were adopted, i.e. $C_D = 2.5$, $C_D = 5$ (default and recommended value; see Section 7.3.2) and $C_D = 10$.

Figure 10.33 includes predictions of the concentration and the effective cloud half-width (B_{eff}) for base case A. The following is concluded:

- In the revised model ($C_D > 0$) the predictions are extremely insensitive to the precise value of the adjustable parameter C_D . Virtually identical results are obtained for C_{AV} and B_{eff} for $C_D = 2.5$, 5 and 10. This is caused by the fact that only a (unlikely) large value of C_D in eq. (7.25) will lead to a significant amount of spreading downwind of the point of collapse of gravitational spreading.
- The inclusion of gravitational collapse leads to a considerable reduction of the increase of cloud width downwind of the point of collapse (Figure 10.33b). The reduced spreading in the crosswind direction leads to higher predictions for the centre-line ground-level concentration (Figure 10.33a).
- Far downwind the dispersion processes approach the passive limit and the differences in predictions between the old and new crosswind spreading models disappear.

Formula for crosswind dispersion coefficient σ_y

The use of different empirical formulae for the non-dense crosswind dispersion coefficient σ_y and their implementation in HEGADAS has been discussed in detail in Section 7.3.1. In HEGADAS two different formulae are implemented:

- a power-law for σ_y (MODSY = 1; see Table 7.1 for details); this formula is recommended for distances less than 1000 m
- a formula proposed by Briggs (MODSY = 2; see Table 7.2 for details); this formula is recommended by Briggs for open-country conditions and $100 < x < 10000$ m.

For the above two types of formulae Figures 10.34 and 10.35 include predictions of the concentration and the effective cloud half-width for the base cases A and B, respectively. Note that the difference in predictions for both formulae is very small. The following is observed.

- In accordance with the underlying theoretical equations (entrainment law, gravity-spreading law; see Section 7.3 and Appendix 3) the concentration and cloud-width predictions are identical upwind of the downwind position x_{tr}^b at which the middle part of the concentration profile disappears.
- The formula $\sigma_y(x)$ depends on stability class and averaging time (see Tables 7.1 and 7.2). It is recalled that for both base cases neutral conditions (stability class D) and averaging times of 60 seconds are adopted. It is seen from Table 9.4 that for $200 < x < 10000$ m the dispersion coefficient $\sigma_y(x)$ is larger for the Briggs formula than for the power-law. This results in larger cloud half-widths for the Briggs formula downwind of the transition point $x = x_{tr}^b$ up to $x = 10000$ m (Figure 10.35b). The larger predictions for the cloud half-width (somewhat more spreading in the crosswind directions) are accompanied with smaller predictions of the centre-line ground-level concentration (Figure 10.35a).
- Downwind of $x = 10000$ m the dispersion coefficient $\sigma_y(x)$ is smaller for the Briggs formula than for the power-law. This results in smaller cloud widths and larger centre-line ground-level concentrations for the Briggs formula.

It must be noted that the above conclusions are dependent on the adopted formulas for $\sigma_y(x)$. Thus the conclusions may be somewhat changed if a different stability class and/or averaging time is adopted.

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Table 10.1a. BASE CASE A. CONTRIBUTIONS TO VOLUMETRIC ENTRAINMENT DURING VARIOUS STAGES OF "HFPLUME" PLUME (part of .HP2 file)

Interpretation:							Interpretation:				
dx: plume centroid displacement (m); entr: total entrainment/unit axis length (kg/s/m); jet: proportion jet entrainment (-); pass: proportion passive entrainment (-); cross: proportion cross-wind entrainment (-); slump: gravity-slumping entrainment part (-); heavy: heavy-gas advection entrainment (-); Ri: heavy-gas (bulk) Richardson number (-).							aspect: plume cross-section aspect-ratio (-); u/u_atm: ratio of plume to ambient speed stage: stage (geometry) of plume development (-);				
dx	entr	jet	pass	cross	slump	heavy	Ri	u/u_atm	aspect	phase	stage
1.0	3.3	0.97	0.03	0.00	0.00	0.00	0.000E-01	14.25	1.0	airborne	
2.0	4.2	0.94	0.06	0.00	0.00	0.00	0.000E-01	9.81	1.0	airborne	
3.0	4.6	0.91	0.08	0.00	0.00	0.00	0.000E-01	7.35	1.0	airborne	
4.0	4.9	0.88	0.11	0.01	0.00	0.00	0.000E-01	5.88	1.0	airborne	
5.0	5.2	0.84	0.14	0.01	0.00	0.00	0.000E-01	4.92	1.0	airborne	
6.0	5.5	0.80	0.18	0.02	0.00	0.00	0.000E-01	4.25	1.0	airborne	
7.0	5.7	0.76	0.21	0.03	0.00	0.00	0.000E-01	3.76	1.0	airborne	
8.0	6.1	0.71	0.24	0.05	0.00	0.00	0.000E-01	3.39	1.0	airborne	
9.0	6.4	0.67	0.27	0.07	0.00	0.00	0.000E-01	3.10	1.0	airborne	
10.0	6.5	0.65	0.25	0.10	0.00	0.00	0.000E-01	2.87	1.0	airborne	
11.	4.6	0.73	0.26	0.00	0.01	0.01	106.	2.72	0.89	touchdown	<-- touchdown
12.	4.0	0.78	0.19	0.00	0.02	0.01	97.0	2.62	0.78	touchdown	
13.	3.5	0.84	0.12	0.00	0.03	0.01	90.6	2.53	0.68	touchdown	
14.	3.2	0.90	0.06	0.00	0.03	0.02	85.9	2.47	0.60	touchdown	
15.	3.1	0.92	0.02	0.00	0.03	0.02	82.3	2.41	0.53	touchdown	
16.	3.0	0.93	0.00	0.00	0.05	0.02	79.1	2.35	0.48	slumped	<-- slumping
17.	3.0	0.93	0.00	0.00	0.05	0.03	76.4	2.30	0.44	slumped	
18.	3.0	0.92	0.00	0.00	0.05	0.03	73.7	2.25	0.40	slumped	
19.	3.0	0.92	0.00	0.00	0.05	0.03	71.1	2.21	0.37	slumped	
20.	3.0	0.92	0.00	0.00	0.05	0.03	68.6	2.17	0.34	slumped	
25.	3.2	0.91	0.00	0.00	0.04	0.05	57.7	2.00	0.24	slumped	
30.	3.3	0.89	0.00	0.00	0.04	0.07	48.9	1.86	0.18	slumped	
35.	3.4	0.88	0.00	0.00	0.04	0.08	42.0	1.74	0.14	slumped	
40.	3.5	0.86	0.00	0.00	0.04	0.10	36.7	1.65	0.12	slumped	
45.	3.5	0.84	0.00	0.00	0.03	0.12	32.8	1.57	0.11	slumped	
46.	3.5	0.84	0.00	0.00	0.03	0.13	32.1	1.55	0.10	slumped	
47.	3.5	0.83	0.00	0.00	0.03	0.13	31.5	1.54	0.10	slumped	<-- RU = 0.10 = RULST
48.	3.5	0.83	0.00	0.00	0.03	0.14	30.9	1.53	9.96E-02	slumped	
50.	3.6	0.82	0.00	0.00	0.03	0.14	29.8	1.50	9.53E-02	slumped	
55.	3.5	0.80	0.00	0.00	0.03	0.17	27.5	1.45	8.62E-02	slumped	
60.	3.5	0.78	0.00	0.00	0.03	0.19	25.7	1.41	7.89E-02	slumped	
65.	3.5	0.76	0.00	0.00	0.03	0.21	24.4	1.37	7.28E-02	slumped	
70.	3.5	0.74	0.00	0.00	0.03	0.22	23.3	1.34	6.76E-02	slumped	
75.	3.5	0.73	0.00	0.00	0.03	0.24	22.5	1.31	6.31E-02	slumped	
80.	3.4	0.71	0.00	0.00	0.03	0.26	21.8	1.29	5.91E-02	slumped	
85.	3.4	0.69	0.00	0.00	0.03	0.28	21.2	1.27	5.56E-02	slumped	
90.	3.4	0.68	0.00	0.00	0.03	0.29	20.8	1.25	5.24E-02	slumped	
95.	3.3	0.66	0.00	0.00	0.03	0.31	20.4	1.23	4.96E-02	slumped	
100.	3.3	0.65	0.00	0.00	0.03	0.32	20.1	1.22	4.71E-02	slumped	
1.05E+02	3.3	0.63	0.00	0.00	0.03	0.34	19.8	1.20	4.47E-02	slumped	
1.10E+02	3.2	0.62	0.00	0.00	0.03	0.35	19.5	1.19	4.26E-02	slumped	
1.15E+02	3.2	0.60	0.00	0.00	0.03	0.37	19.3	1.18	4.06E-02	slumped	
1.20E+02	3.2	0.59	0.00	0.00	0.03	0.38	19.1	1.17	3.88E-02	slumped	
1.25E+02	3.1	0.58	0.00	0.00	0.03	0.39	18.9	1.16	3.71E-02	slumped	
1.30E+02	3.1	0.56	0.00	0.00	0.03	0.41	18.6	1.15	3.56E-02	slumped	
1.35E+02	3.1	0.55	0.00	0.00	0.03	0.42	18.4	1.15	3.41E-02	slumped	
1.40E+02	3.0	0.54	0.00	0.00	0.03	0.43	18.2	1.14	3.28E-02	slumped	
1.45E+02	3.0	0.52	0.00	0.00	0.03	0.45	18.0	1.13	3.16E-02	slumped	
1.50E+02	3.0	0.51	0.00	0.00	0.03	0.46	17.8	1.13	3.04E-02	slumped	
1.55E+02	3.0	0.50	0.00	0.00	0.03	0.47	17.6	1.12	2.93E-02	slumped	
1.60E+02	2.9	0.49	0.00	0.00	0.03	0.48	17.4	1.12	2.83E-02	slumped	
1.65E+02	3.0	0.47	0.00	0.00	0.03	0.49	17.3	1.11	2.74E-02	slumped	
1.70E+02	3.2	0.46	0.00	0.00	0.03	0.51	16.9	1.11	2.65E-02	slumped	
1.75E+02	3.4	0.44	0.00	0.00	0.03	0.53	16.5	1.10	2.57E-02	slumped	
1.80E+02	3.5	0.43	0.00	0.00	0.03	0.55	16.1	1.10	2.51E-02	slumped	
1.85E+02	3.7	0.41	0.00	0.00	0.03	0.57	15.7	1.09	2.45E-02	slumped	
1.90E+02	3.9	0.39	0.00	0.00	0.02	0.58	15.3	1.09	2.40E-02	slumped	
1.95E+02	4.0	0.37	0.00	0.00	0.02	0.60	15.0	1.08	2.35E-02	slumped	
2.00E+02	4.2	0.36	0.00	0.00	0.02	0.62	14.6	1.08	2.31E-02	slumped	
2.05E+02	4.3	0.34	0.00	0.00	0.02	0.64	14.3	1.07	2.28E-02	slumped	
2.10E+02	4.4	0.32	0.00	0.00	0.02	0.65	14.0	1.07	2.24E-02	slumped	
2.15E+02	4.6	0.31	0.00	0.00	0.02	0.67	13.7	1.06	2.21E-02	slumped	
2.20E+02	4.7	0.29	0.00	0.00	0.02	0.69	13.4	1.06	2.19E-02	slumped	
2.24E+02	4.8	0.28	0.00	0.00	0.02	0.70	13.2	1.05	2.17E-02	slumped	< RE = 0.30 = RELST

Table 10.1b. BASE CASE A. PREDICTIONS BY HEGADAS-S DOWNWIND OF HFPLUME/HEGADAS-S TRANSITION

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[part of .HSR file; see HEGADAS user's guide (Appendix 8.D in User's Manual) for precise meaning of data;

x = xtrhp: HFPLUME/HEGADAS-S transition;

x = xtrcd: collapse of gravity spreading (CE/CD formulation);

x = xtrb: half-width b = MDP of middle part of concentration profile becomes 0;

x = xtrri: Richardson number RIB becomes zero (onset of buoyant flow)

DISTANCE (M)	CONC (% VOL.)	SZ (M)	SY (M)	MIDP (M)	YCU (M)	ZCU (M)	YCL (M)	ZCL (M)	RIB	TMP (DEG.C)	CA (KG/M3)	
- breakpoint at DIST = 224. m											--> x = xtrhp	
224.	1.28	1.58	0.000E-01	41.4	41.4	7.10	41.4	9.79	14.6	22.2	1.06E-02	VISIBLE
230.	1.25	1.57	5.59	37.8	50.7	7.03	53.3	9.71	14.4	22.4	1.03E-02	
240.	1.19	1.56	9.24	36.8	58.1	6.95	62.3	9.61	13.7	22.9	9.81E-03	
250.	1.14	1.56	11.9	36.6	63.9	6.89	69.4	9.56	13.0	23.5	9.36E-03	
260.	1.09	1.57	14.2	36.8	69.1	6.86	75.6	9.54	12.4	24.0	8.92E-03	
270.	1.04	1.58	16.2	37.1	73.8	6.85	81.2	9.55	11.9	24.6	8.49E-03	
280.	0.988	1.59	18.1	37.5	78.2	6.85	86.5	9.58	11.4	25.1	8.08E-03	
290.	0.941	1.61	19.8	37.9	82.3	6.87	91.5	9.64	11.0	25.6	7.69E-03	
300.	0.897	1.63	21.4	38.4	86.3	6.91	96.3	9.71	10.6	26.0	7.31E-03	
312.	0.846	1.67	23.3	39.1	90.8	6.96	102.	9.82	10.1	26.6	6.89E-03	
326.	0.789	1.71	25.5	39.8	96.0	7.04	108.	9.97	9.63	27.2	6.41E-03	
344.	0.726	1.76	27.9	40.8	102.	7.16	115.	10.2	9.11	27.8	5.89E-03	
364.	0.658	1.84	30.7	41.9	108.	7.32	123.	10.5	8.56	28.5	5.32E-03	
389.	0.587	1.94	34.0	43.3	116.	7.54	132.	10.9	7.99	29.3	4.73E-03	
419.	0.513	2.07	37.6	44.9	124.	7.84	142.	11.4	7.40	30.0	4.13E-03	
455.	0.440	2.24	41.9	46.6	133.	8.21	154.	12.1	6.81	30.8	3.53E-03	
498.	0.369	2.46	46.7	48.6	143.	8.68	167.	13.0	6.22	31.5	2.96E-03	
											--> x = xtrcd	
550.	0.304	2.78	52.3	49.3	152.	9.38	179.	14.2	5.72	32.1	2.43E-03	
612.	0.249	3.32	58.4	44.1	156.	10.7	187.	16.5	5.54	32.7	1.99E-03	
686.	0.204	3.97	64.9	38.6	160.	12.1	195.	19.2	5.35	33.1	1.62E-03	
775.	0.167	4.73	72.1	32.6	163.	13.7	203.	22.1	5.16	33.5	1.33E-03	
882.	0.137	5.64	79.8	26.2	166.	15.5	211.	25.5	4.97	33.8	1.09E-03	
1.010E+03	0.112	6.72	88.2	19.4	169.	17.4	220.	29.4	4.77	34.0	8.89E-04	
1.164E+03	9.156E-02	8.00	97.4	12.0	171.	19.3	229.	33.8	4.56	34.2	7.26E-04	
1.349E+03	7.472E-02	9.52	108.	4.12	173.	21.4	239.	38.7	4.33	34.4	5.92E-04	
											--> x = xtrb	
1.454E+03	6.752E-02	10.4	113.	0.000E-01	174.	22.5	244.	41.3	4.21	34.5	5.35E-04	
1.720E+03	4.809E-02	12.7	126.	0.000E-01	180.	24.0	263.	47.4	3.48	34.7	3.81E-04	
2.040E+03	3.383E-02	15.7	142.	0.000E-01	184.	25.0	283.	54.2	2.79	34.8	2.68E-04	
2.423E+03	2.349E-02	19.5	161.	0.000E-01	184.	24.9	305.	61.8	2.12	34.9	1.86E-04	
2.883E+03	1.609E-02	24.4	183.	0.000E-01	177.	23.0	329.	70.0	1.47	35.0	1.27E-04	
3.435E+03	1.083E-02	30.9	209.	0.000E-01	153.	17.7	352.	78.8	0.825	35.0	8.57E-05	
4.098E+03	7.118E-03	39.8	240.	0.000E-01	82.7	5.90	373.	87.9	0.148	35.0	5.63E-05	
											--> x = xtrri	
4.893E+03	4.517E-03	52.7	276.	0.000E-01	0.000E-01	0.000E-01	387.	96.6	-0.622	35.1	3.57E-05	
5.847E+03	2.817E-03	70.6	319.	0.000E-01	0.000E-01	0.000E-01	390.	101.	-1.52	35.1	2.23E-05	
6.991E+03	1.747E-03	94.9	370.	0.000E-01	0.000E-01	0.000E-01	373.	96.3	-2.60	35.1	1.38E-05	
8.365E+03	1.083E-03	127.	431.	0.000E-01	0.000E-01	0.000E-01	316.	73.1	-3.92	35.1	8.57E-06	
1.001E+04	6.726E-04	170.	502.	0.000E-01	0.000E-01	0.000E-01	125.	14.1	-5.58	35.1	5.32E-06	
1.199E+04	4.184E-04	227.	586.	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	-7.69	35.1	3.31E-06	
1.437E+04	2.605E-04	301.	685.	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	-10.4	35.1	2.06E-06	
1.721E+04	1.624E-04	400.	802.	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	-13.9	35.1	1.28E-06	
2.063E+04	1.012E-04	530.	941.	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	-18.6	35.1	8.00E-07	
2.473E+04	6.300E-05	702.	1.104E+03	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	-24.7	35.1	4.98E-07	
2.966E+04	3.919E-05	930.	1.296E+03	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	-32.7	35.1	3.10E-07	
3.556E+04	2.435E-05	1.233E+03	1.523E+03	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	-43.3	35.1	1.93E-07	
4.265E+04	1.510E-05	1.636E+03	1.791E+03	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	-57.4	35.1	1.19E-07	
5.116E+04	9.353E-06	2.174E+03	2.107E+03	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	-76.2	35.1	7.40E-08	

Table 10.2a. BASE CASE B. CONTRIBUTIONS TO VOLUMETRIC ENTRAINMENT DURING VARIOUS STAGES OF "HFPLUME" PLUME (part of .HP2 file)

Interpretation:						Interpretation:					
dx: plume centroid displacement (m);						aspect: plume cross-section aspect-ratio (-);					
entr: total entrainment/unit axis length (kg/s/m);						u/u_atm: ratio of plume to ambient speed					
jet: proportion jet entrainment (-);						stage: stage (geometry) of plume development (-);					
pass: proportion passive entrainment (-);											
cross: proportion cross-wind entrainment (-);											
slump: gravity-slumping entrainment part (-);											
heavy: heavy-gas advection entrainment (-)											
Ri: heavy-gas (bulk) Richardson number (-).											
dx	entr	jet	pass	cross	slump	heavy	Ri	u/u_atm	aspect	phase	stage
1.0	3.8	0.94	0.06	0.00	0.00	0.00	0.000E-01	16.87	1.0	airborne	
2.0	4.9	0.90	0.10	0.00	0.00	0.00	0.000E-01	11.18	1.0	airborne	
3.0	5.5	0.84	0.15	0.00	0.00	0.00	0.000E-01	8.16	1.0	airborne	
4.0	6.1	0.79	0.21	0.01	0.00	0.00	0.000E-01	6.39	1.0	airborne	
5.0	6.6	0.73	0.26	0.01	0.00	0.00	0.000E-01	5.24	1.0	airborne	
6.0	7.3	0.66	0.32	0.02	0.00	0.00	0.000E-01	4.46	1.0	airborne	
7.0	8.0	0.60	0.37	0.03	0.00	0.00	0.000E-01	3.89	1.0	airborne	
8.0	8.7	0.55	0.41	0.04	0.00	0.00	0.000E-01	3.46	1.0	airborne	
9.0	7.1	0.55	0.43	0.00	0.00	0.02	24.9	3.15	0.95	touchdown	<-- touchdown
10.0	5.7	0.58	0.36	0.00	0.01	0.05	22.0	2.96	0.83	touchdown	
11.	4.8	0.63	0.27	0.00	0.02	0.08	20.1	2.82	0.73	touchdown	
12.	4.2	0.68	0.18	0.00	0.03	0.11	18.7	2.72	0.64	touchdown	
13.	3.7	0.74	0.09	0.00	0.03	0.14	17.6	2.63	0.57	touchdown	
14.	3.4	0.77	0.02	0.00	0.04	0.17	16.6	2.55	0.52	touchdown	
15.	3.3	0.76	0.00	0.00	0.05	0.19	15.8	2.48	0.47	slumped	<-- slumping
16.	3.3	0.74	0.00	0.00	0.05	0.21	14.9	2.41	0.43	slumped	
17.	3.3	0.73	0.00	0.00	0.05	0.22	14.1	2.35	0.40	slumped	
18.	3.3	0.71	0.00	0.00	0.05	0.24	13.4	2.29	0.37	slumped	
19.	3.3	0.70	0.00	0.00	0.05	0.25	12.7	2.24	0.35	slumped	
20.	3.3	0.69	0.00	0.00	0.05	0.27	12.0	2.19	0.32	slumped	
21.	3.2	0.67	0.00	0.00	0.05	0.28	11.3	2.14	0.30	slumped	
22.	3.2	0.66	0.00	0.00	0.05	0.29	10.8	2.10	0.29	slumped	
23.	3.2	0.65	0.00	0.00	0.05	0.30	10.2	2.06	0.27	slumped	<-- RI = 10
24.	3.1	0.67	0.00	0.00	0.00	0.33	9.69	2.02	0.26	slumped	switch off gravity-slumping entrainment
25.	3.1	0.65	0.00	0.00	0.00	0.35	9.17	1.98	0.24	slumped	
30.	3.0	0.60	0.00	0.00	0.00	0.40	7.15	1.82	0.20	slumped	
35.	3.1	0.54	0.00	0.00	0.00	0.46	5.64	1.68	0.17	slumped	
40.	3.6	0.47	0.00	0.00	0.00	0.53	4.37	1.57	0.15	slumped	
45.	4.2	0.41	0.00	0.00	0.00	0.59	3.26	1.46	0.14	slumped	
50.	4.9	0.35	0.00	0.00	0.00	0.65	2.29	1.37	0.13	slumped	
55.	5.1	0.31	0.00	0.00	0.00	0.69	1.50	1.29	0.12	slumped	
56.	5.1	0.30	0.00	0.00	0.00	0.70	1.36	1.28	0.12	slumped	<-- RE = 0.30 = RELST
57.	5.1	0.29	0.00	0.00	0.00	0.71	1.23	1.27	0.12	slumped	
60.	5.2	0.27	0.00	0.00	0.00	0.73	0.874	1.23	0.12	slumped	
65.	5.4	0.24	0.00	0.00	0.00	0.76	0.384	1.19	0.12	slumped	
68.	5.4	0.22	0.00	0.00	0.00	0.78	0.131	1.16	0.12	slumped	
69.	5.4	0.21	0.00	0.00	0.00	0.79	6.111E-02	1.15	0.12	slumped	<-- RI=0 (gas becomes buoyant)
70.	5.4	0.20	0.00	0.00	0.00	0.80	-7.901E-03	1.14	0.12	slumped	
75.	5.7	0.15	0.00	0.00	0.00	0.85	-0.320	1.10	0.13	slumped	<-- RU = 0.10 = RULST

Table 10.2b. BASE CASE B. PREDICTIONS BY HEGADAS-S DOWNWIND OF HFPLUME/HEGADAS-S TRANSITION

 [part of .HSR file; see HEGADAS user's guide (Appendix 8.D in User's Manual) for precise meaning of data;
 x = xtrhp: HFPLUME/HEGADAS-S transition;
 x = xtrb: half-width b = MIDP of middle part of concentration profile becomes 0;

DISTANCE (M)	CONC (% VOL.)	SZ (M)	SY (M)	MIDP (M)	YCU (M)	ZCU (M)	YCL (M)	ZCL (M)	RIB	TMP (DEG.C)	CA (KG/M3)
- breakpoint at DIST = 74.9 m											--> x = xtrhp
74.9	2.98	2.84	0.000E-01	11.2	11.2	12.6	11.2	16.3	1.46	16.4	2.51E-02 VISIBLE
80.0	2.77	2.88	2.89	9.32	16.5	12.7	17.7	16.4	0.946	17.1	2.33E-02 VISIBLE
90.0	2.36	3.16	5.07	8.05	20.5	13.6	22.6	17.7	8.272E-02	18.0	1.98E-02 VISIBLE
											--> x = xtrri
100.	1.98	3.66	6.59	6.71	22.6	15.3	25.5	20.1	-0.647	18.4	1.65E-02 VISIBLE
110.	1.66	4.23	7.81	5.62	24.1	17.3	27.6	22.9	-1.59	19.0	1.38E-02 VISIBLE
120.	1.40	4.88	8.87	4.68	25.4	19.4	29.4	25.9	-2.49	19.3	1.17E-02 VISIBLE
130.	1.19	5.57	9.81	3.85	26.4	21.7	30.9	29.1	-3.26	19.4	9.92E-03 VISIBLE
140.	1.03	6.29	10.7	3.08	27.3	23.9	32.2	32.3	-3.92	19.4	8.56E-03 VISIBLE
150.	0.896	7.03	11.5	2.38	28.0	26.1	33.4	35.6	-4.47	19.3	7.47E-03 VISIBLE
160.	0.792	7.78	12.2	1.72	28.7	28.3	34.5	38.8	-4.94	19.1	6.60E-03 VISIBLE
170.	0.706	8.53	12.9	1.10	29.3	30.5	35.5	42.0	-5.33	19.0	5.90E-03 VISIBLE
180.	0.636	9.29	13.6	0.505	29.8	32.6	36.4	45.2	-5.65	18.8	5.31E-03 VISIBLE
											--> x = xtrb
189.	0.583	9.97	14.2	0.000E-01	30.3	34.5	37.1	48.1	-5.90	18.7	4.87E-03 VISIBLE
190.	0.575	10.1	14.2	0.000E-01	30.4	34.7	37.3	48.4	-5.91	18.6	4.81E-03 VISIBLE
200.	0.504	10.8	14.8	0.000E-01	31.3	36.4	38.5	51.2	-6.00	18.4	4.22E-03 VISIBLE
210.	0.446	11.6	15.5	0.000E-01	32.1	38.0	39.8	53.9	-6.01	18.1	3.73E-03 VISIBLE
220.	0.397	12.3	16.1	0.000E-01	32.9	39.6	41.0	56.5	-5.95	17.9	3.33E-03 VISIBLE
230.	0.357	13.0	16.7	0.000E-01	33.8	41.0	42.2	59.0	-5.83	17.7	2.99E-03 VISIBLE
240.	0.323	13.7	17.3	0.000E-01	34.6	42.3	43.4	61.4	-5.67	17.5	2.71E-03 VISIBLE
250.	0.294	14.4	17.9	0.000E-01	35.4	43.6	44.6	63.7	-5.48	17.3	2.47E-03 VISIBLE
260.	0.269	15.0	18.5	0.000E-01	36.1	44.8	45.8	65.8	-5.26	17.1	2.26E-03 VISIBLE
270.	0.247	15.7	19.1	0.000E-01	36.9	45.9	47.0	67.9	-5.01	16.9	2.08E-03 VISIBLE
280.	0.228	16.3	19.7	0.000E-01	37.7	46.9	48.1	69.9	-4.75	16.7	1.92E-03 VISIBLE
290.	0.212	16.9	20.3	0.000E-01	38.4	47.8	49.3	71.7	-4.47	16.6	1.78E-03 VISIBLE
300.	0.197	17.5	20.9	0.000E-01	39.2	48.7	50.4	73.5	-4.19	16.5	1.66E-03 VISIBLE
312.	0.182	18.2	21.6	0.000E-01	40.0	49.6	51.8	75.5	-3.84	16.3	1.53E-03 VISIBLE
326.	0.166	19.0	22.5	0.000E-01	41.1	50.7	53.4	77.7	-3.41	16.1	1.40E-03 VISIBLE
344.	0.150	19.9	23.5	0.000E-01	42.3	51.7	55.3	80.2	-2.90	15.9	1.26E-03 VISIBLE
364.	0.134	20.9	24.7	0.000E-01	43.7	52.8	57.6	82.8	-2.29	15.7	1.13E-03 VISIBLE
389.	0.119	22.0	26.2	0.000E-01	45.4	53.8	60.3	85.6	-1.58	15.5	1.01E-03 VISIBLE
419.	0.105	23.1	27.9	0.000E-01	47.4	54.6	63.6	88.2	-0.785	15.3	8.87E-04 VISIBLE
455.	9.211E-02	24.2	30.0	0.000E-01	49.7	55.2	67.4	90.6	7.903E-02	15.2	7.79E-04 VISIBLE
498.	8.080E-02	25.2	32.5	0.000E-01	52.5	55.3	72.0	92.5	0.974	15.0	6.84E-04 VISIBLE
550.	7.063E-02	26.3	35.4	0.000E-01	55.8	55.1	77.5	94.1	1.90	14.8	5.98E-04 VISIBLE
612.	6.130E-02	27.3	38.9	0.000E-01	59.5	54.6	83.8	95.4	2.87	14.6	5.20E-04 VISIBLE
686.	5.275E-02	28.4	43.0	0.000E-01	63.7	53.8	91.2	96.6	3.28	14.6	4.47E-04
775.	4.472E-02	29.7	48.0	0.000E-01	68.3	52.9	99.8	98.2	2.88	14.6	3.79E-04
882.	3.728E-02	31.4	53.8	0.000E-01	73.0	51.7	110.	100.	2.49	14.7	3.16E-04
1.010E+03	3.053E-02	33.5	60.7	0.000E-01	77.8	50.3	121.	103.	2.12	14.8	2.59E-04
1.164E+03	2.455E-02	36.1	68.9	0.000E-01	82.2	48.2	133.	106.	1.77	14.8	2.08E-04
1.349E+03	1.937E-02	39.4	78.6	0.000E-01	85.6	45.3	147.	109.	1.44	14.9	1.64E-04
1.571E+03	1.499E-02	43.4	90.0	0.000E-01	86.9	41.0	162.	113.	1.14	14.9	1.27E-04
1.837E+03	1.139E-02	48.5	104.	0.000E-01	84.0	34.4	178.	117.	0.848	15.0	9.64E-05
2.157E+03	8.494E-03	54.7	120.	0.000E-01	72.1	24.0	195.	122.	0.576	15.0	7.19E-05
2.540E+03	6.217E-03	62.6	139.	0.000E-01	31.3	5.53	213.	126.	0.314	15.0	5.26E-05
3.000E+03	4.466E-03	72.6	161.	0.000E-01	0.000E-01	0.000E-01	229.	129.	5.656E-02	15.1	3.78E-05
3.552E+03	3.153E-03	85.2	187.	0.000E-01	0.000E-01	0.000E-01	242.	130.	-0.206	15.1	2.67E-05
4.215E+03	2.198E-03	101.	219.	0.000E-01	0.000E-01	0.000E-01	251.	126.	-0.479	15.1	1.86E-05
5.010E+03	1.517E-03	120.	255.	0.000E-01	0.000E-01	0.000E-01	248.	115.	-0.771	15.1	1.28E-05
5.964E+03	1.040E-03	144.	299.	0.000E-01	0.000E-01	0.000E-01	225.	90.3	-1.09	15.1	8.80E-06
7.109E+03	7.088E-04	173.	350.	0.000E-01	0.000E-01	0.000E-01	149.	43.0	-1.45	15.1	6.00E-06
8.482E+03	4.806E-04	208.	411.	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	-1.87	15.1	4.07E-06
1.013E+04	3.245E-04	252.	482.	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	-2.35	15.1	2.75E-06
1.211E+04	2.182E-04	305.	567.	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	-2.93	15.1	1.85E-06
1.448E+04	1.462E-04	370.	666.	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	-3.63	15.1	1.24E-06
1.733E+04	9.753E-05	451.	784.	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	-4.47	15.1	8.25E-07
2.075E+04	6.483E-05	551.	922.	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	-5.51	15.1	5.48E-07
2.485E+04	4.292E-05	675.	1.086E+03	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	-6.78	15.1	3.63E-07
2.977E+04	2.830E-05	830.	1.279E+03	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	-8.36	15.1	2.39E-07
3.568E+04	1.858E-05	1.024E+03	1.506E+03	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	-10.3	15.1	1.57E-07
4.277E+04	1.215E-05	1.266E+03	1.774E+03	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	-12.8	15.1	1.03E-07
5.127E+04	7.918E-06	1.571E+03	2.091E+03	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	-15.8	15.1	6.70E-08

Predictions of concentration for basecase A by HFPLUME/HEGADAS-S

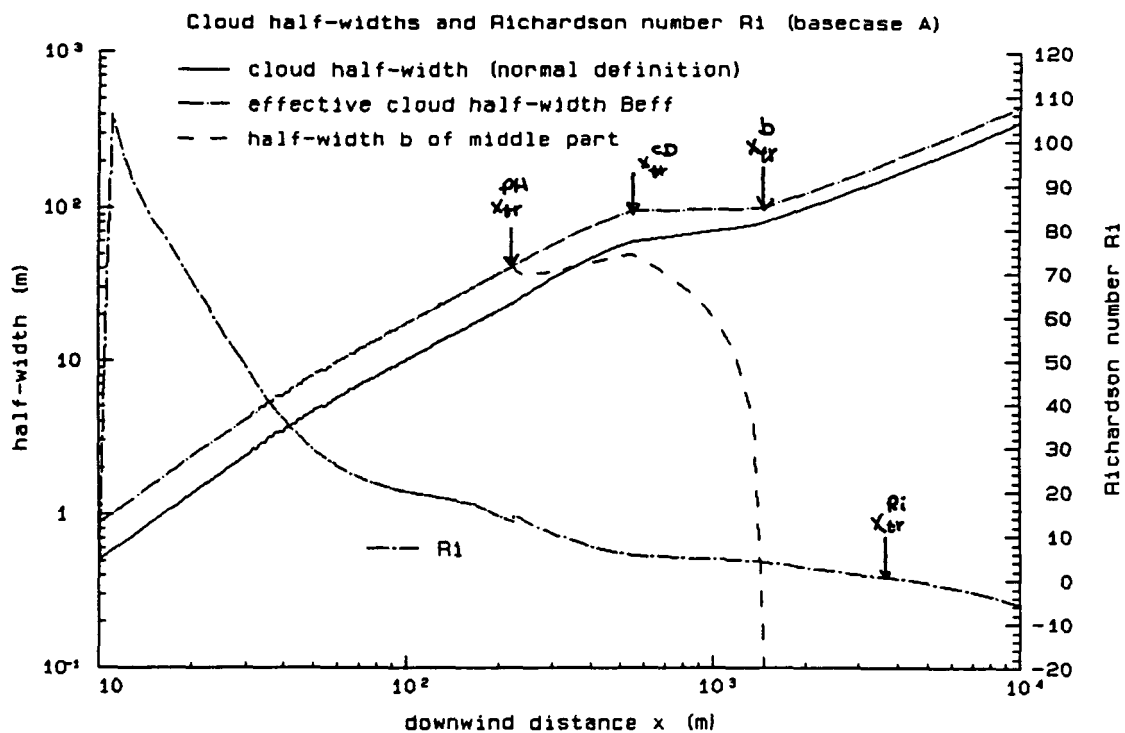
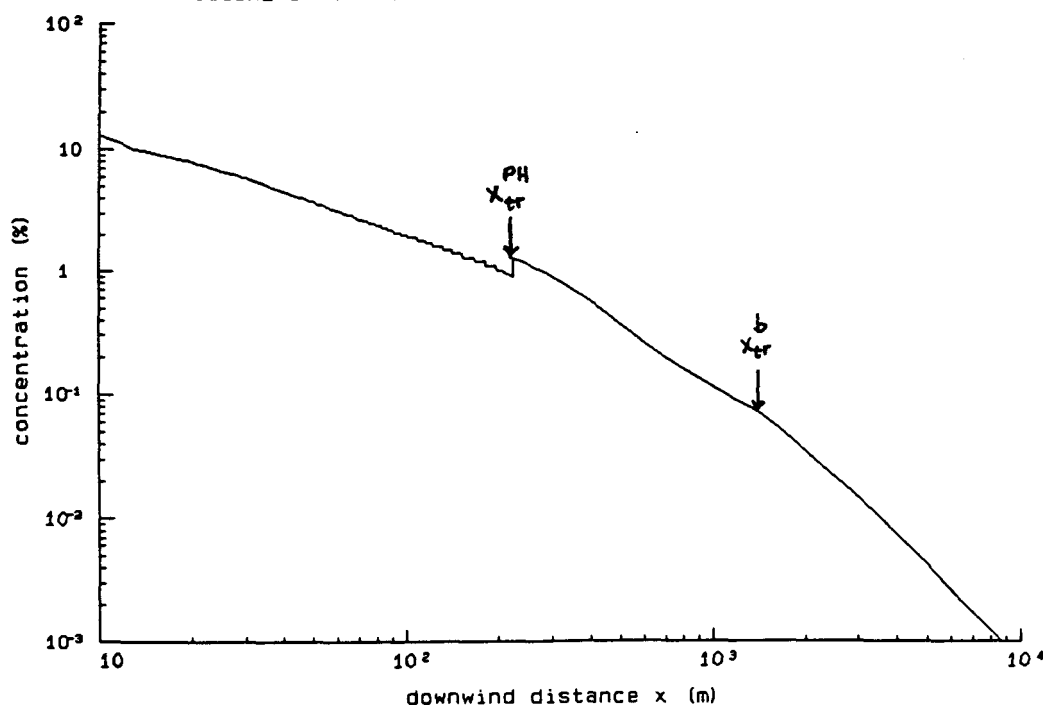
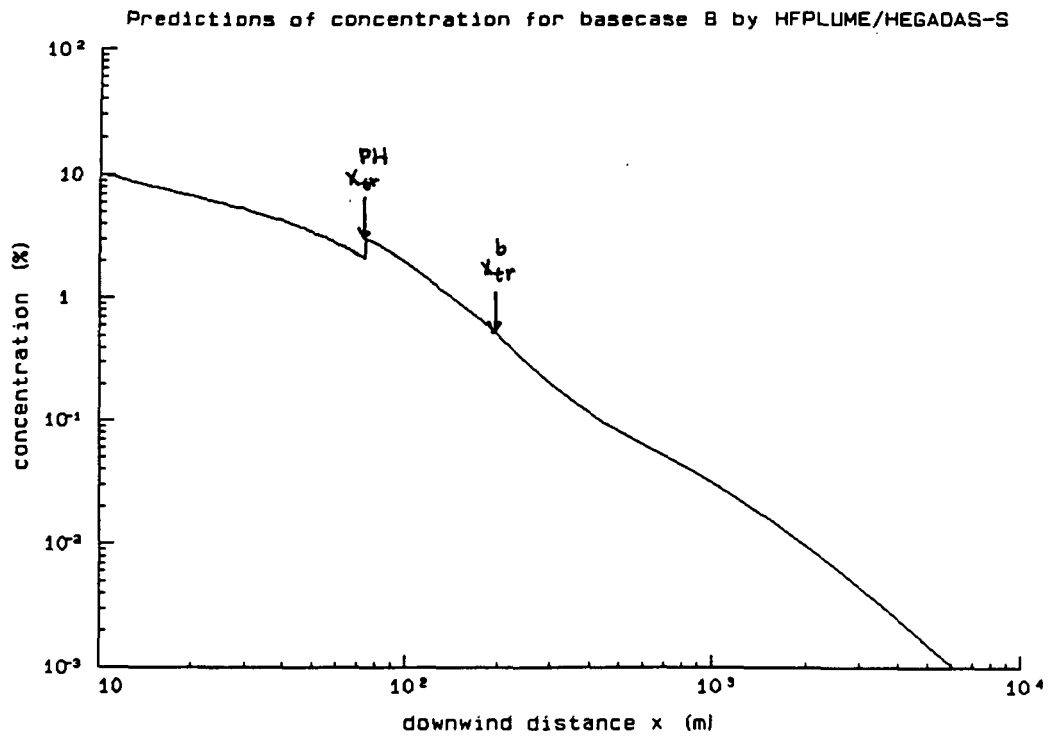
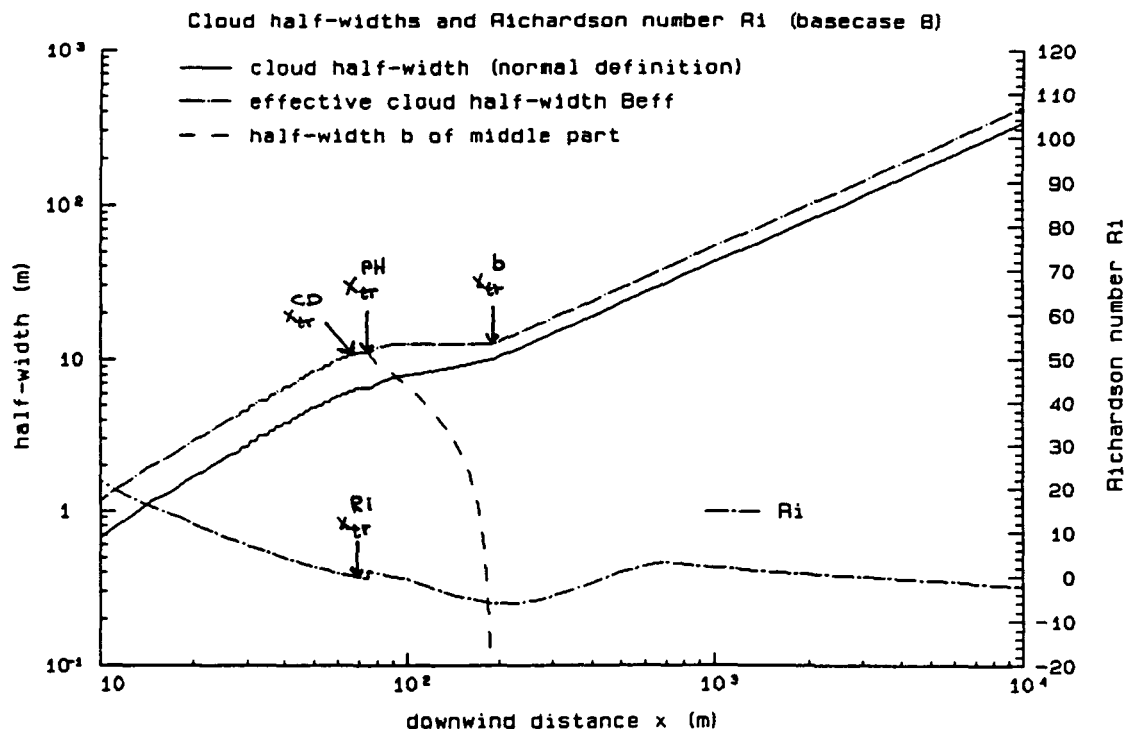


Fig. 10.1. HFPLUME/HEGADAS-S concentration predictions for base case A;
 (a) centre-line concentration (% molar fraction; HFPLUME sectional-mean value and HEGADAS value at ground level)
 (b) cloud half-width (from usually adopted definition), effective half-width B_{eff} of cloud (adopted in HEGADAS), half-width b of middle part of crosswind concentration profile, and bulk Richardson number Ri_*

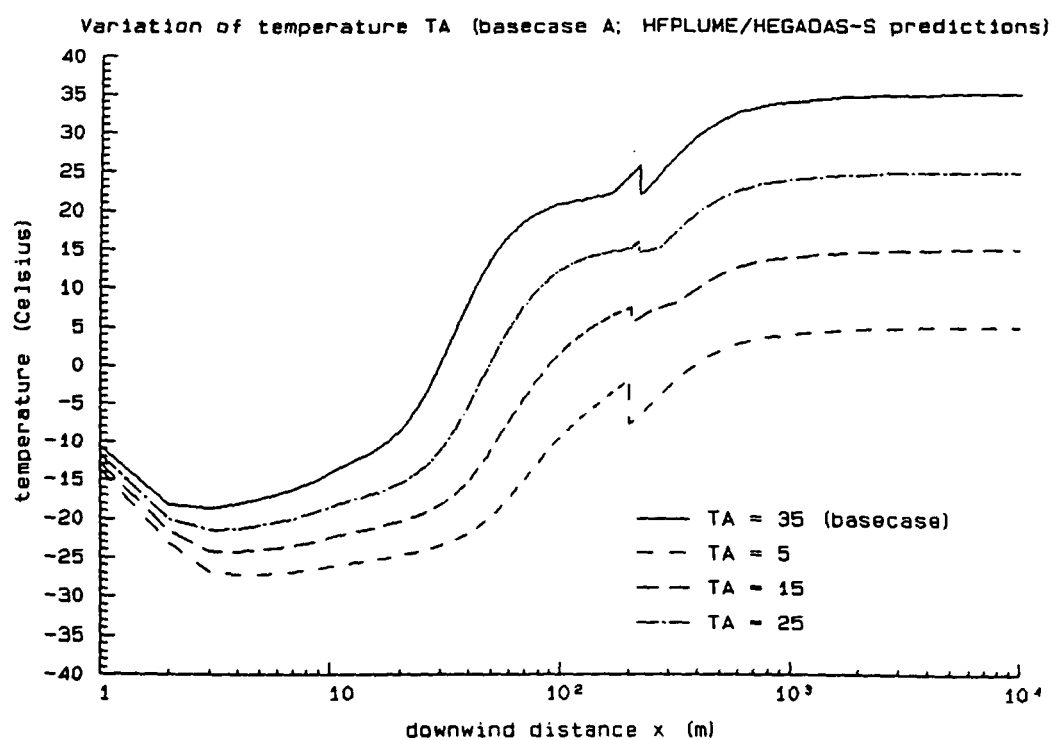


(a)

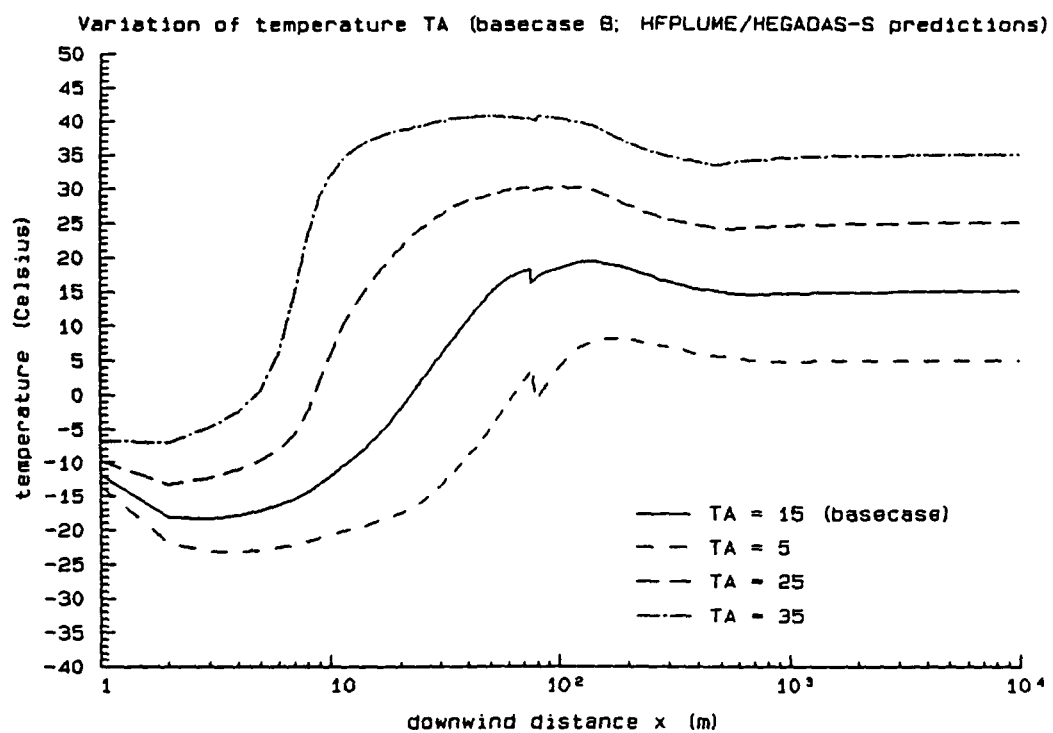


(b)

Fig. 10.2. HFPLUME/HEGADAS-S concentration predictions for base case B;
 (a) centre-line concentration (% molar fraction; HFPLUME sectional-mean value and HEGADAS value at ground level)
 (b) cloud half-width (from usually adopted definition), effective half-width B_{eff} of cloud (adopted in HEGADAS), half-width b of middle part of crosswind concentration profile, and bulk Richardson number Ri_*

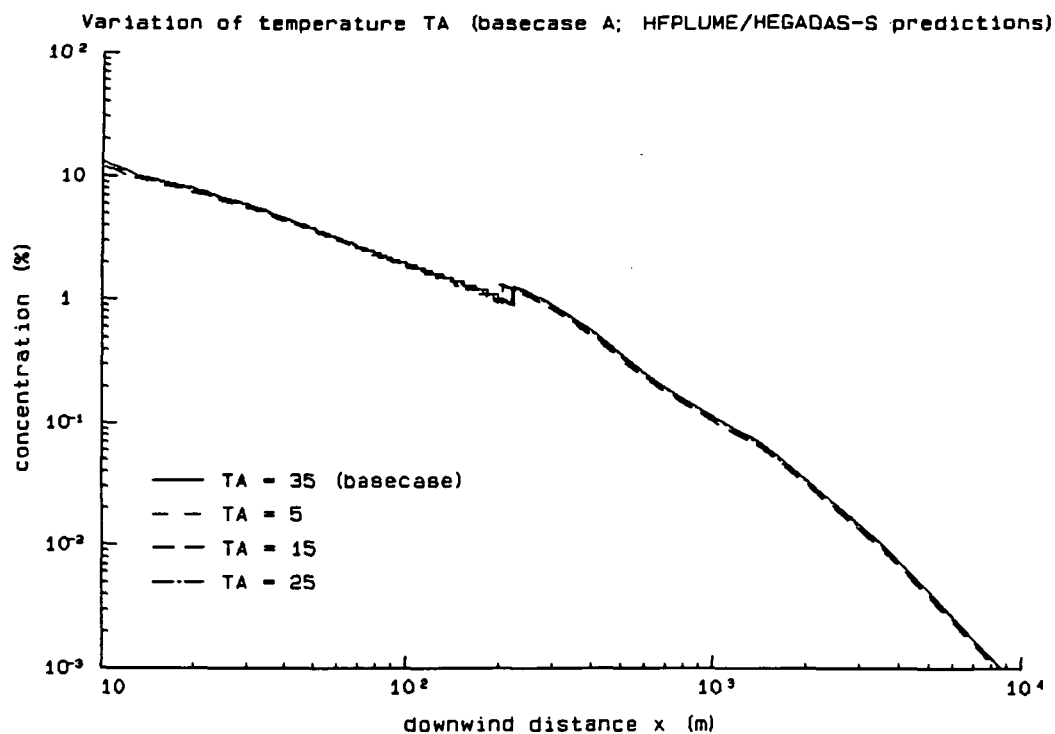


(a)

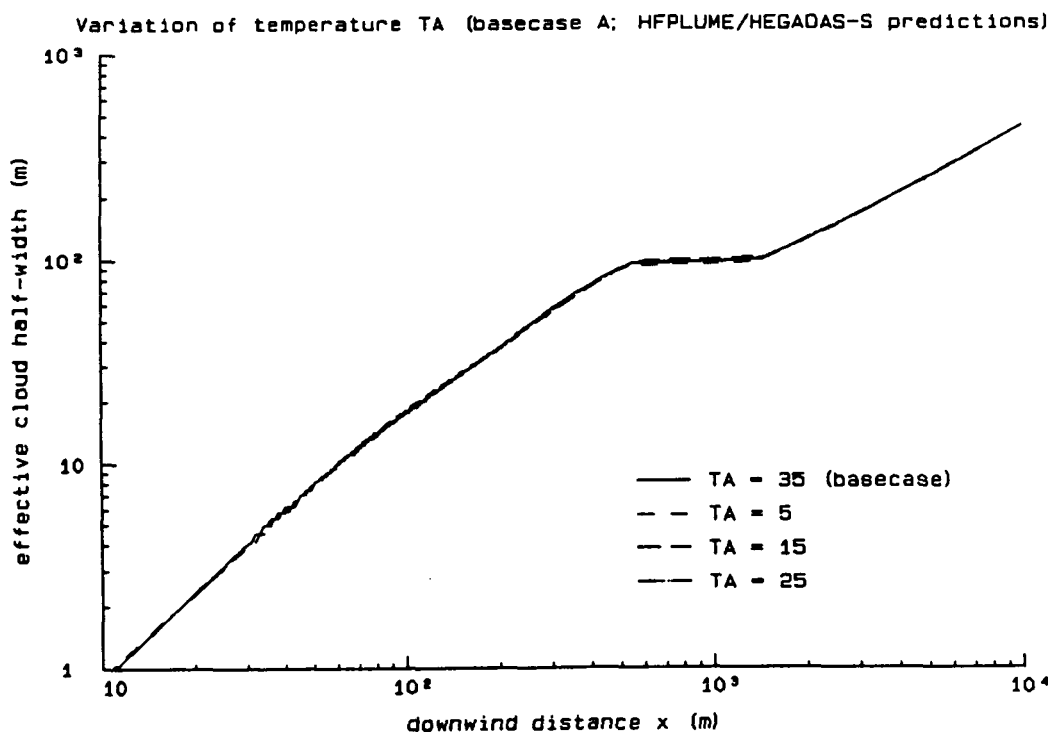


(b)

Fig. 10.3. Effect of ambient temperature T_a on predictions of HFPLUME (sectional-mean) and HEGADAS-S (ground-level) temperature; $T_a = 5, 15, 25$ or 35°C ;
 (a) base case A
 (b) base case B

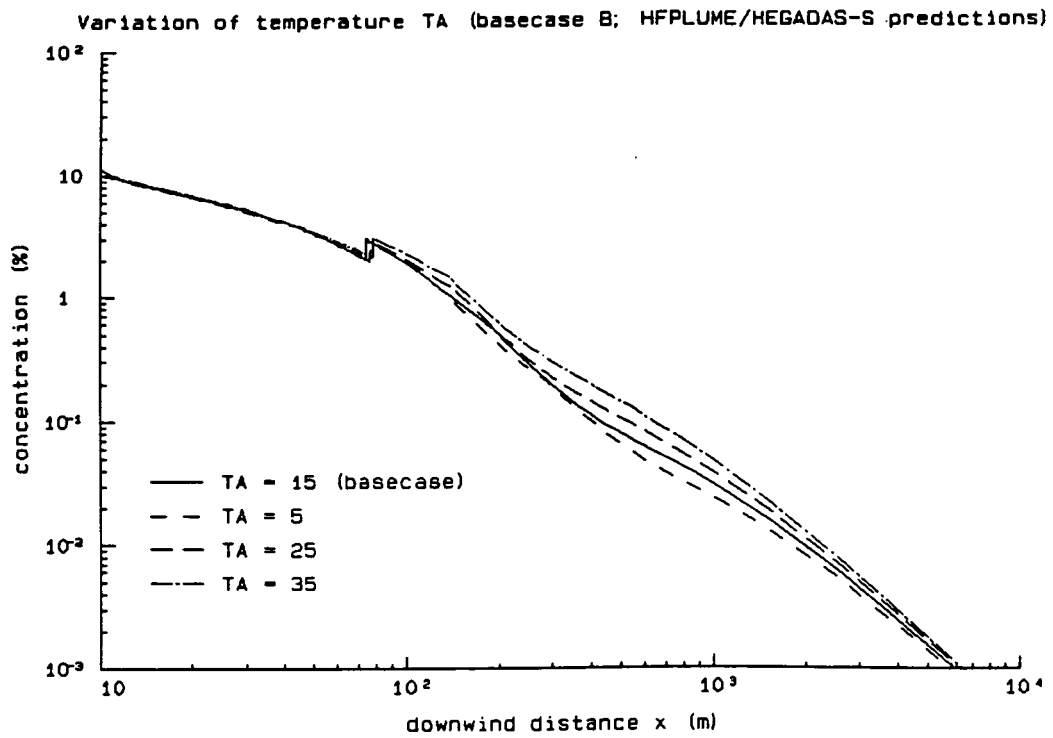


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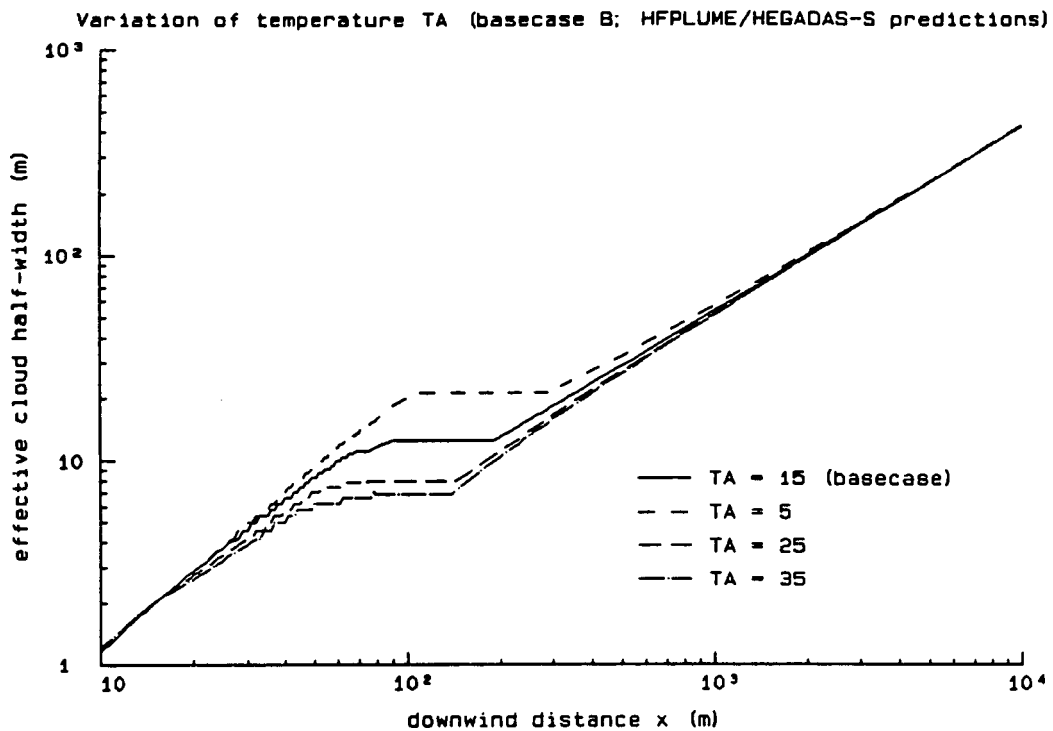


(b)

Fig. 10.4. Effect of ambient temperature T_a on HFPLUME/HEGADAS-S concentration predictions; $T_a = 5, 15, 25$ or 35°C ; base case A; (a) centre-line concentration (% molar fraction; HFPLUME sectional-mean value and HEGADAS value at ground level) (b) effective half-width B_{eff} of cloud

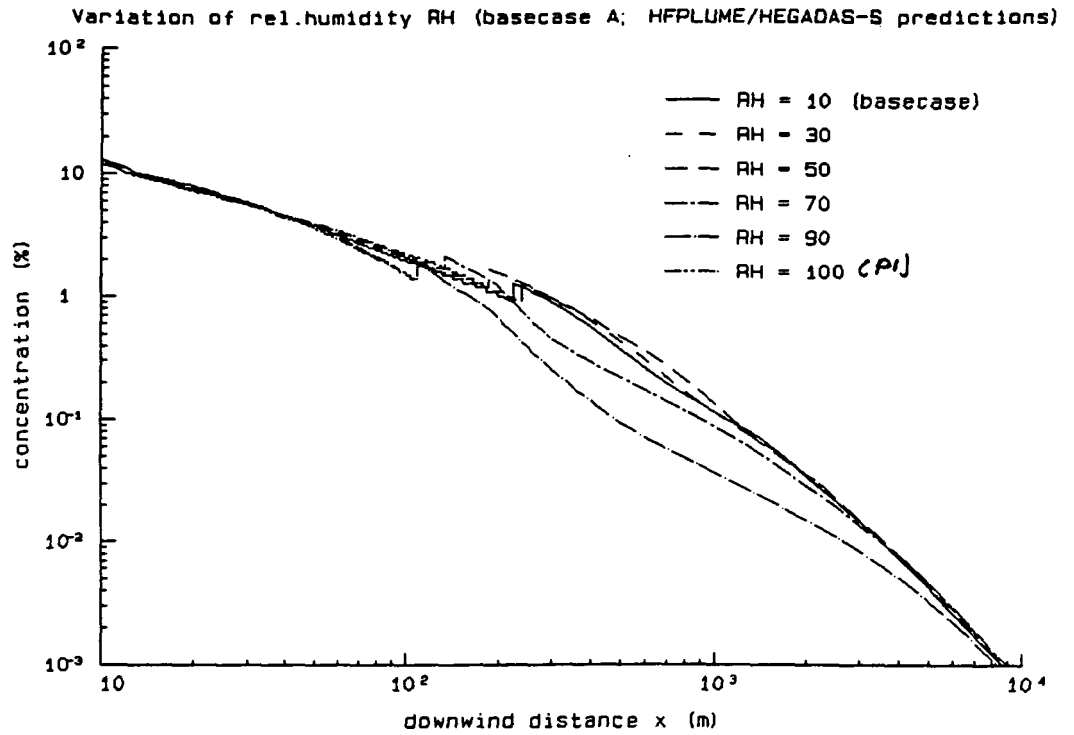


(a)

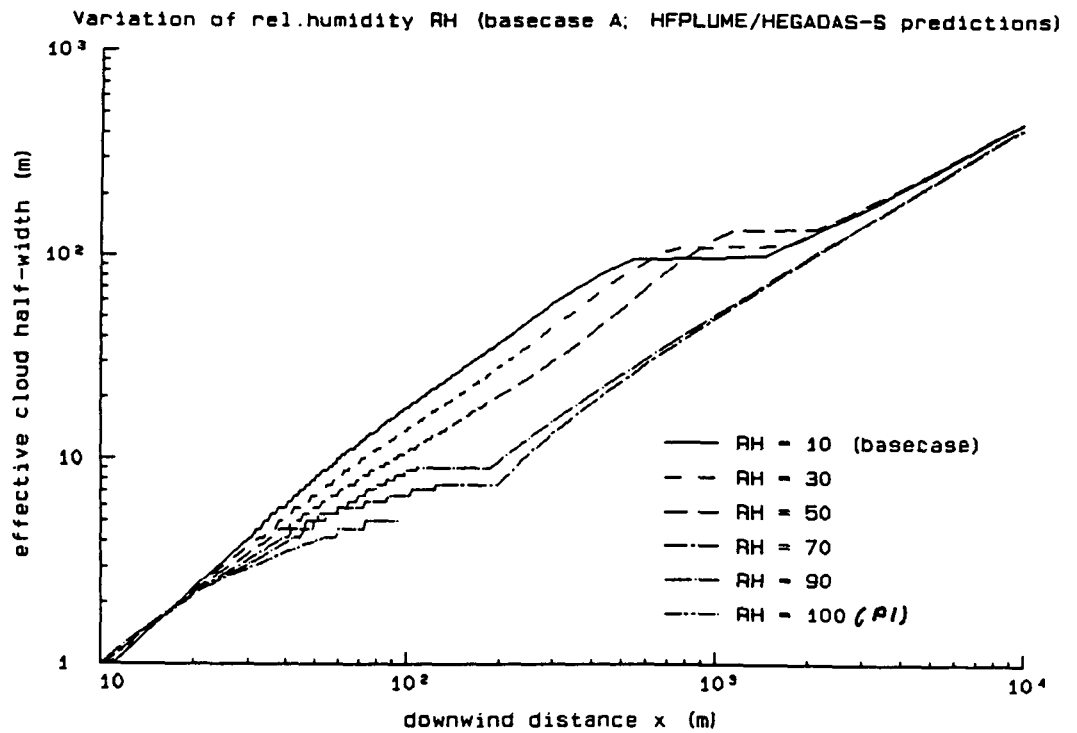


(b)

Fig. 10.5. Effect of ambient temperature T_a on HFPLUME/HEGADAS-S concentration predictions; $T_a = 5, 15, 25$ or 35°C ; base case B
 (a) centre-line concentration (% molar fraction; HFPLUME sectional-mean value and HEGADAS value at ground level)
 (b) effective half-width B_{eff} of cloud



(a)

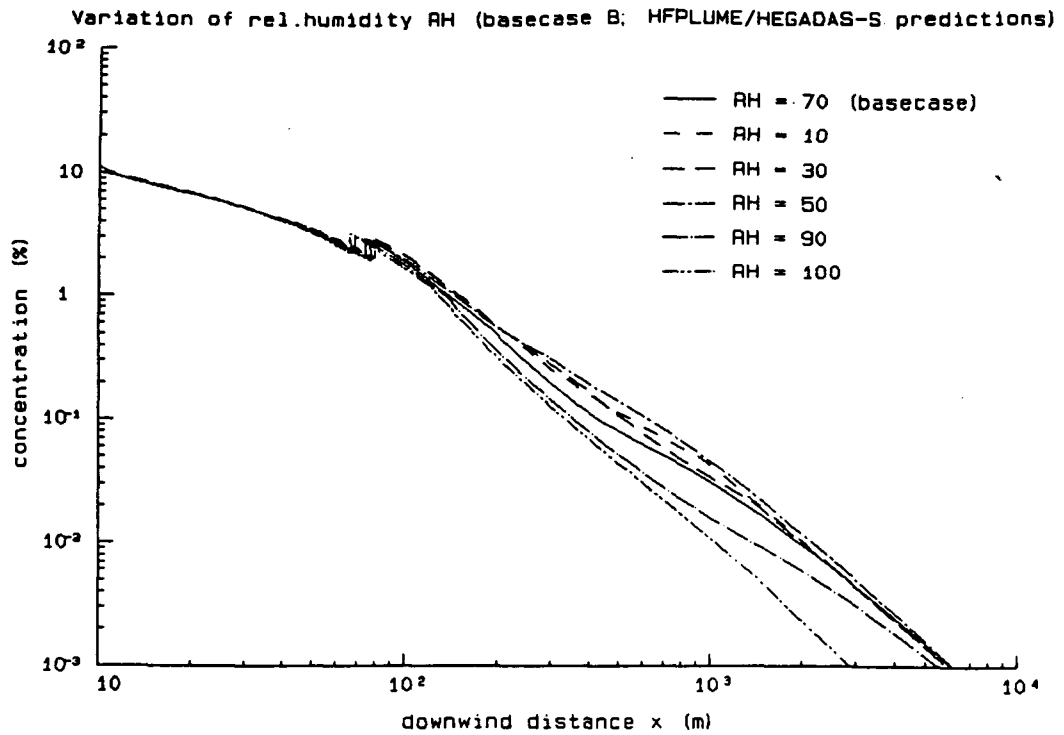


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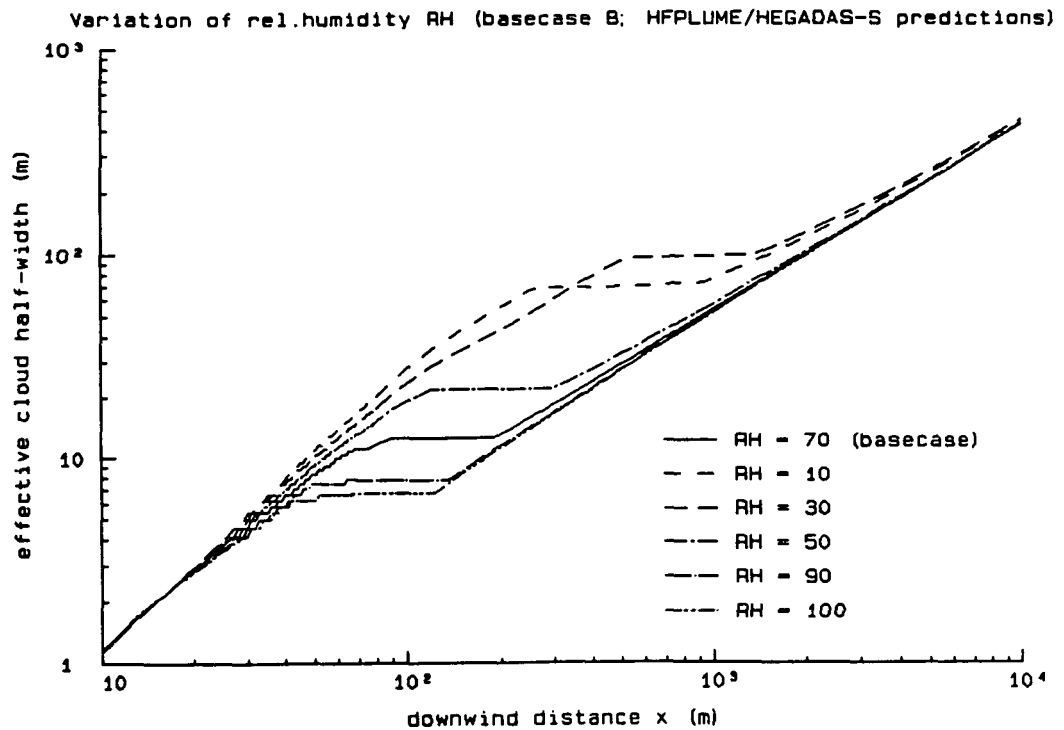
Fig. 10.6. Effect of relative humidity r_H on HFPLUME/HEGADAS-S concentration predictions; $r_H = 10, 30, 50, 70, 90$ or 100% ; base case A

(a) centre-line concentration (% molar fraction; HFPLUME sectional-mean value and HEGADAS value at ground level)

(b) effective half-width B_{eff} of cloud



(a)

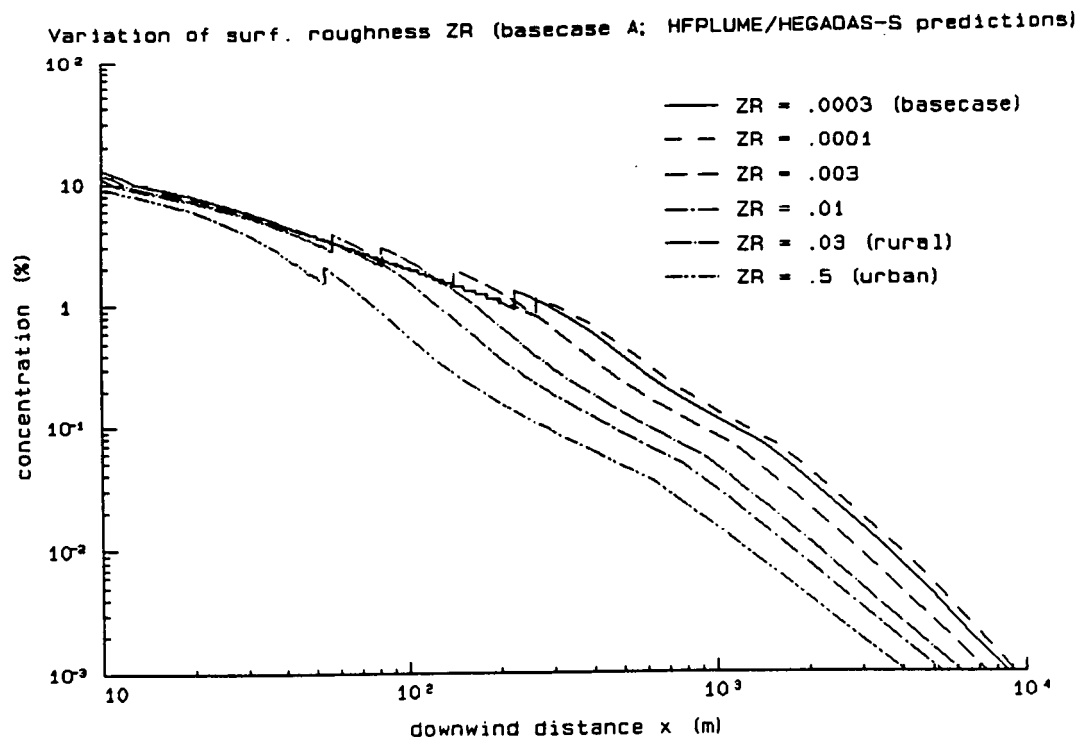


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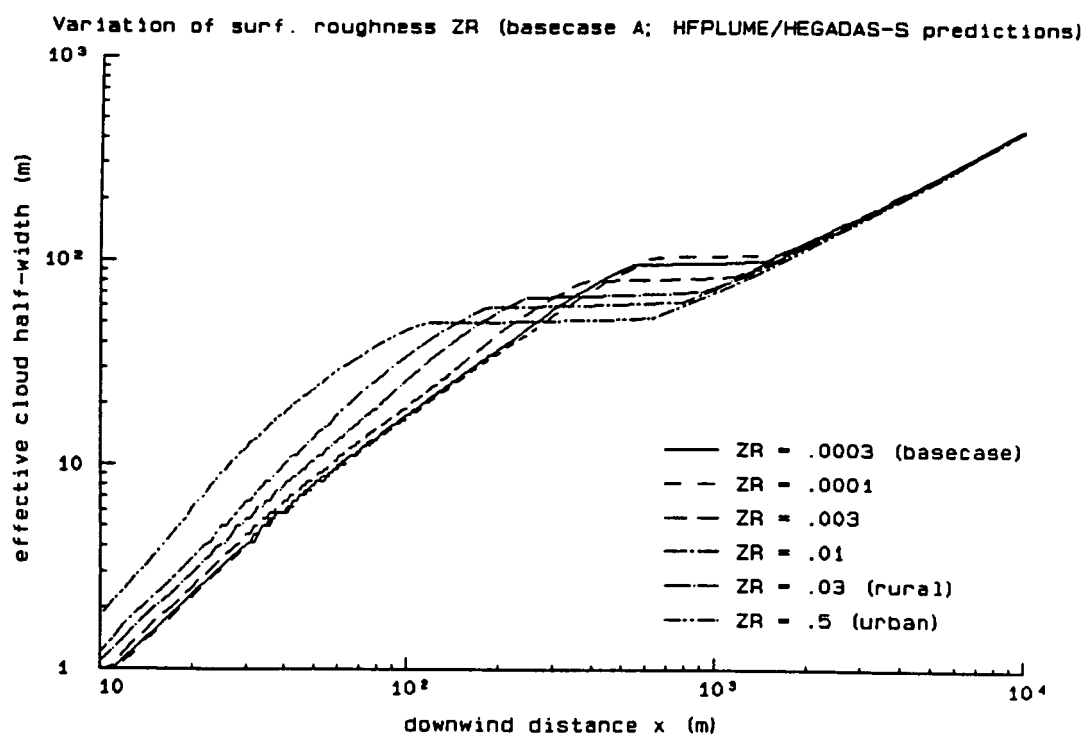
Fig. 10.7. Effect of relative humidity r_H on HFPLUME/HEGADAS-S concentration predictions; $r_H = 10, 30, 50, 70, 90$ or 100% ; base case B

(a) centre-line concentration (% molar fraction; HFPLUME sectional-mean value and HEGADAS value at ground level)

(b) effective half-width B_{eff} of cloud

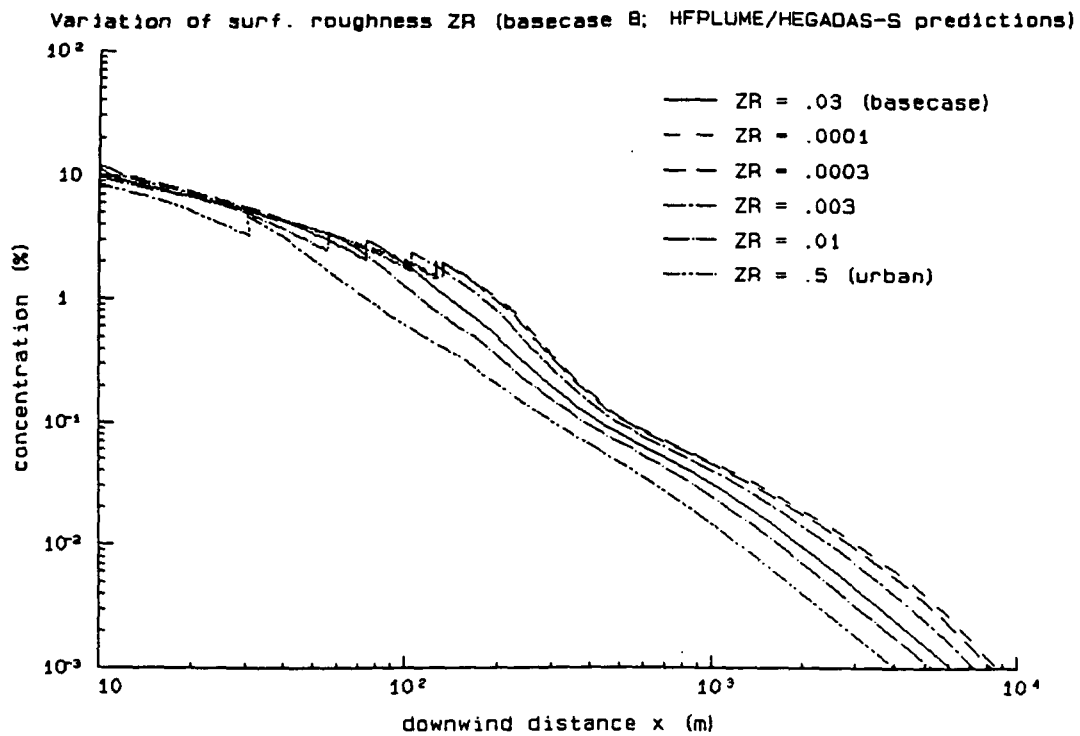


(a)

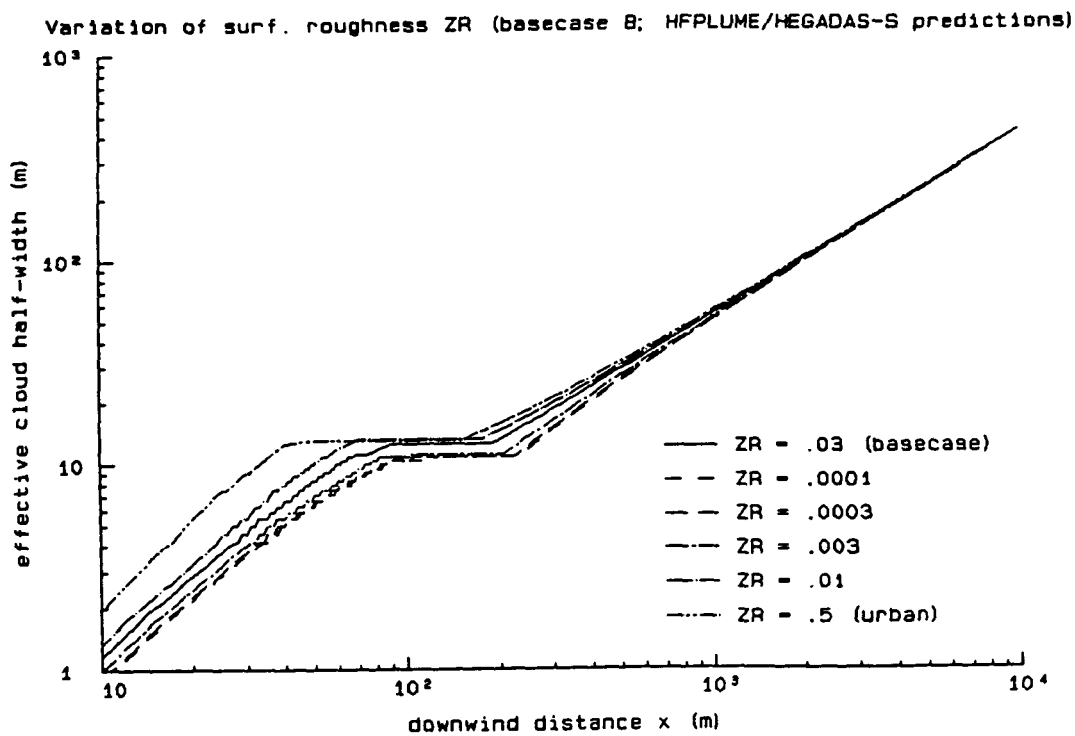


(b)

Fig. 10.8. Effect of surface roughness z_R on HFPLUME/HEGADAS-S concentration predictions; $z_R = .0001, .0003, .003, .01, .03$ or $.5$ m; base case A
 (a) centre-line concentration (% molar fraction; HFPLUME sectional-mean value and HEGADAS value at ground level)
 (b) effective half-width B_{eff} of cloud

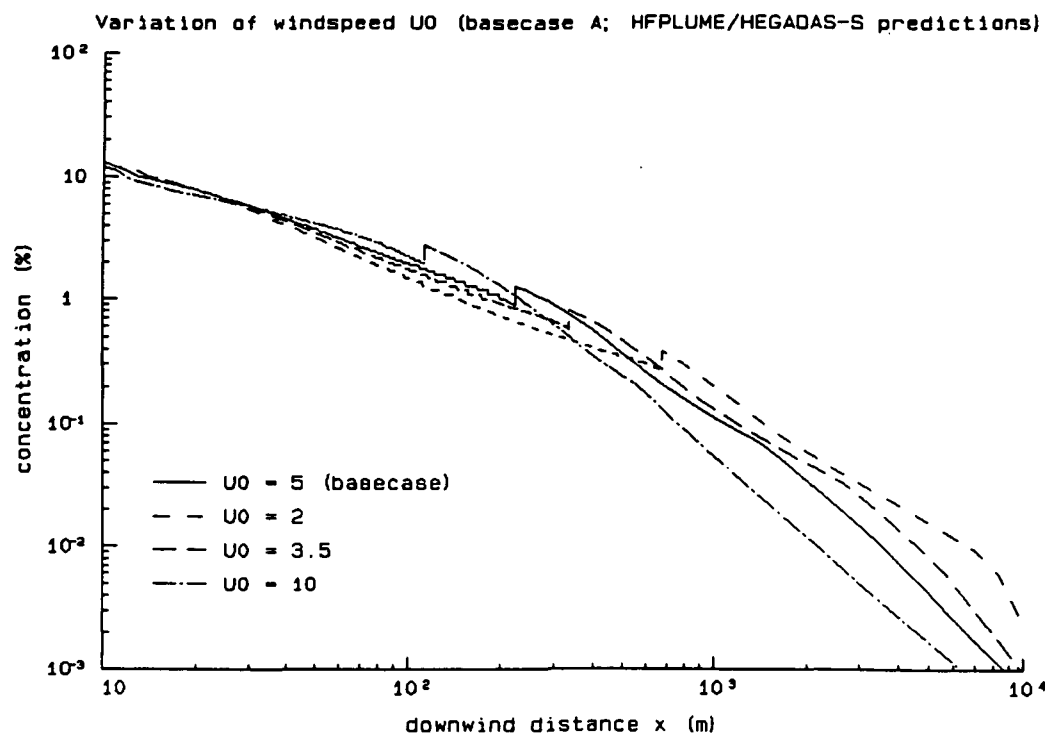


(a)

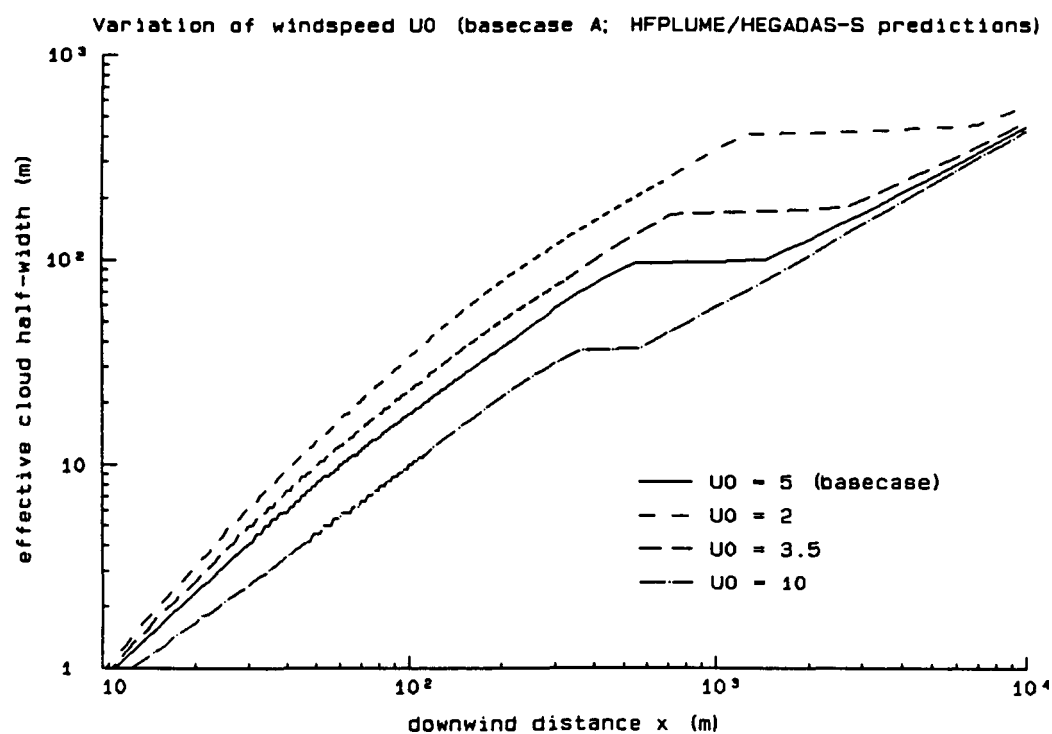


(b)

Fig. 10.9. Effect of surface roughness z_R on HFPLUME/HEGADAS-S concentration predictions; $z_R = .0001, .0003, .003, .01, .03$ or $.5$ m; base case B
 (a) centre-line concentration (% molar fraction; HFPLUME sectional-mean value and HEGADAS value at ground level)
 (b) effective half-width B_{eff} of cloud

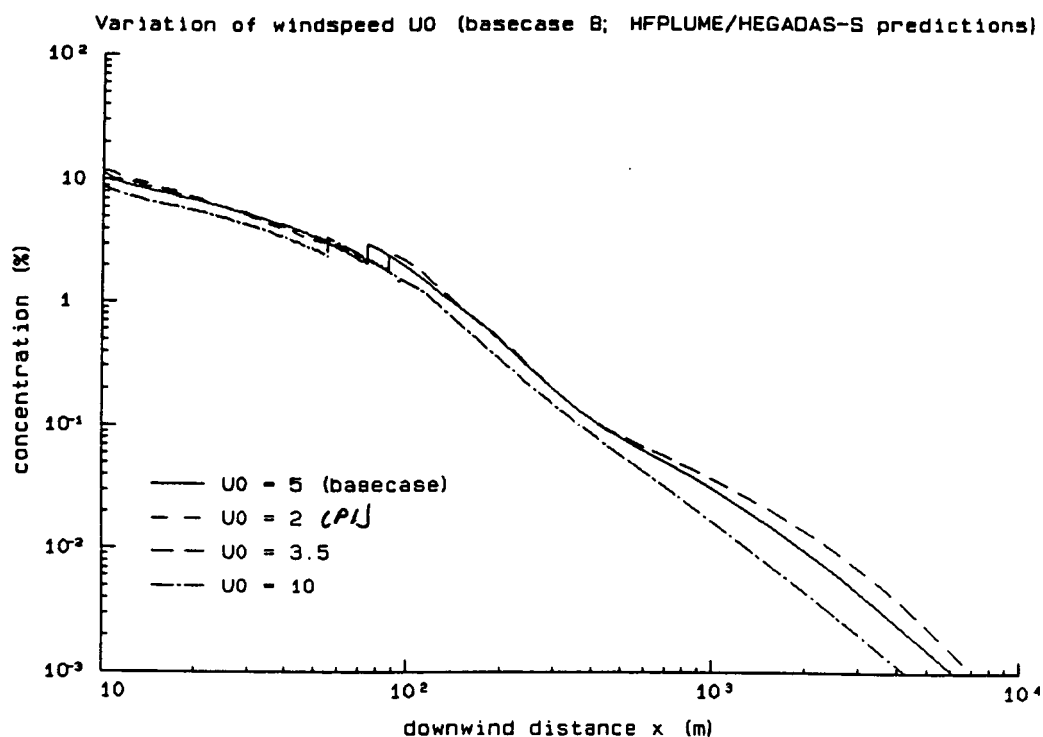


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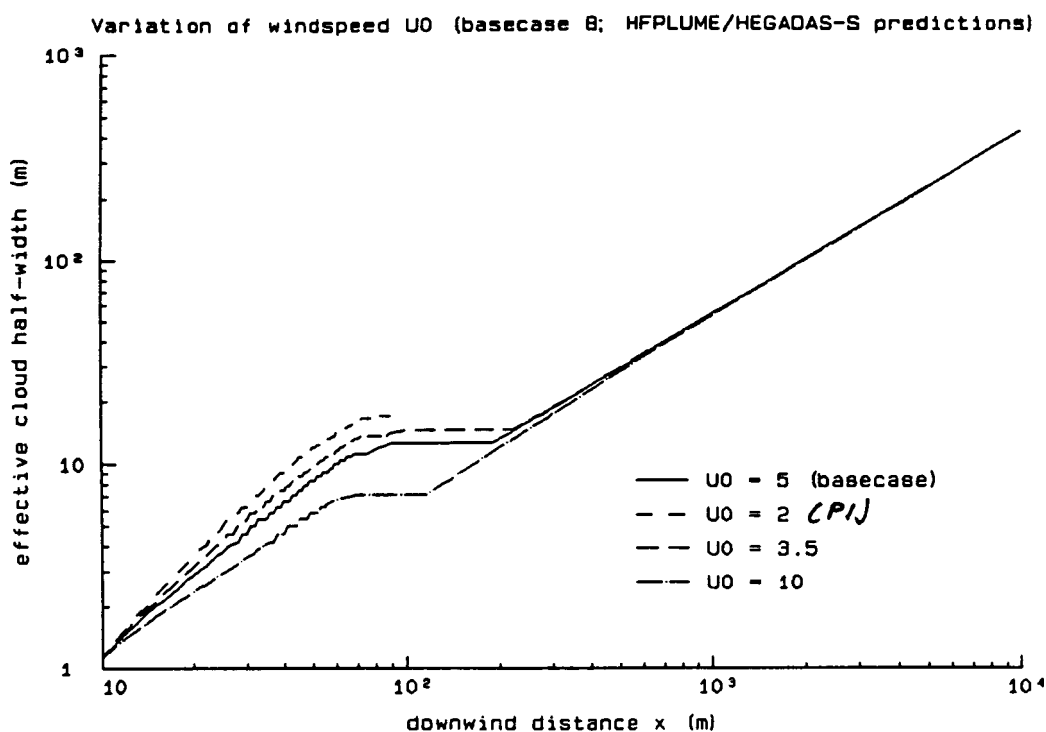


(b)

Fig. 10.10. Effect of windspeed u_0 on HFPLUME/HEGADAS-S concentration predictions; $u_0 = 2, 3.5, 5$ or 10 m/s; base case A
 (a) centre-line concentration (% molar fraction; HFPLUME sectional-mean value and HEGADAS value at ground level)
 (b) effective half-width B_{eff} of cloud

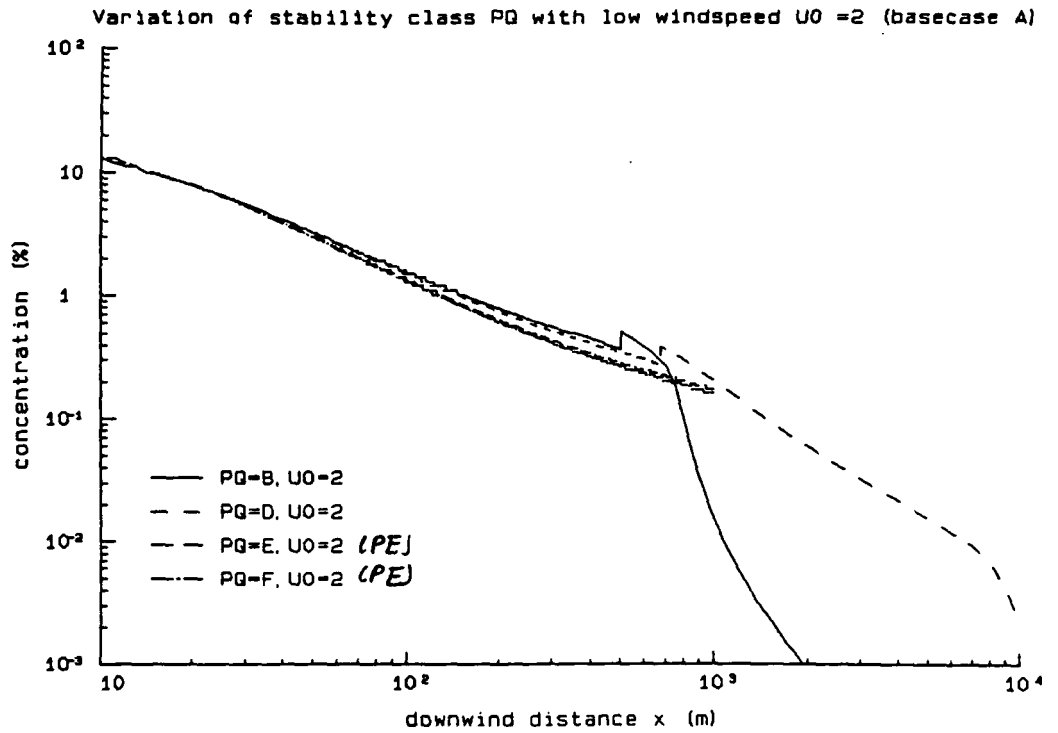


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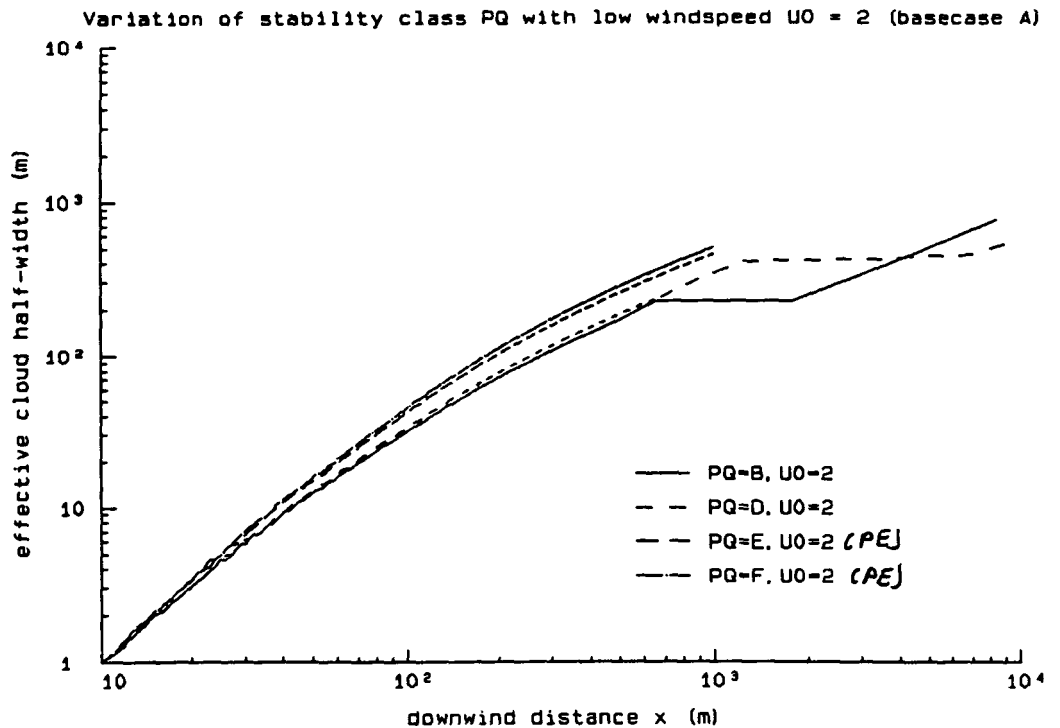


(b)

Fig. 10.11. Effect of windspeed u_0 on HFPLUME/HEGADAS-S concentration predictions; $u_0 = 2, 3.5, 5$ or 10 m/s; base case B
 (a) centre-line concentration (% molar fraction; HFPLUME sectional-mean value and HEGADAS value at ground level)
 (b) effective half-width B_{eff} of cloud

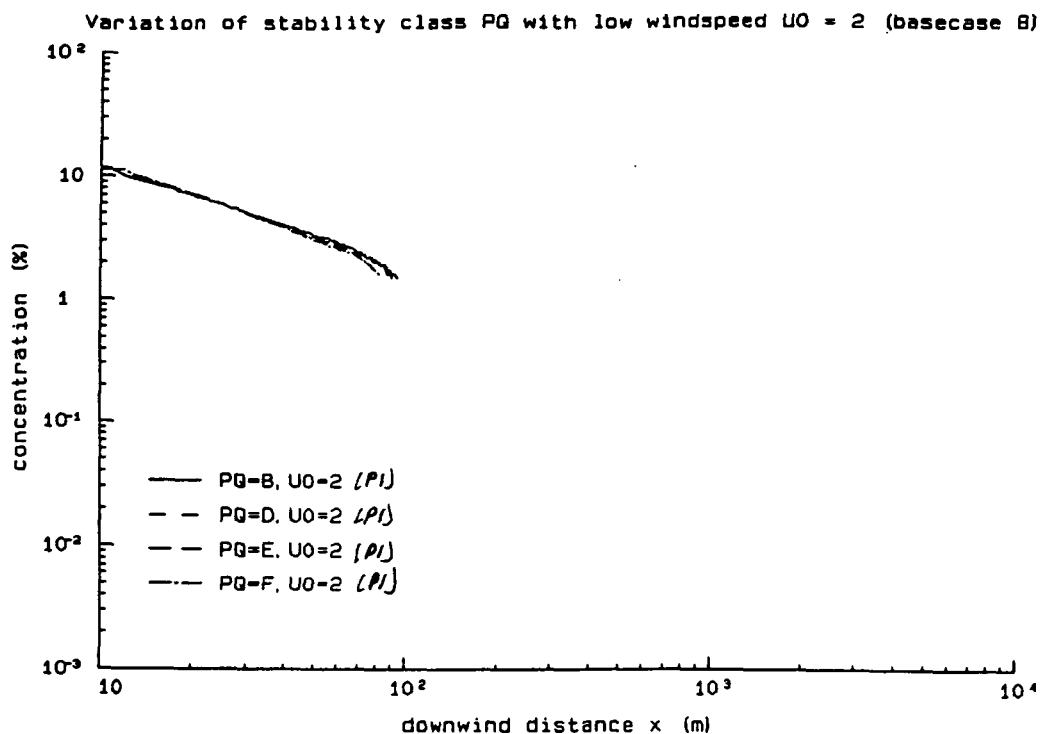


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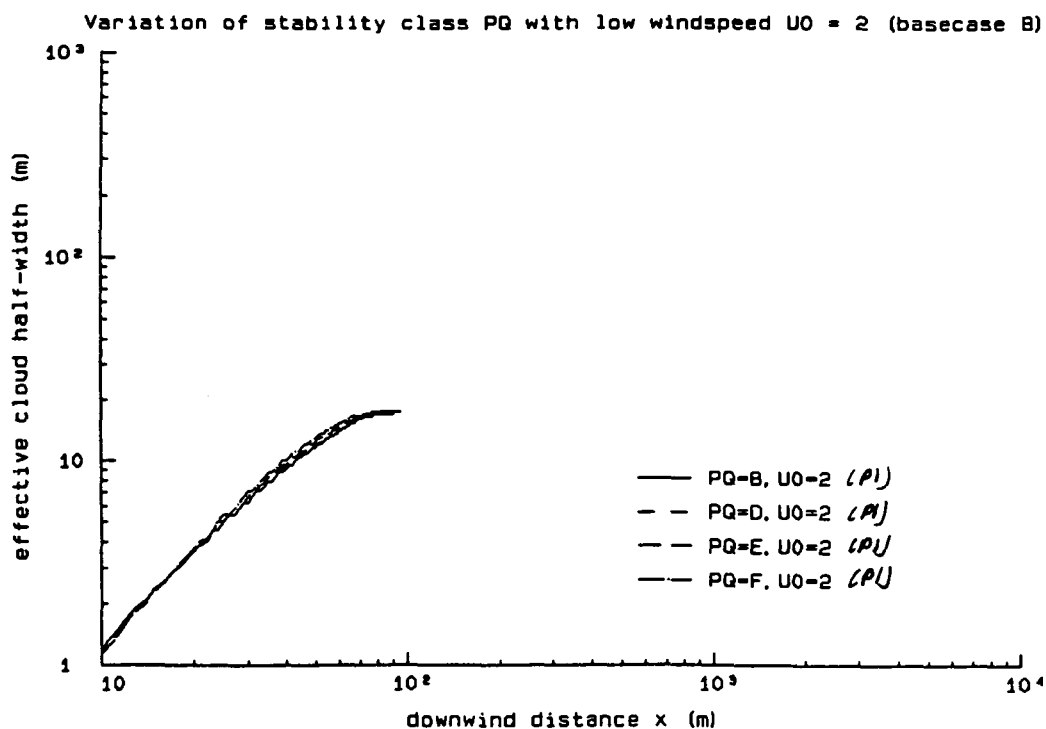


(b)

Fig. 10.12. Effect of stability class PQSTAB on HFPLUME/HEGADAS-S concentration predictions; PQSTAB = B, D, E or F; base case A with low windspeed $u_0 = 2$ m/s;
 (a) centre-line concentration (% molar fraction; HFPLUME sectional-mean value and HEGADAS value at ground level)
 (b) effective half-width B_{eff} of cloud

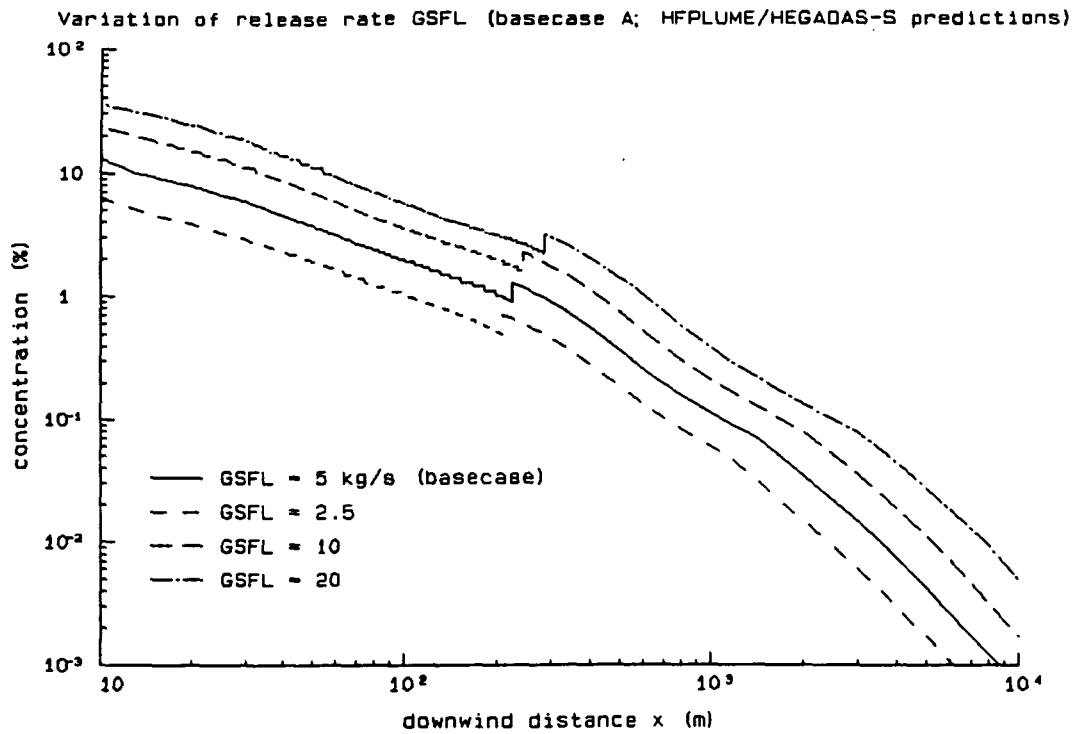


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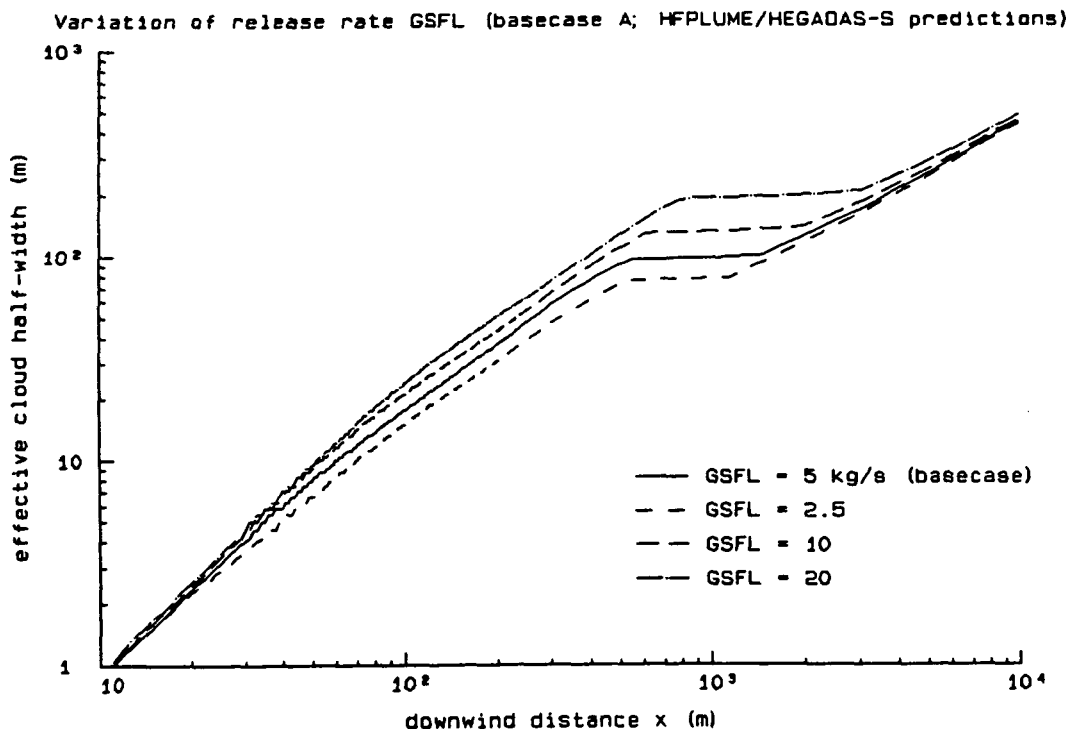


(b)

Fig. 10.13. Effect of stability class PQSTAB on HFPLUME/HEGADAS-S concentration predictions; PQSTAB = B, D, E or F; base case B with low windspeed $u_0 = 2$ m/s;
 (a) centre-line concentration (% molar fraction; HFPLUME sectional-mean value and HEGADAS value at ground level)
 (b) effective half-width B_{eff} of cloud

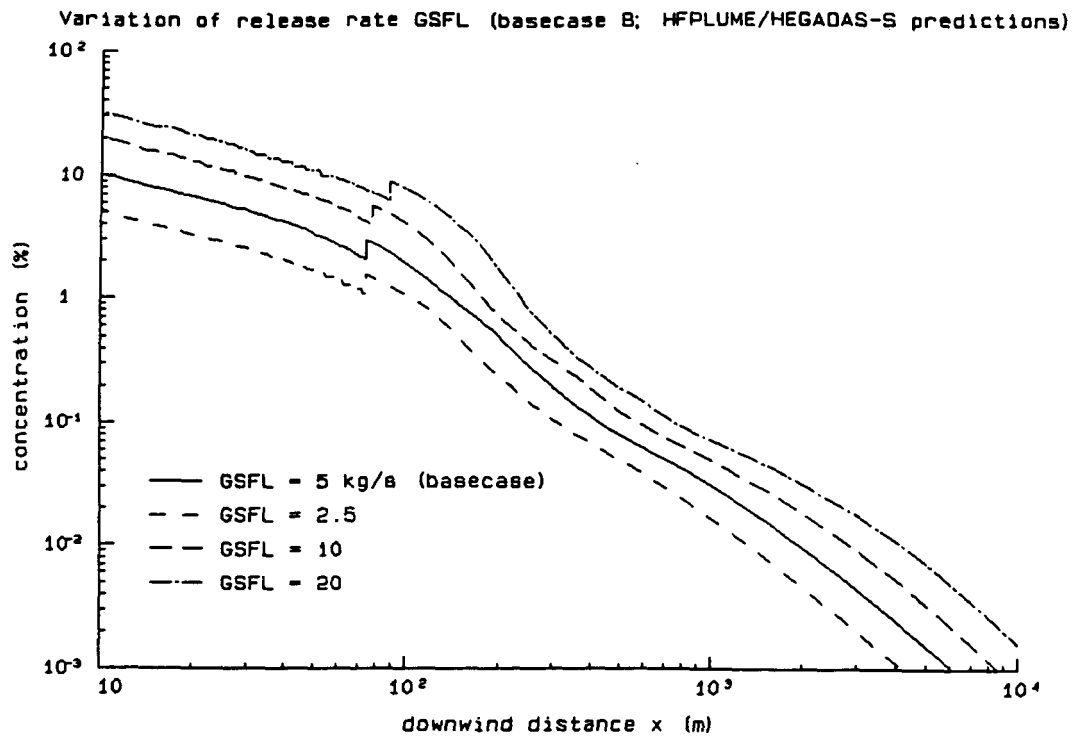


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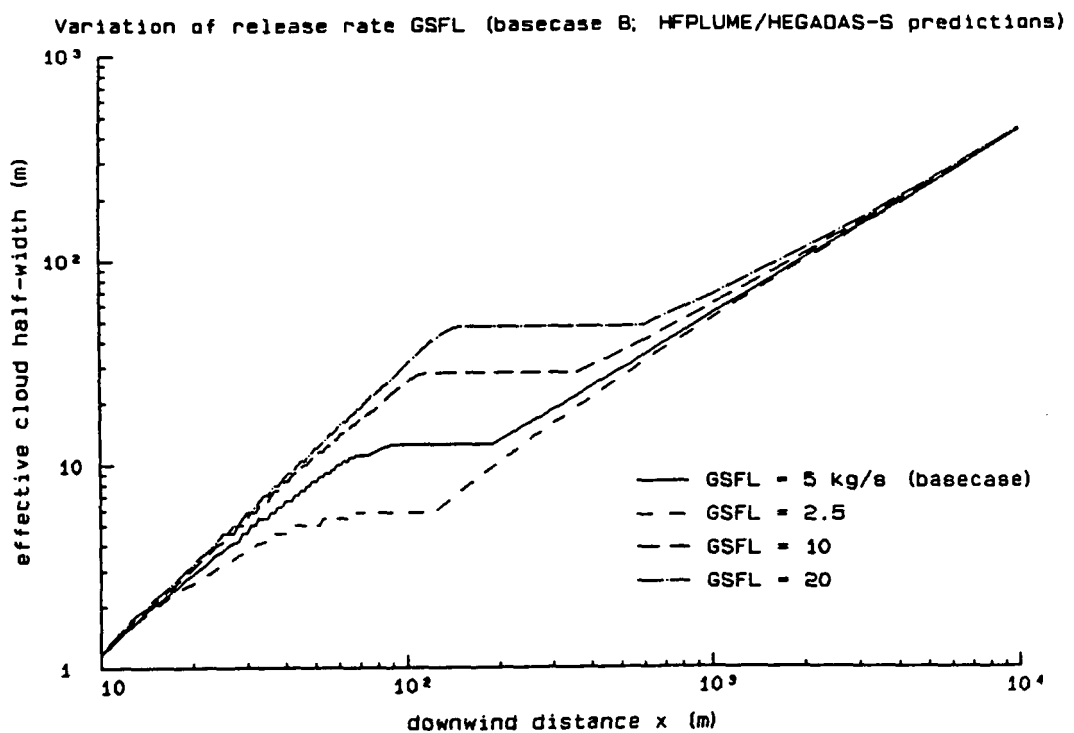


(b)

Fig. 10.14. Effect of release rate E on HFPLUME/HEGADAS-S concentration predictions; $E = 2.5, 5, 10$ or 20 kg/s; base case A;
 (a) centre-line concentration (% molar fraction; HFPLUME sectional-mean value and HEGADAS value at ground level)
 (b) effective half-width B_{eff} of cloud

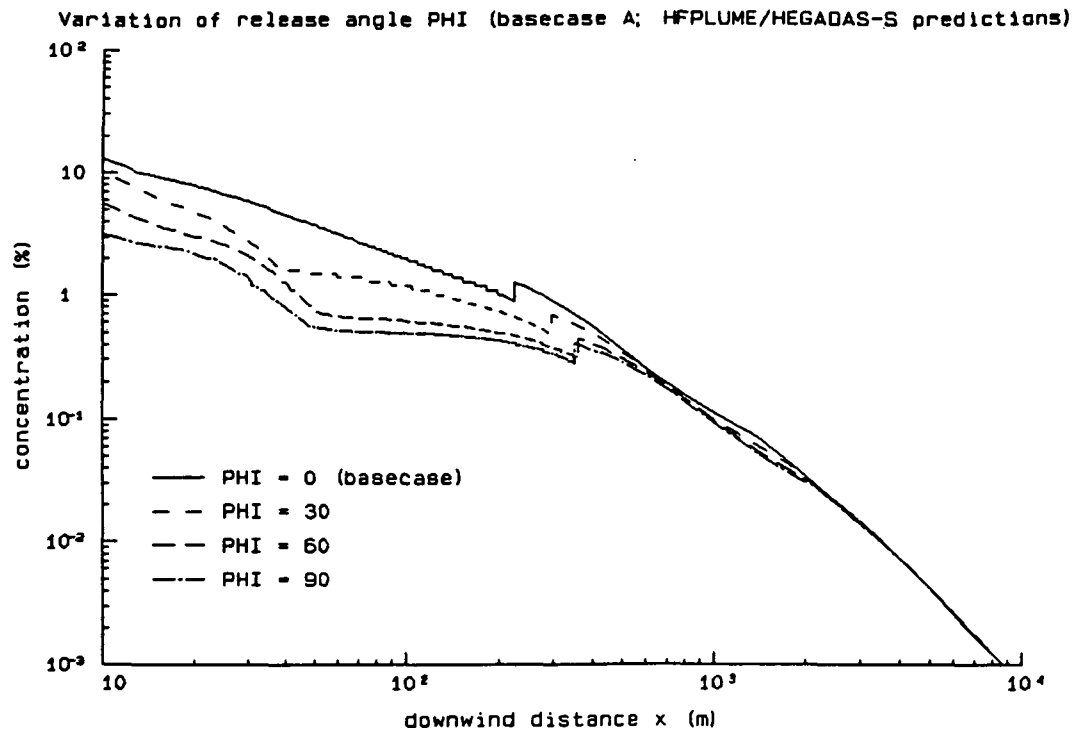


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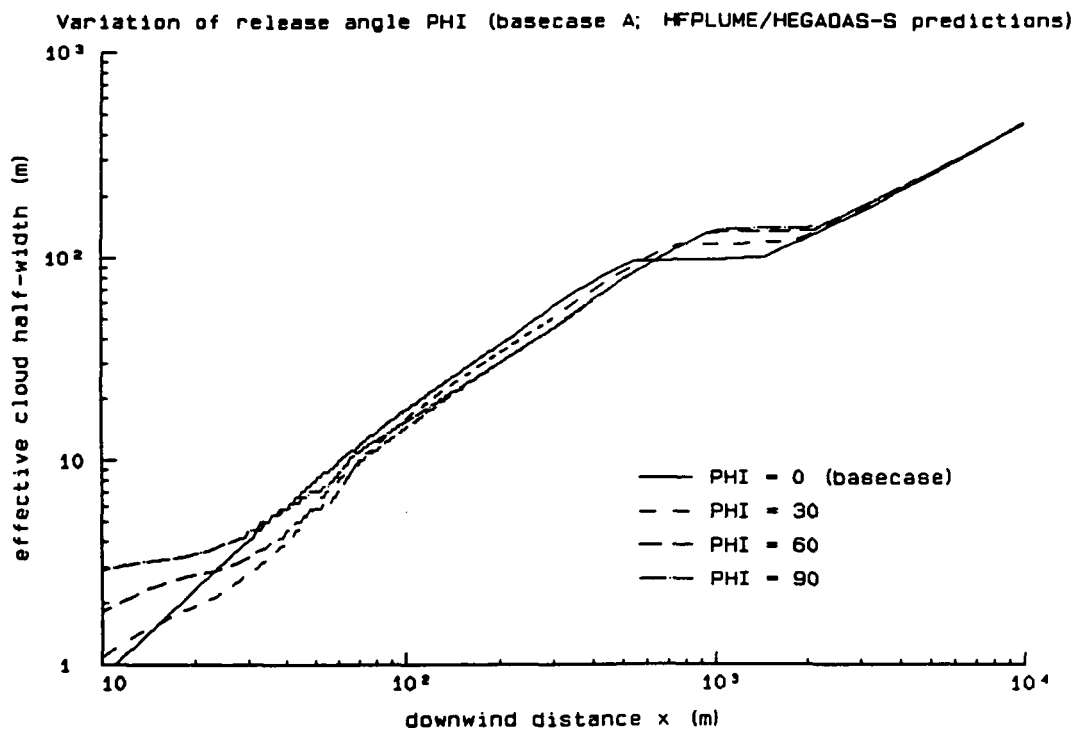


(b)

Fig. 10.15. Effect of release rate E on HFPLUME/HEGADAS-S concentration predictions; $E = 2.5, 5, 10$ or 20 kg/s; base case B;
 (a) centre-line concentration (% molar fraction; HFPLUME sectional-mean value and HEGADAS value at ground level)
 (b) effective half-width B_{eff} of cloud

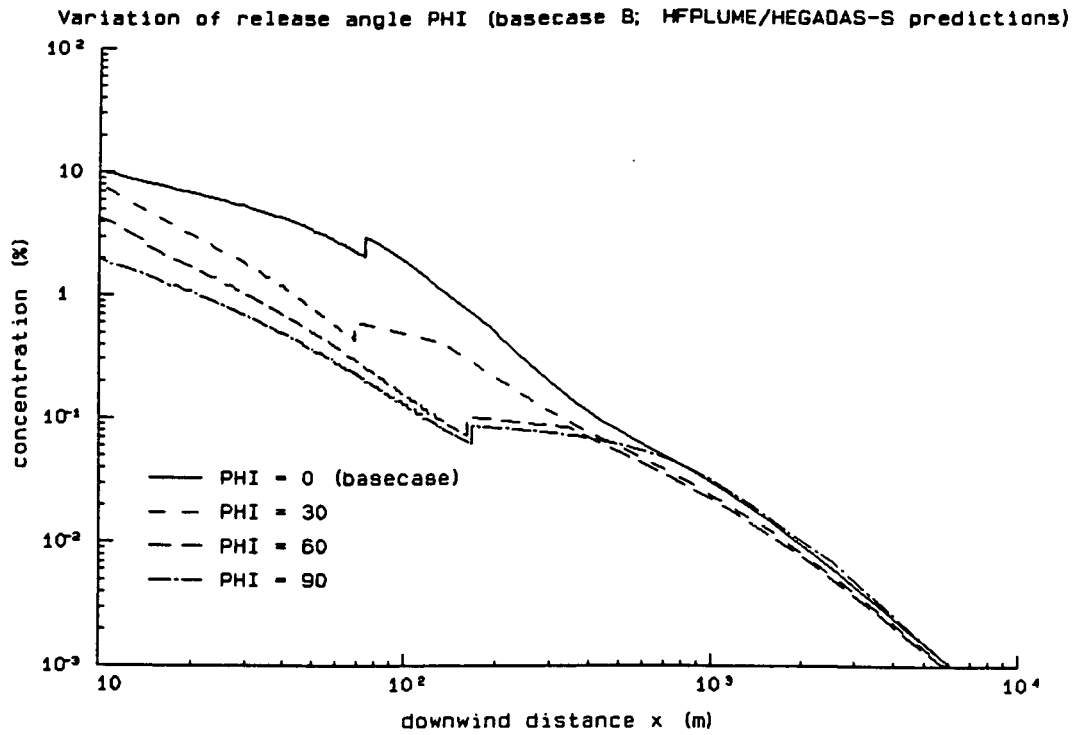


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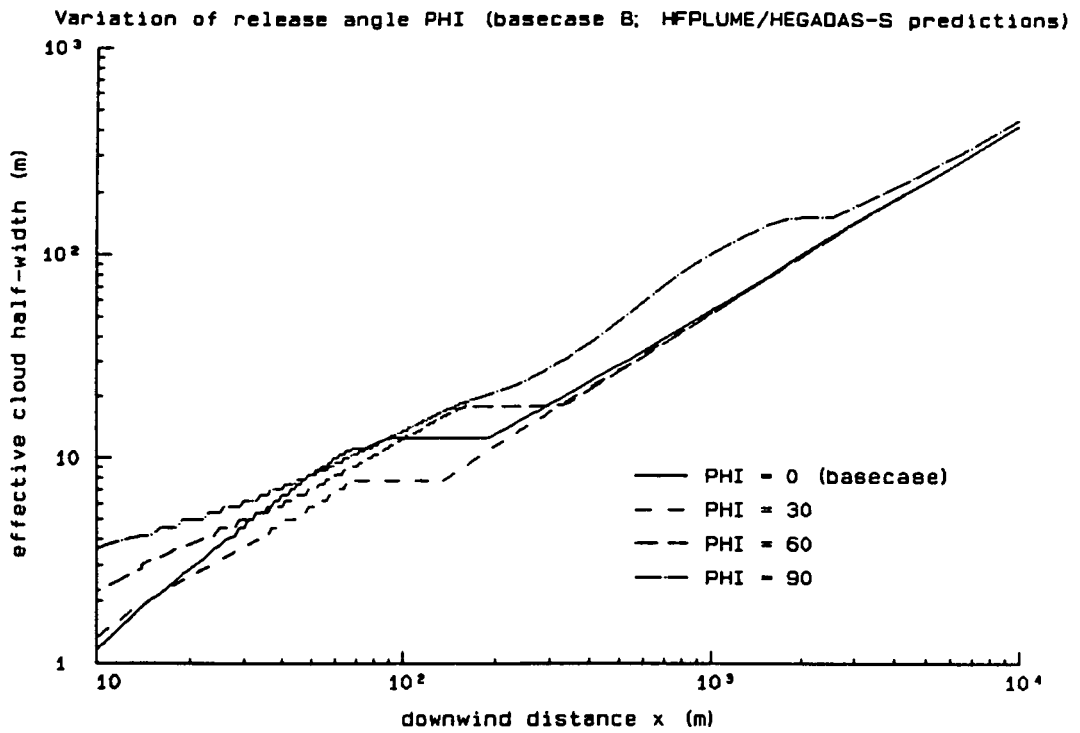


(b)

Fig. 10.16. Effect of release angle ϕ on HFPLUME/HEGADAS-S concentration predictions; $\phi = 0, 30, 60$ or 90 degrees; base case A;
 (a) centre-line concentration (% molar fraction; HFPLUME sectional-mean value and HEGADAS value at ground level)
 (b) effective half-width B_{eff} of cloud



(a)



(b)

Fig. 10.17. Effect of release angle ϕ on HFPLUME/HEGADAS-S concentration predictions; $\phi = 0, 30, 60$ or 90 degrees; base case B;
 (a) centre-line concentration (% molar fraction; HFPLUME sectional-mean value and HEGADAS value at ground level)
 (b) effective half-width B_{eff} of cloud

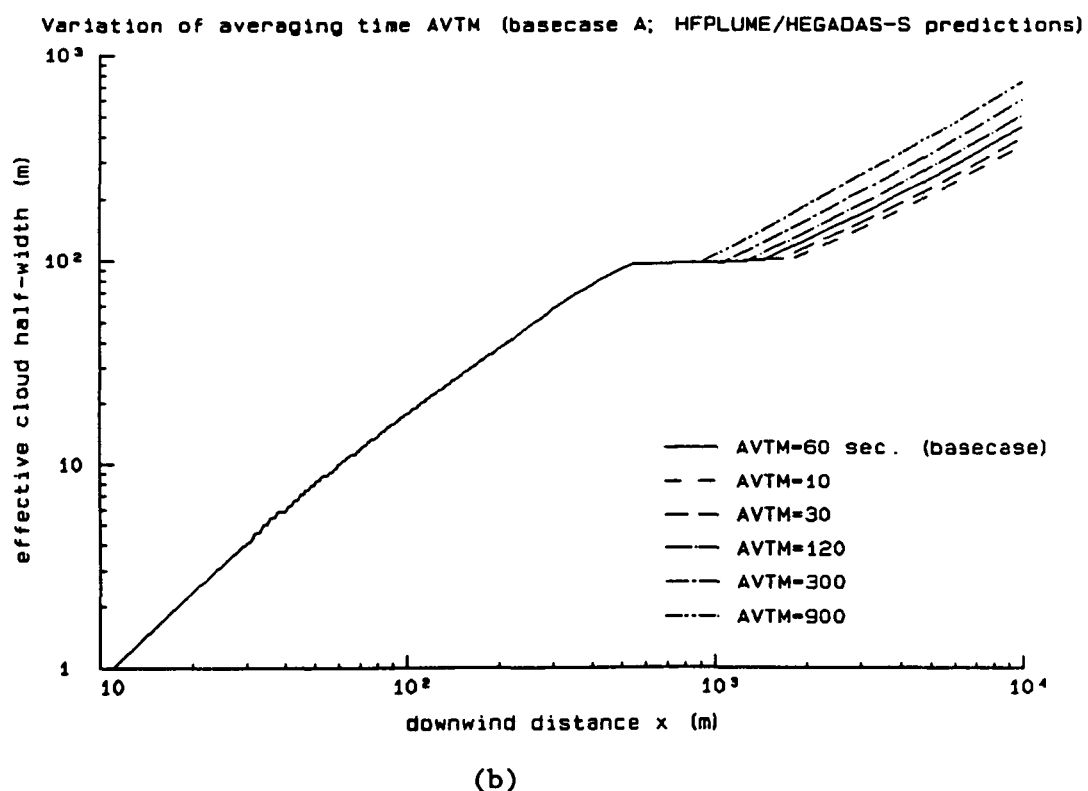
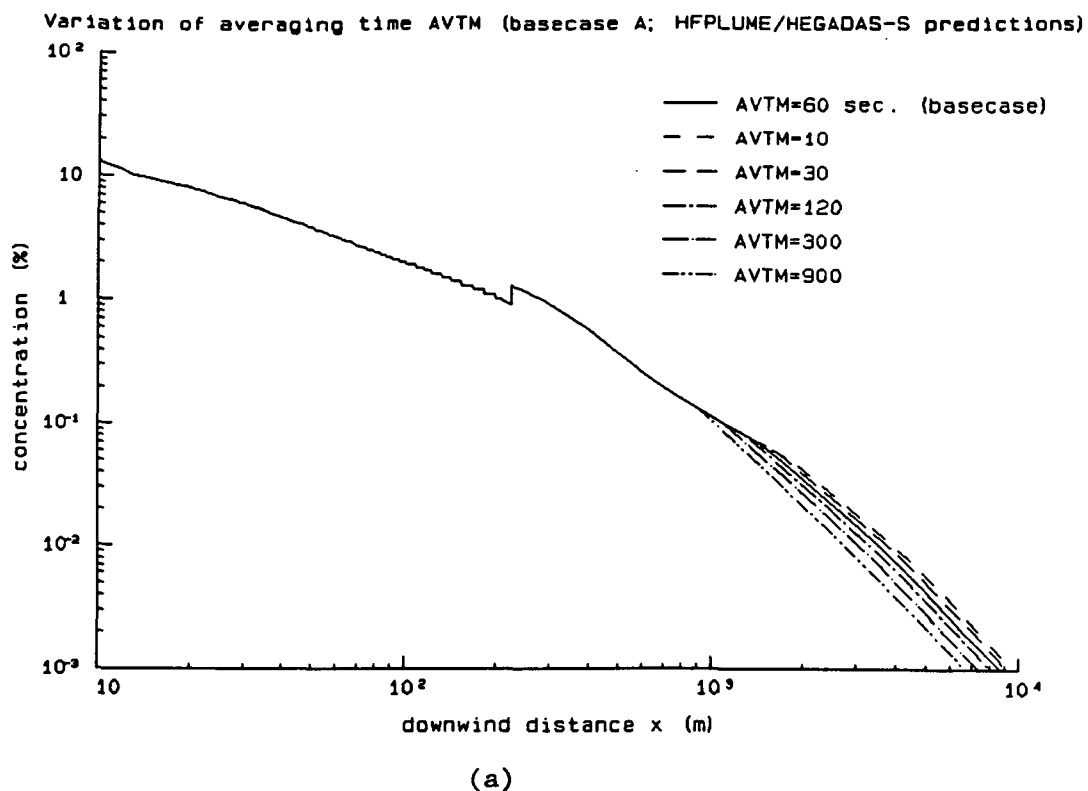
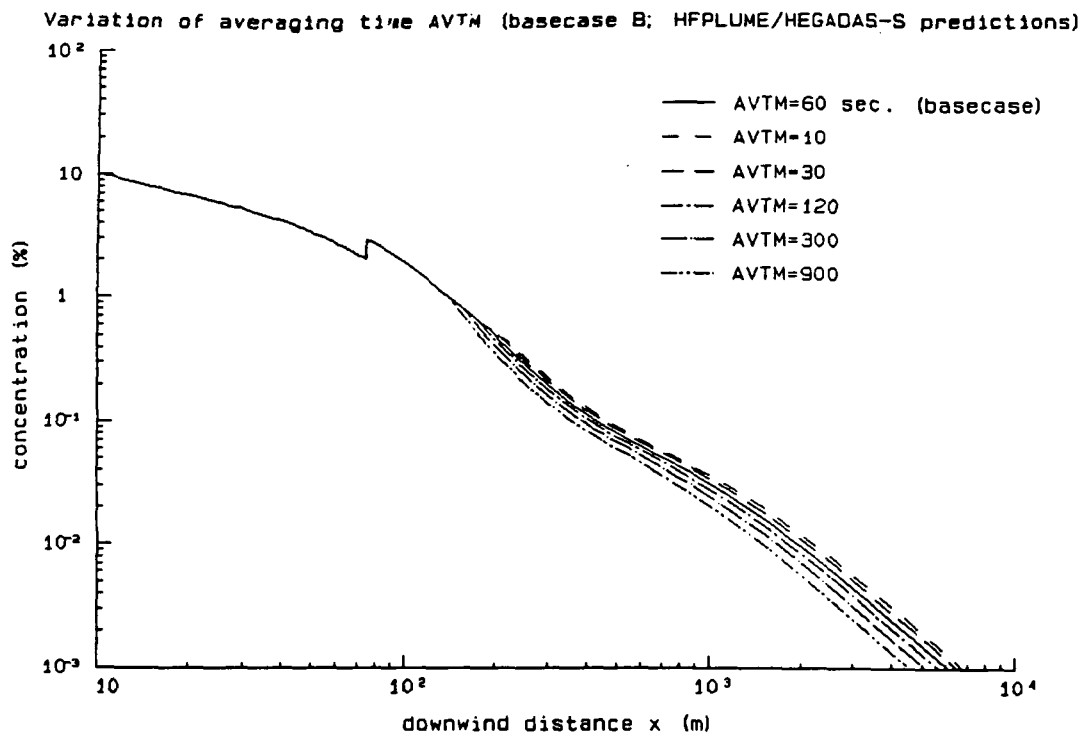


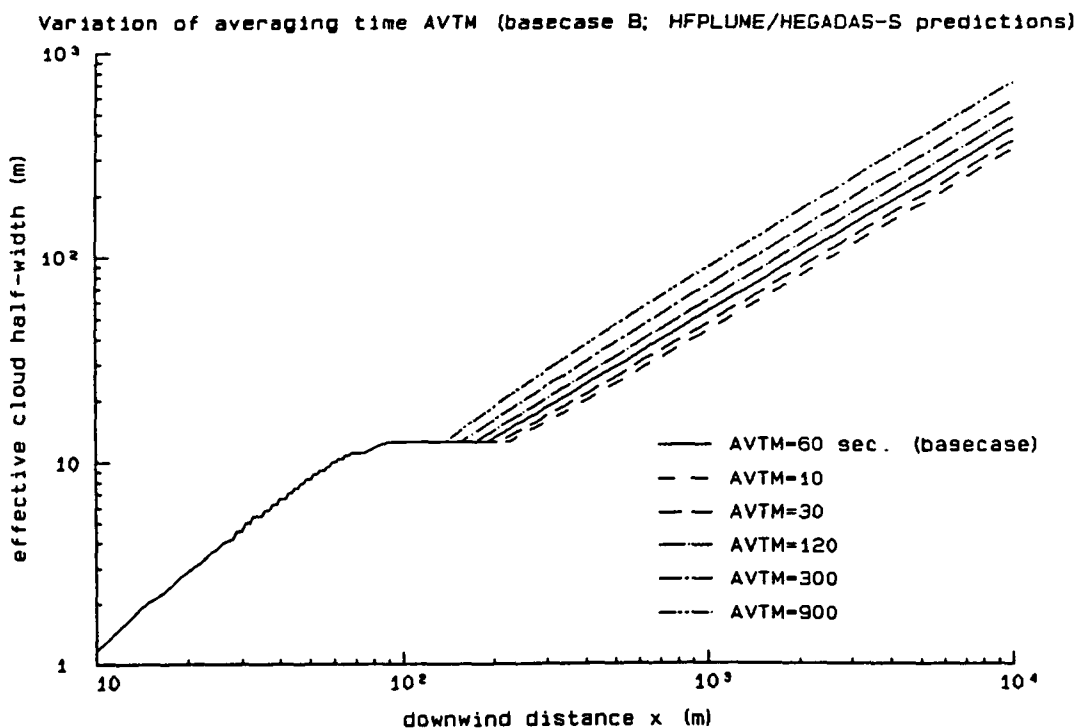
Fig. 10.18. Effect of averaging time AVTIMC on HFPLUME/HEGADAS-S concentration predictions; AVTIMC = 10, 30, 60, 120, 300 or 900 seconds; base case A;

(a) centre-line concentration (% molar fraction; HFPLUME sectional-mean value and HEGADAS value at ground level)

(b) effective half-width B_{eff} of cloud



(a)



(b)

Fig. 10.19. Effect of averaging time AVTIMC on HFPLUME/HEGADAS-S concentration predictions; AVTIMC = 10, 30, 60, 120, 300 or 900 seconds; base case B;
 (a) centre-line concentration (% molar fraction; HFPLUME sectional-mean value and HEGADAS value at ground level)
 (b) effective half-width B_{eff} of cloud

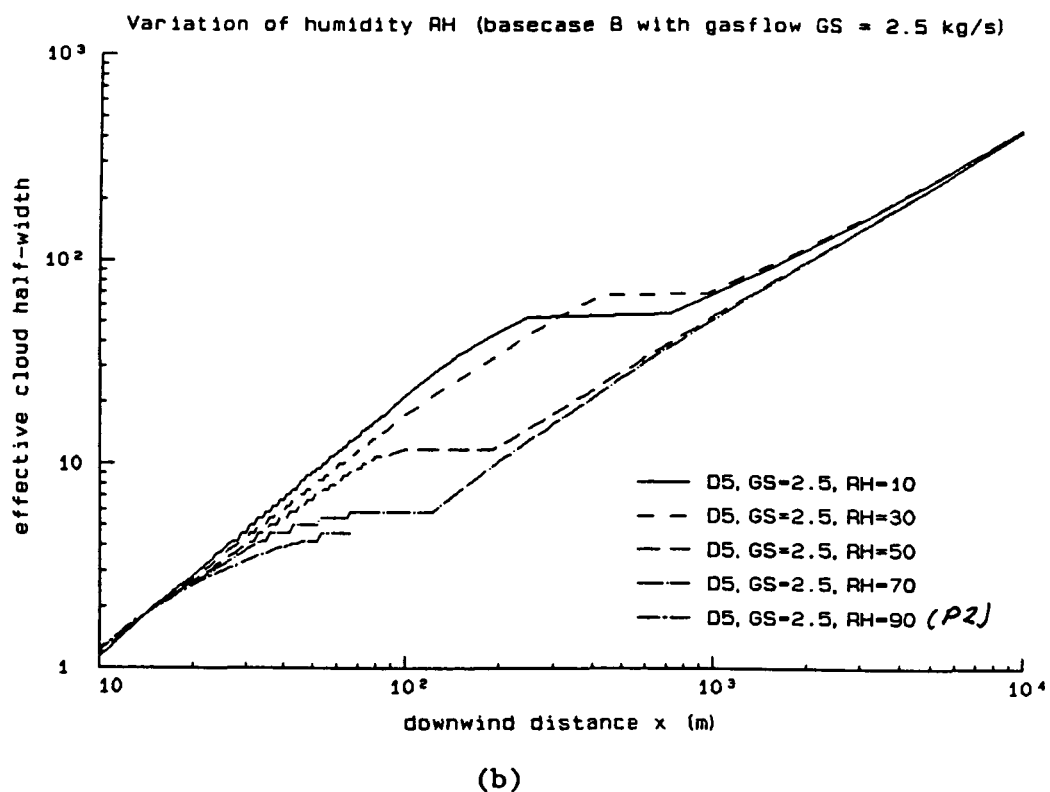
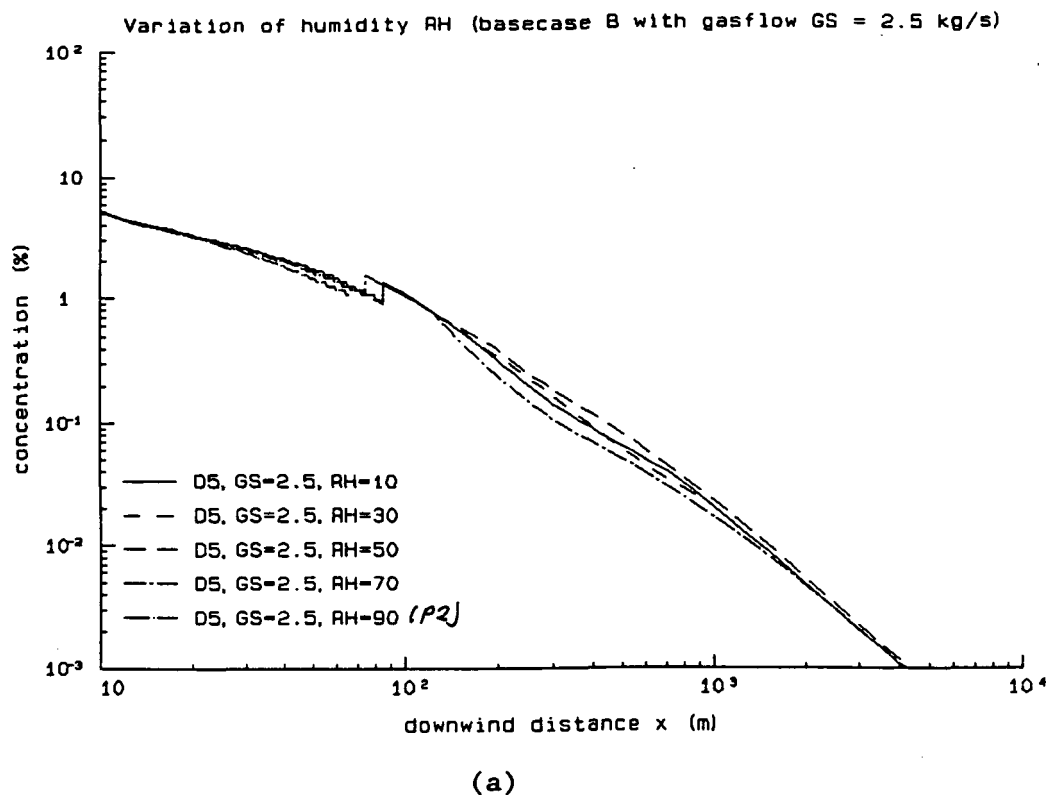
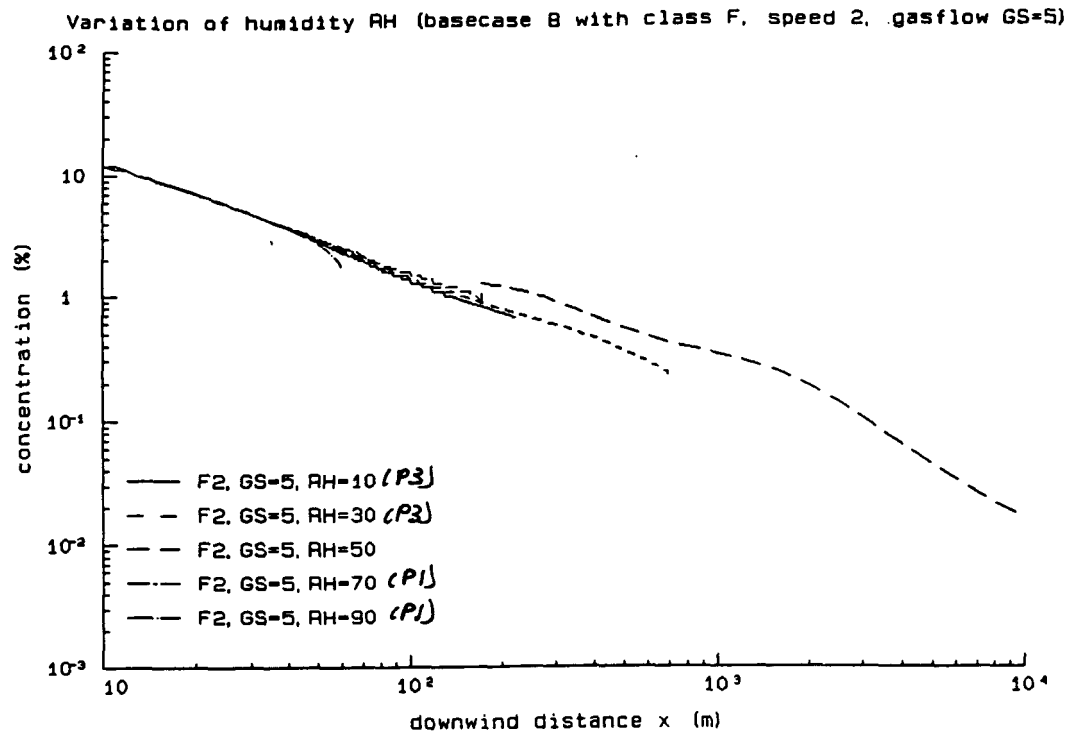
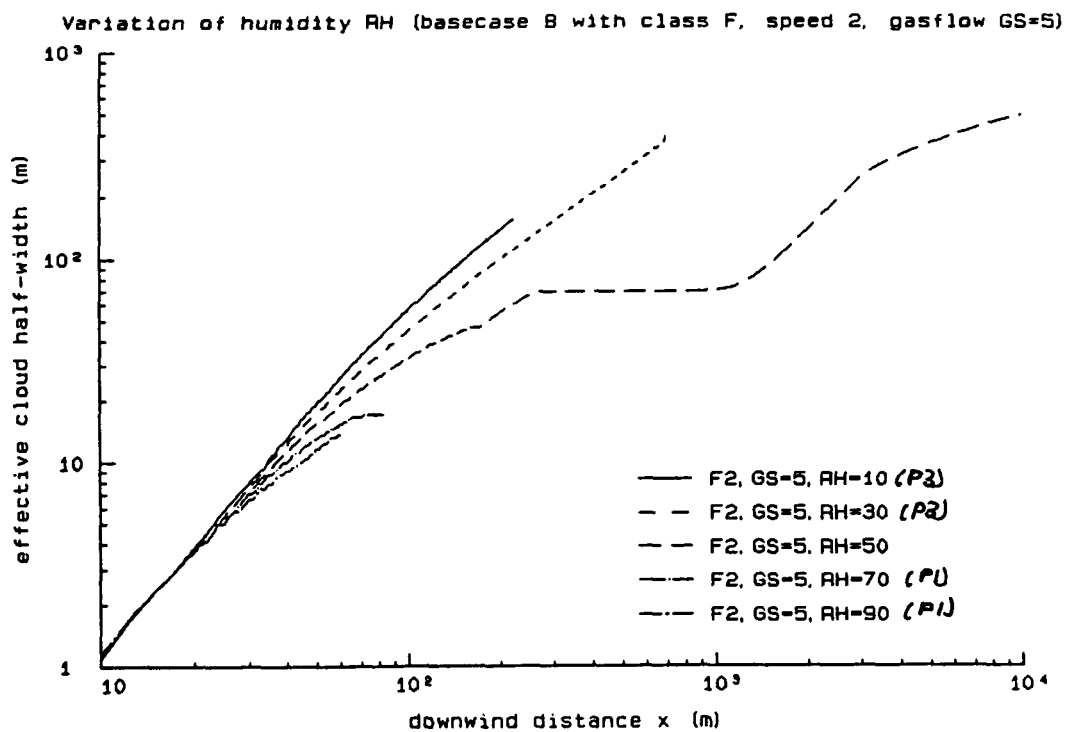


Fig. 10.20. Effect of relative humidity r_H on HFPLUME/HEGADAS-S concentration predictions; $r_H = 10, 30, 50, 70, 90\%$; rural conditions ($z_R = .03$ m) with horizontal release, stability class D, windspeed 5 m/s and release rate 2.5 kg/s; base case B;
 (a) centre-line concentration (% molar fraction; HFPLUME sectional-mean value and HEGADAS value at ground level)
 (b) effective half-width B_{eff} of cloud

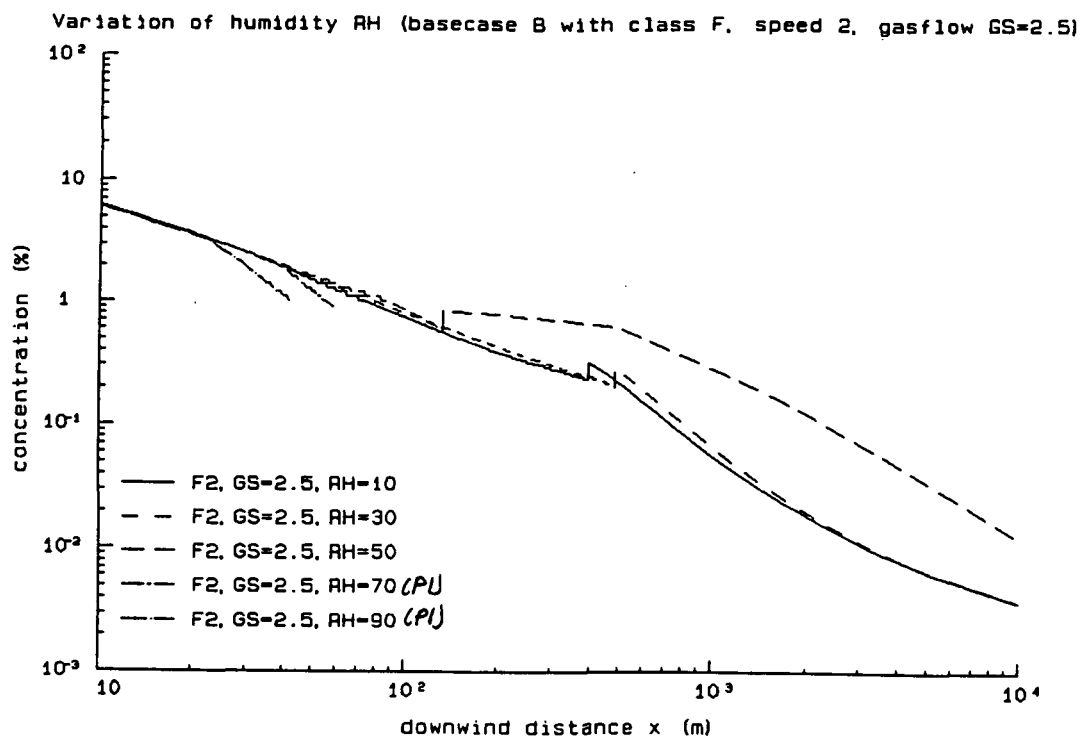


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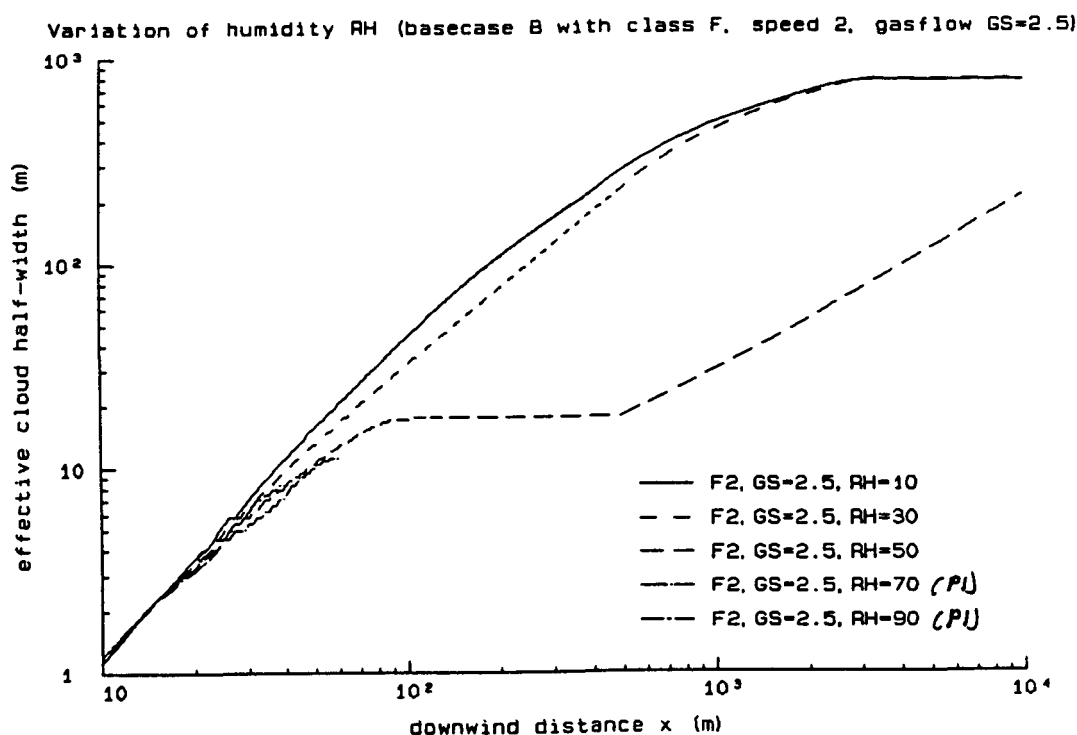


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Fig. 10.21. Effect of relative humidity r_H on HFPLUME/HEGADAS-S concentration predictions; $r_H = 10, 30, 50, 70, 90\%$; rural conditions ($z_R = .03$ m) with horizontal release, stability class F, windspeed 2 m/s and release rate 5 kg/s; base case B;
 (a) centre-line concentration (% molar fraction; HFPLUME sectional-mean value and HEGADAS value at ground level)
 (b) effective half-width B_{eff} of cloud

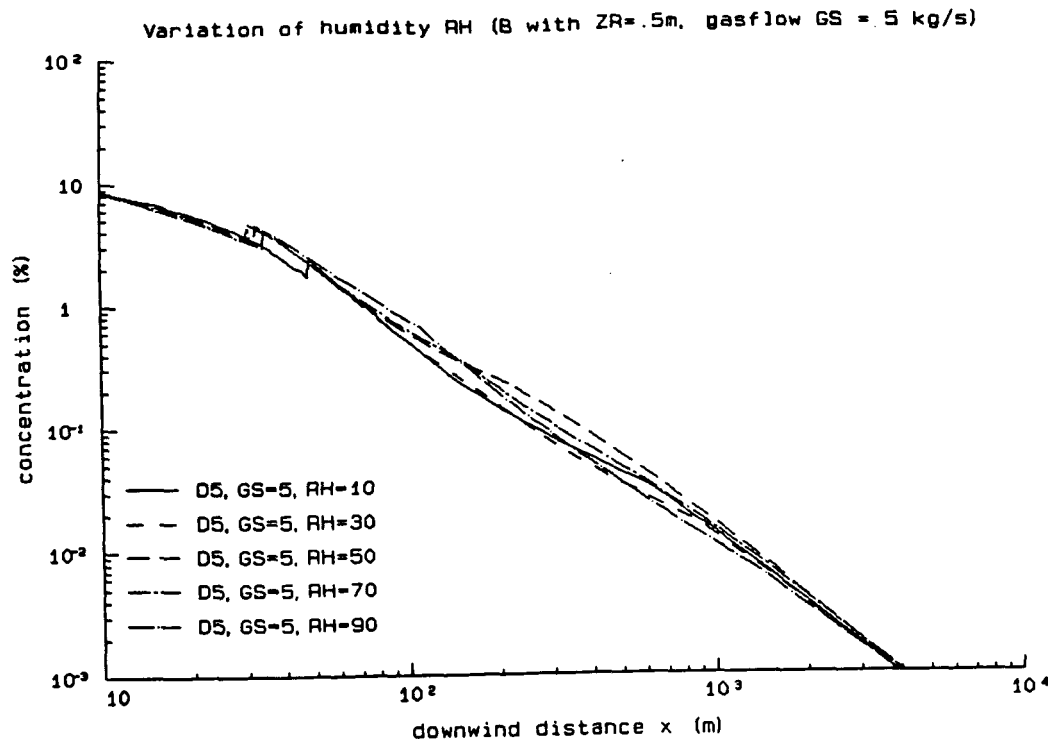


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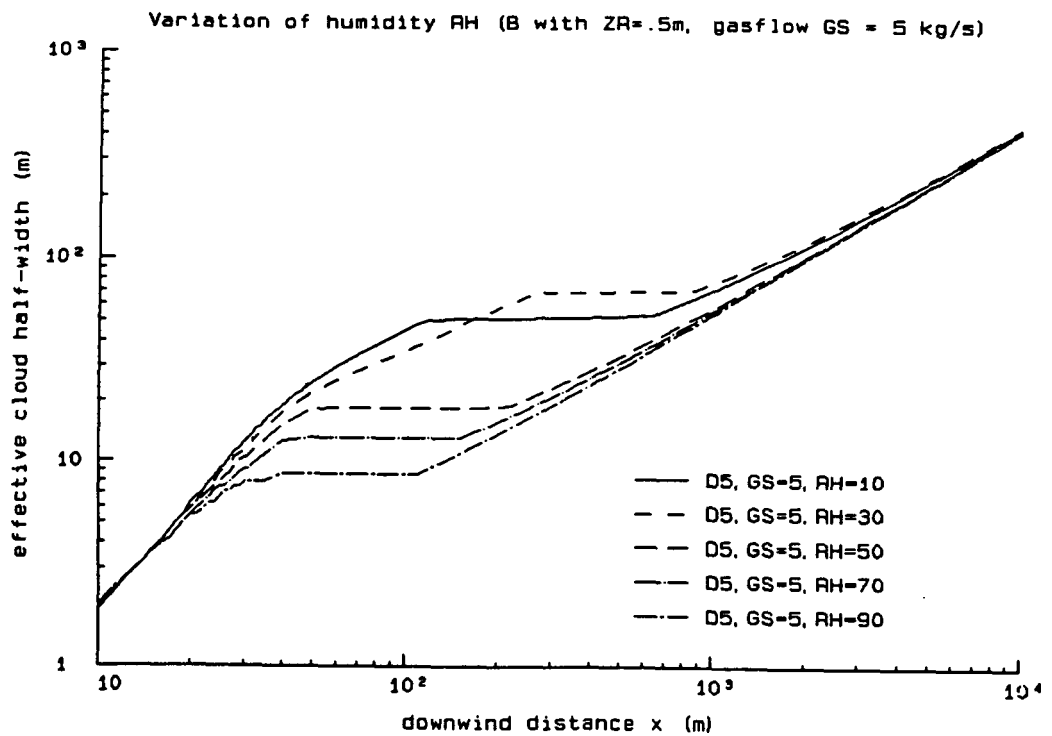


(b)

Fig. 10.22. Effect of relative humidity r_H on HFPLUME/HEGADAS-S concentration predictions; $r_H = 10, 30, 50, 70, 90\%$; rural conditions ($z_R = .03$ m) with horizontal release, stability class F, windspeed 2 m/s and release rate 2.5 kg/s; base case B;
 (a) centre-line concentration (% molar fraction; HFPLUME sectional-mean value and HEGADAS value at ground level)
 (b) effective half-width B_{eff} of cloud

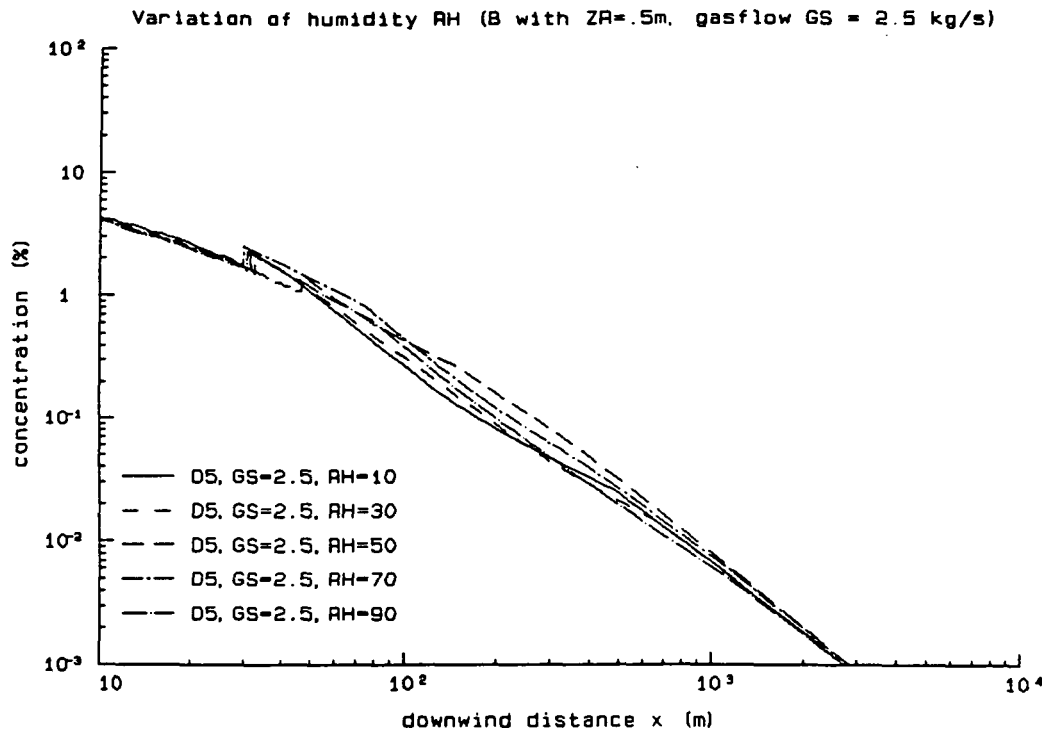


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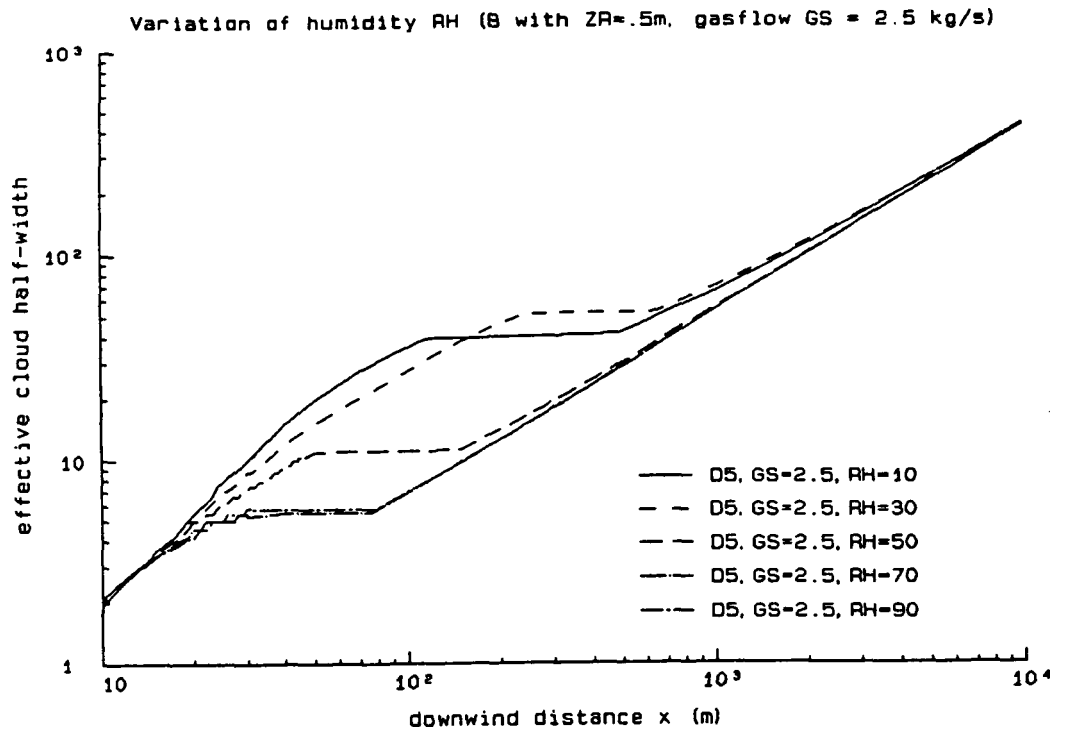


(b)

Fig. 10.23. Effect of relative humidity r_H on HFPLUME/HEGADAS-S concentration predictions; $r_H = 10, 30, 50, 70, 90\%$; urban conditions ($z_R = .5 m$) with horizontal release, stability class D, windspeed 5 m/s and release rate 5 kg/s; base case B;
 (a) centre-line concentration (% molar fraction; HFPLUME sectional-mean value and HEGADAS value at ground level)
 (b) effective half-width B_{eff} of cloud

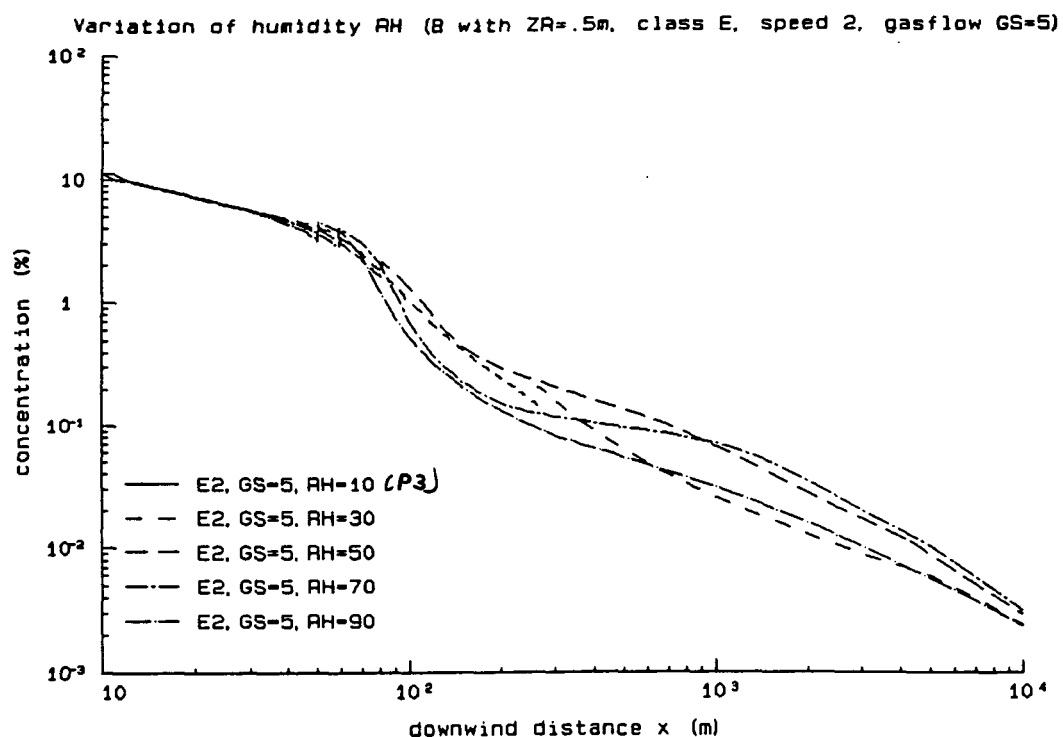


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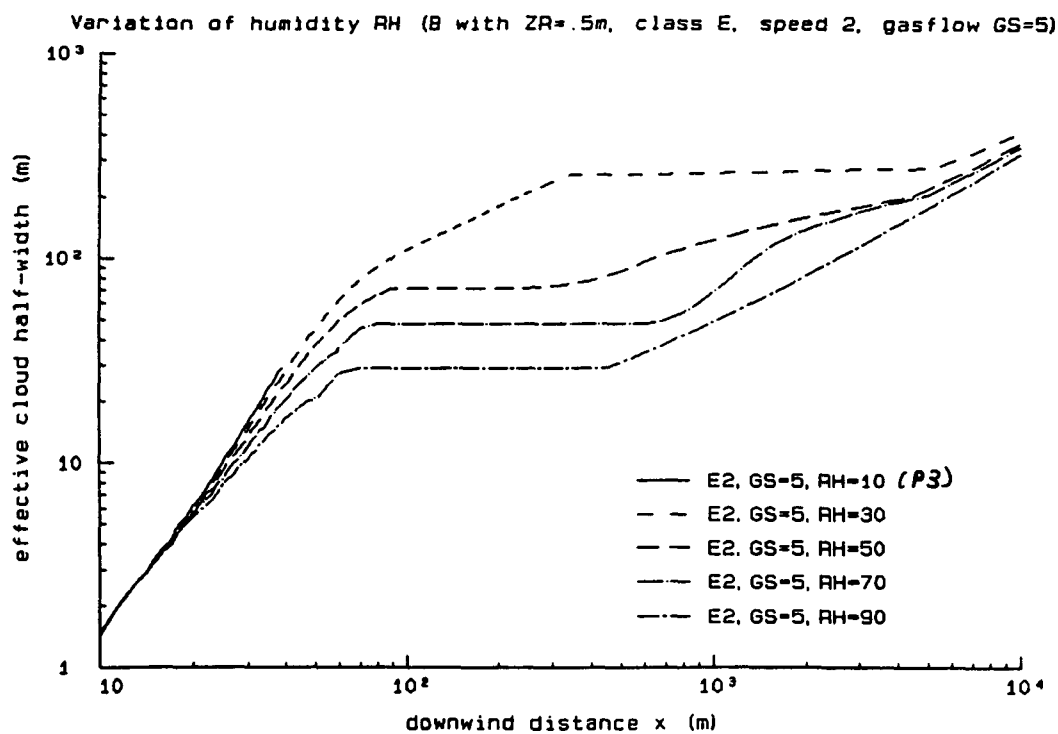


(b)

Fig. 10.24. Effect of relative humidity r_H on HFPLUME/HEGADAS-S concentration predictions; $r_H = 10, 30, 50, 70, 90\%$; urban conditions ($z_R = .5 m$) with horizontal release, stability class D, windspeed 5 m/s and release rate 2.5 kg/s; base case B;
 (a) centre-line concentration (% molar fraction; HFPLUME sectional-mean value and HEGADAS value at ground level)
 (b) effective half-width B_{eff} of cloud

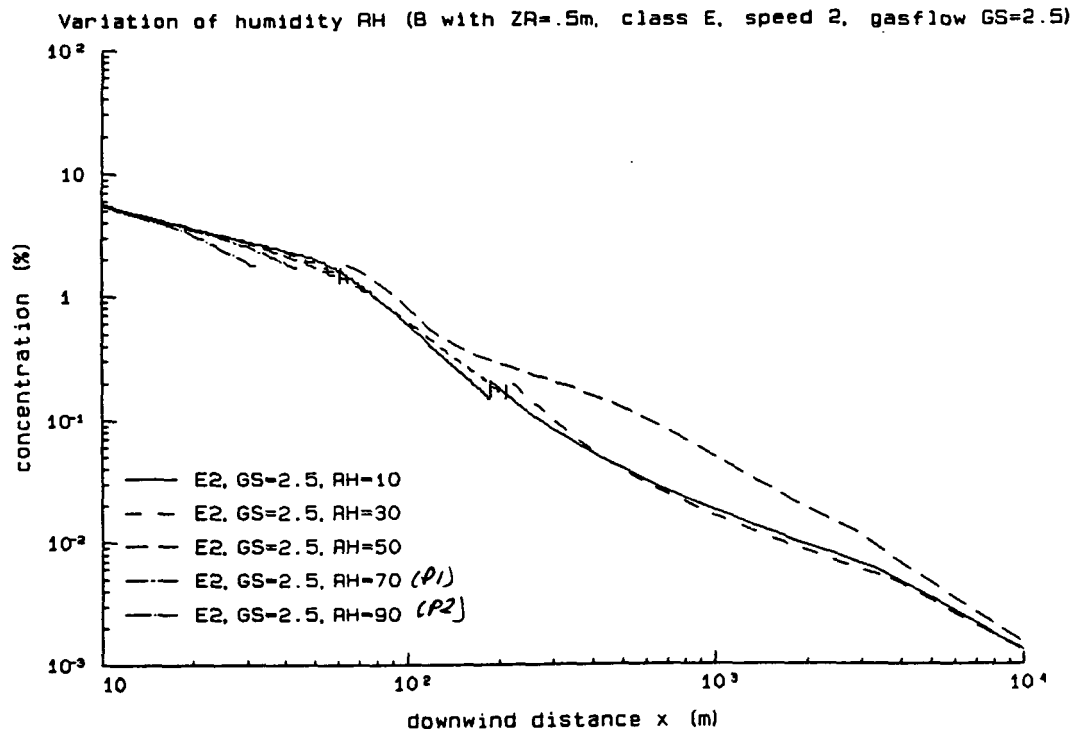


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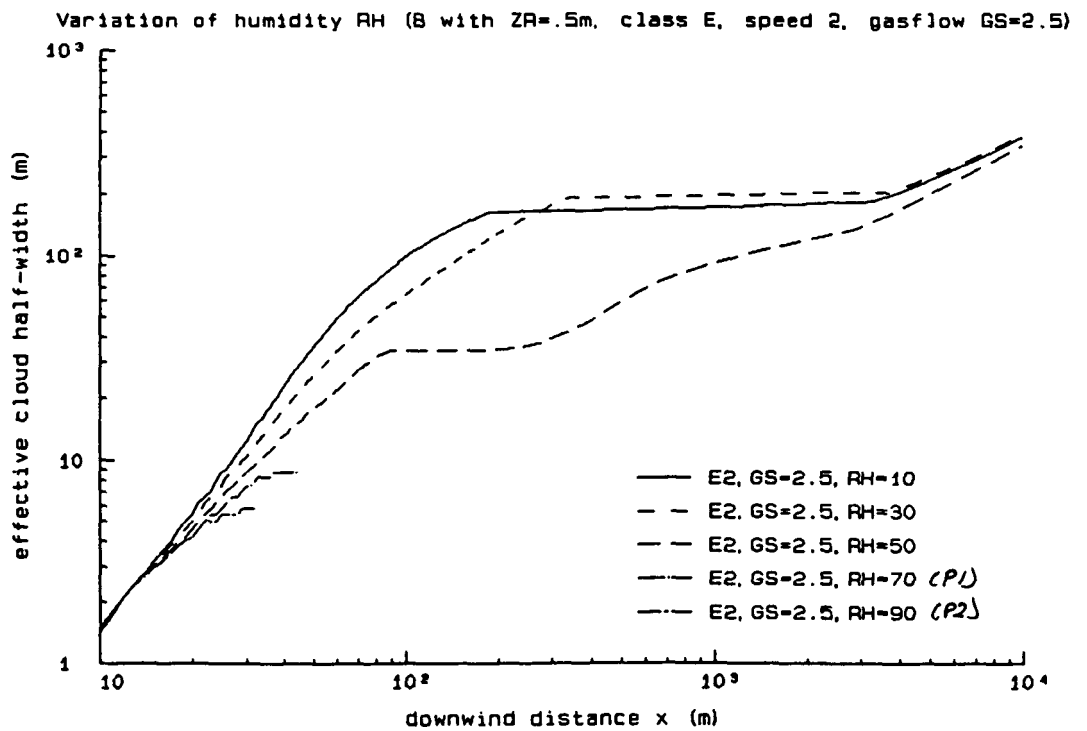


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Fig. 10.25. Effect of relative humidity r_H on HFPLUME/HEGADAS-S concentration predictions; $r_H = 10, 30, 50, 70, 90\%$; urban conditions ($z_R = .5$ m) with horizontal release, stability class E, windspeed 2 m/s and release rate 5 kg/s; base case B;
 (a) centre-line concentration (% molar fraction; HFPLUME sectional-mean value and HEGADAS value at ground level)
 (b) effective half-width B_{eff} of cloud

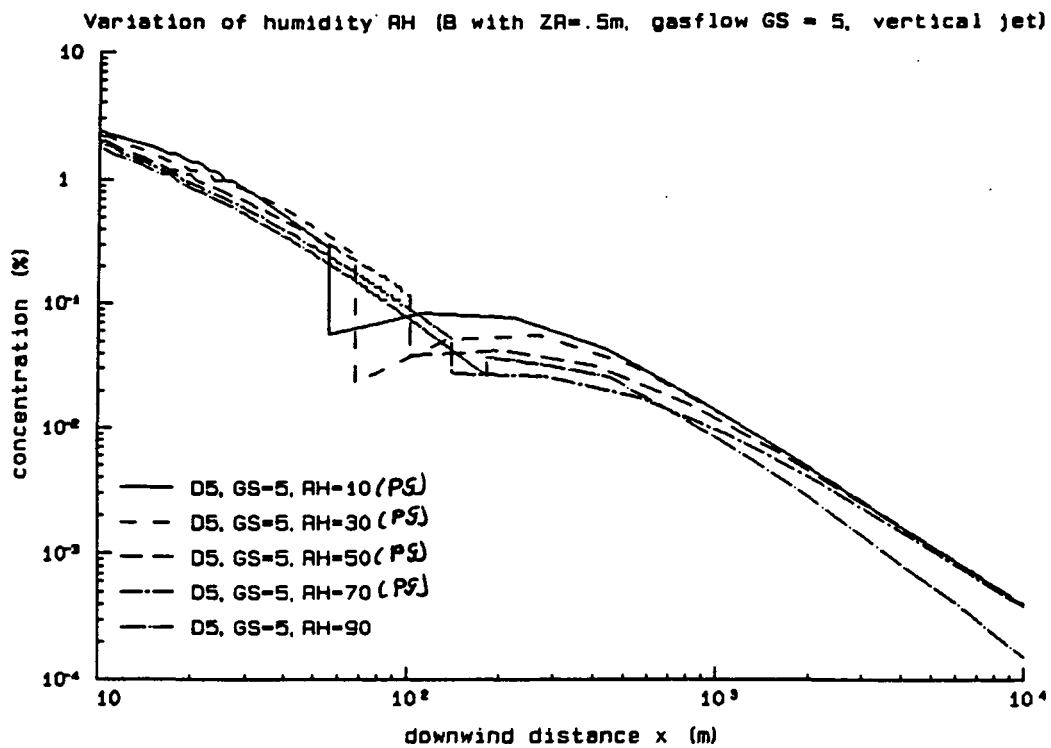


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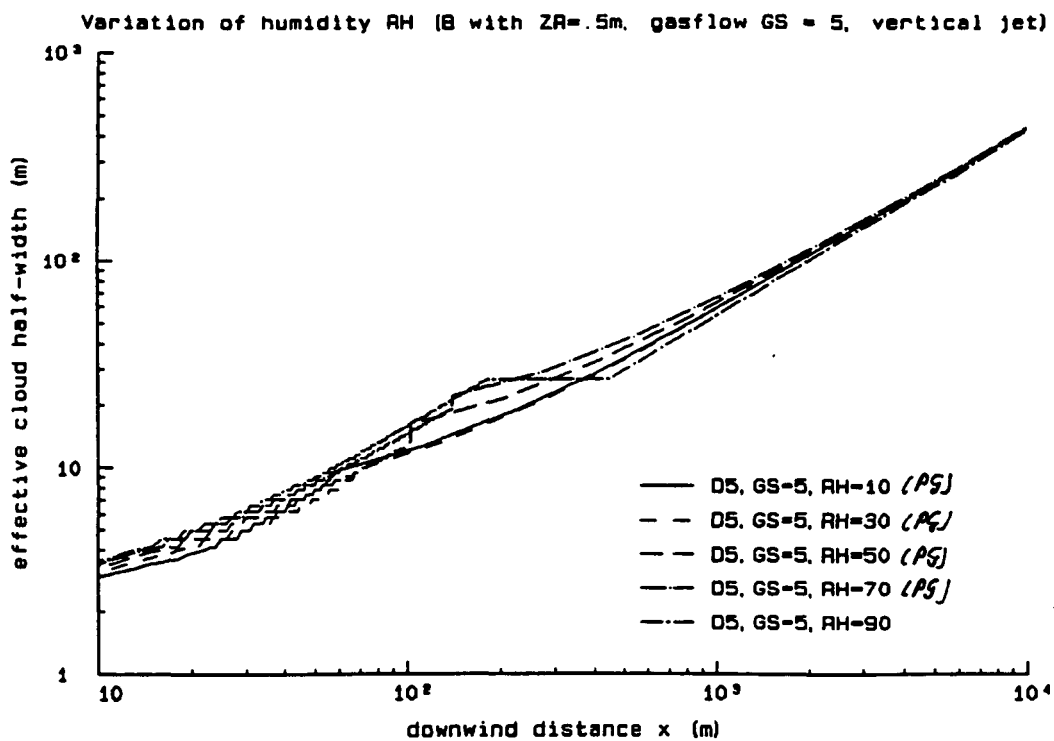


(b)

Fig. 10.26. Effect of relative humidity r_H on HFPLUME/HEGADAS-S concentration predictions; $r_H = 10, 30, 50, 70, 90\%$; urban conditions ($z_R = .5m$) with horizontal release, stability class E, windspeed 2 m/s and release rate 2.5 kg/s; base case B;
 (a) centre-line concentration (% molar fraction; HFPLUME sectional-mean value and HEGADAS value at ground level)
 (b) effective half-width B_{eff} of cloud



(a)

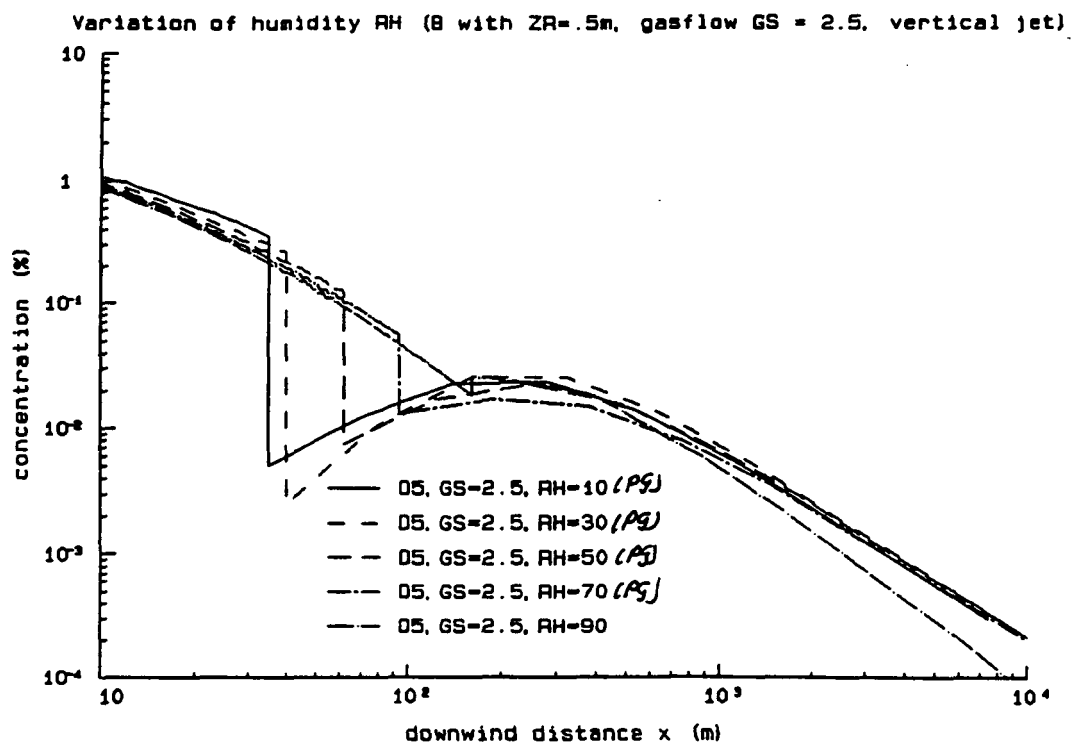


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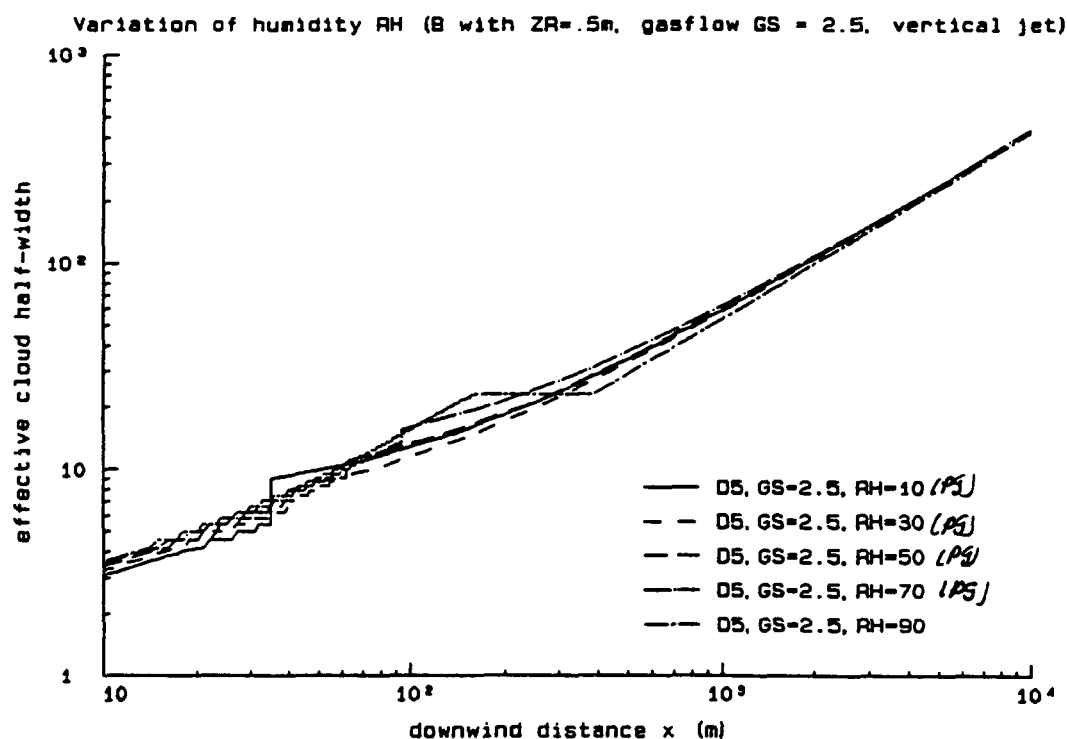
Fig. 10.27. Effect of relative humidity r_H on concentration predictions; urban conditions ($z_R = 0.5$ m) with vertical release at 10 m height, stability class D, windspeed 5 m/s and release rate 5 kg/s; base case B; link from HFPLUME to PGPLUME for $r_H = 10, 30, 50, 70$ % and to HEGADAS-S for $r_H = 90$ %;

(a) centre-line concentration (% molar fraction; HFPLUME sectional-mean value; HEGADAS and PGPLUME values at ground level)

(b) effective half-width B_{eff} of cloud



(a)

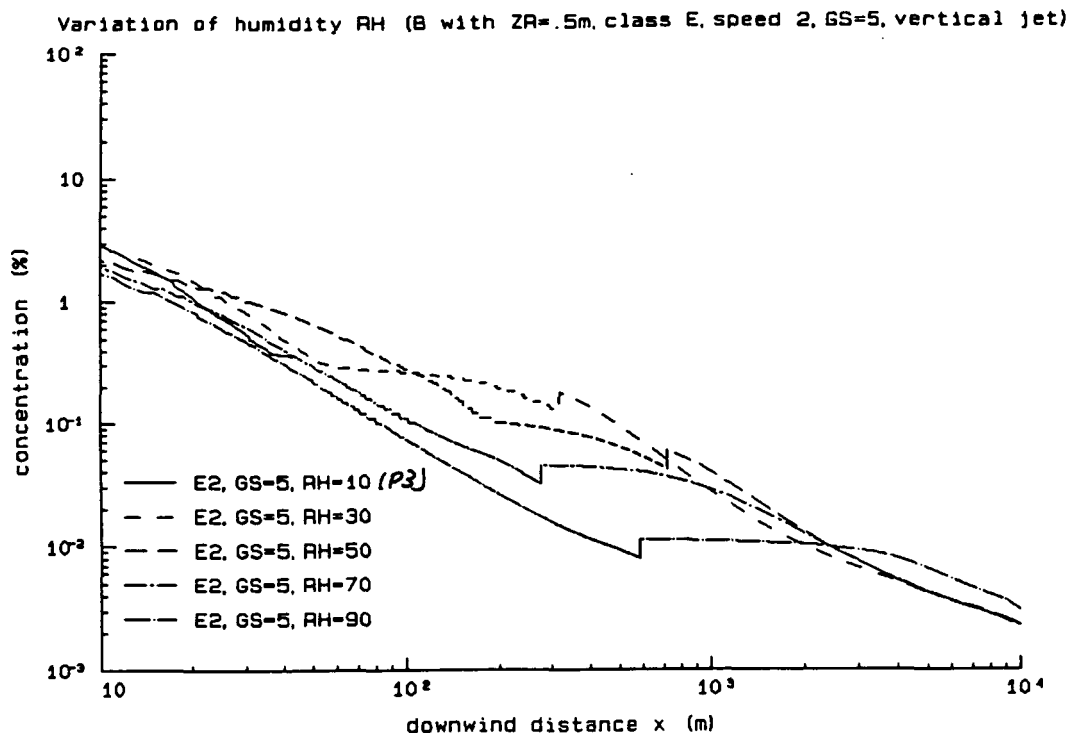


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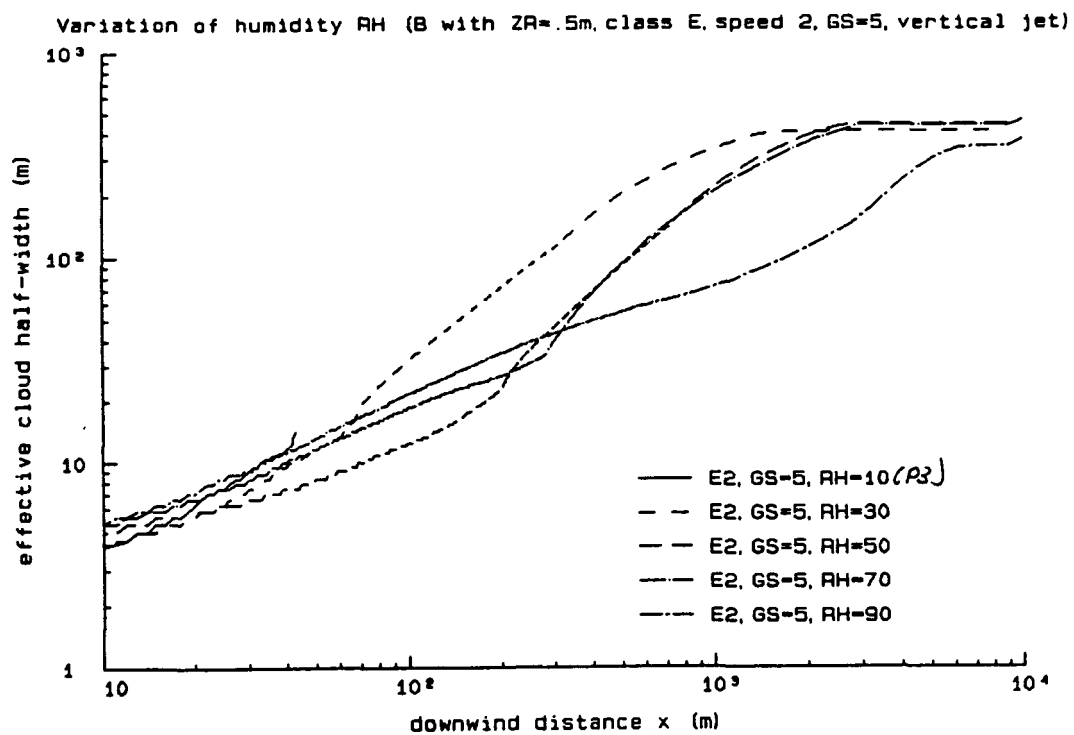
Fig. 10.28. Effect of relative humidity r_H on concentration predictions; urban conditions ($z_R = 0.5$ m) with vertical release at 10 m height, stability class D, windspeed 5 m/s and release rate 2.5 kg/s; base case B; link from HFPLUME to PGPLUME for $r_H = 10, 30, 50, 70$ % and to HEGADAS-S for $r_H = 90$ %;

(a) centre-line concentration (% molar fraction; HFPLUME sectional-mean value; HEGADAS and PGPLUME values at ground level)

(b) effective half-width B_{eff} of cloud



(a)

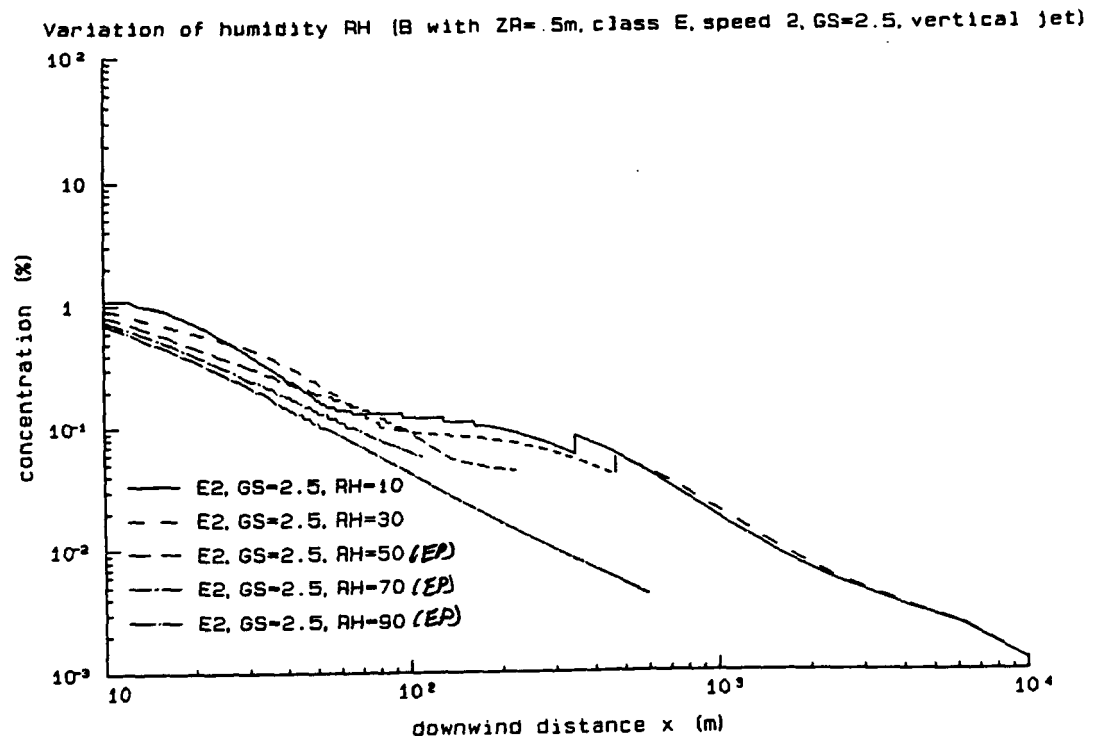


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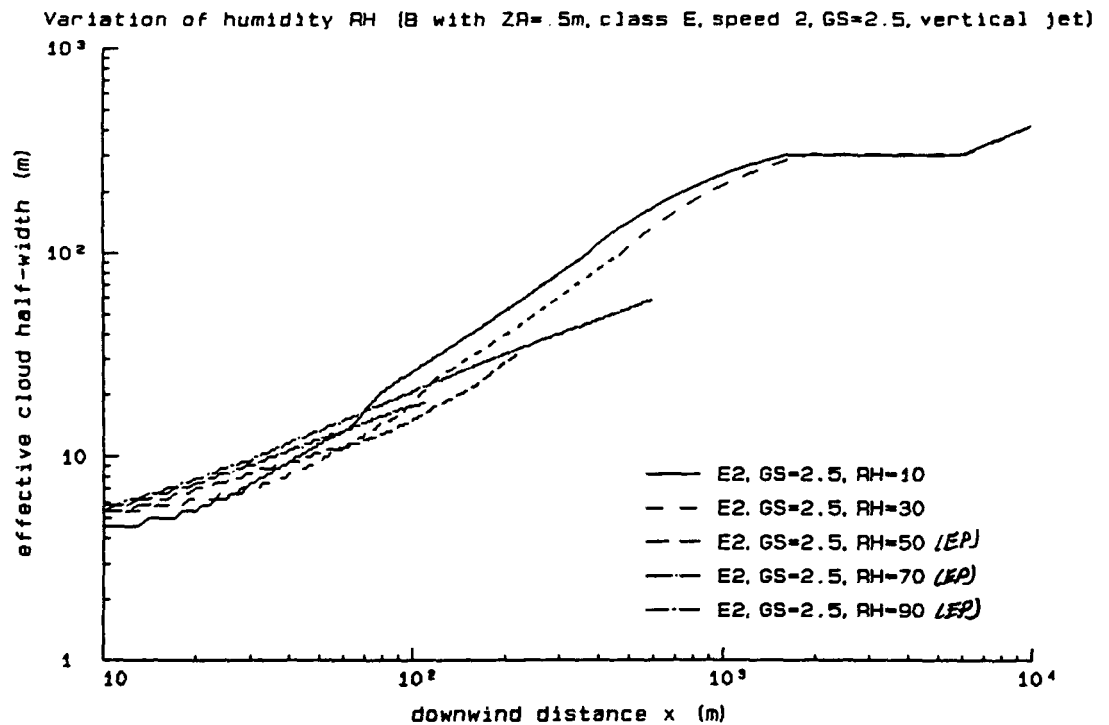
Fig. 10.29. Effect of relative humidity r_H on HFPLUME/HEGADAS-S concentration predictions; $r_H = 10, 30, 50, 70, 90\%$; urban conditions ($z_R = .5$ m) with vertical release at 10 m height, stability class E, windspeed 2 m/s and release rate 5 kg/s; base case B;

(a) centre-line concentration (% molar fraction; HFPLUME sectional-mean value and HEGADAS value at ground level)

(b) effective half-width B_{eff} of cloud



(a)

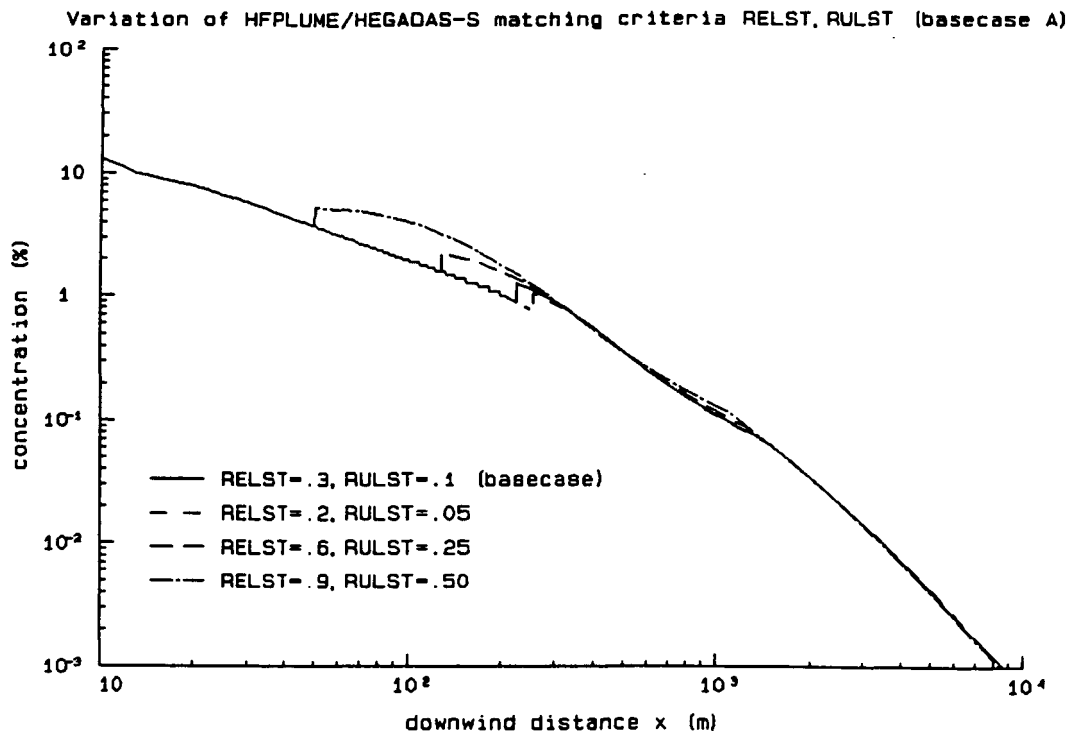


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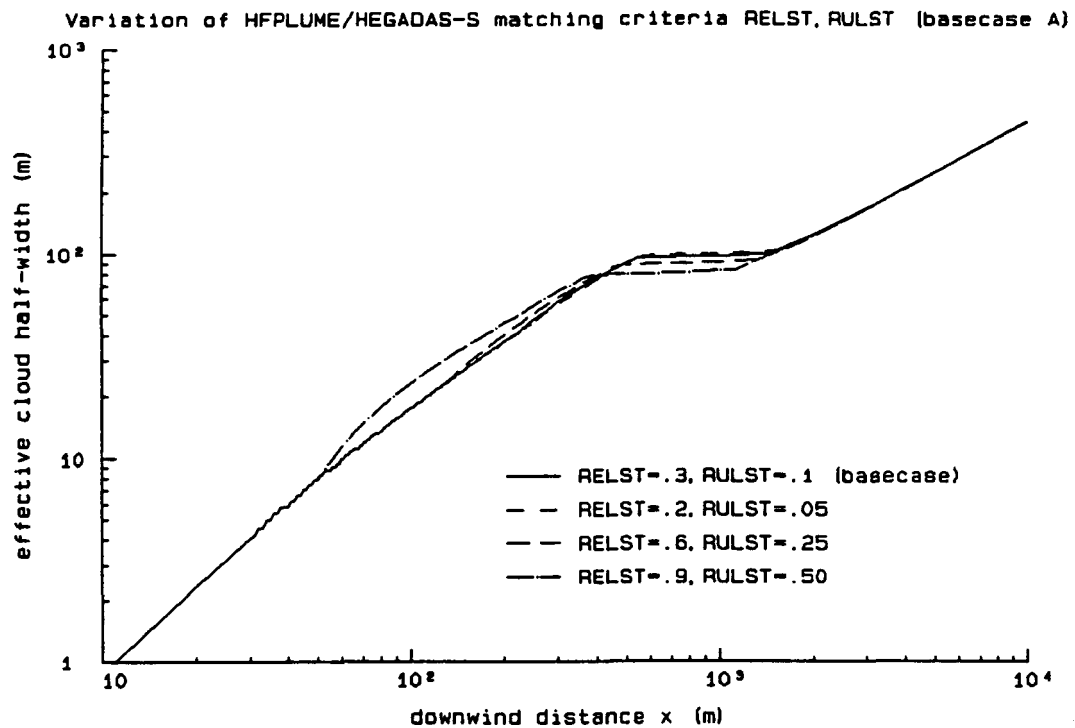
Fig. 10.30. Effect of relative humidity r_H on HFPLUME/HEGADAS-S concentration predictions; $r_H = 10, 30, 50, 70, 90\%$; urban conditions ($z_R = .5 m$) with vertical release at 10 m height, stability class E, windspeed 2 m/s and release rate 2.5 kg/s; base case B;

(a) centre-line concentration (% molar fraction; HFPLUME sectional-mean value and HEGADAS value at ground level)

(b) effective half-width B_{eff} of cloud

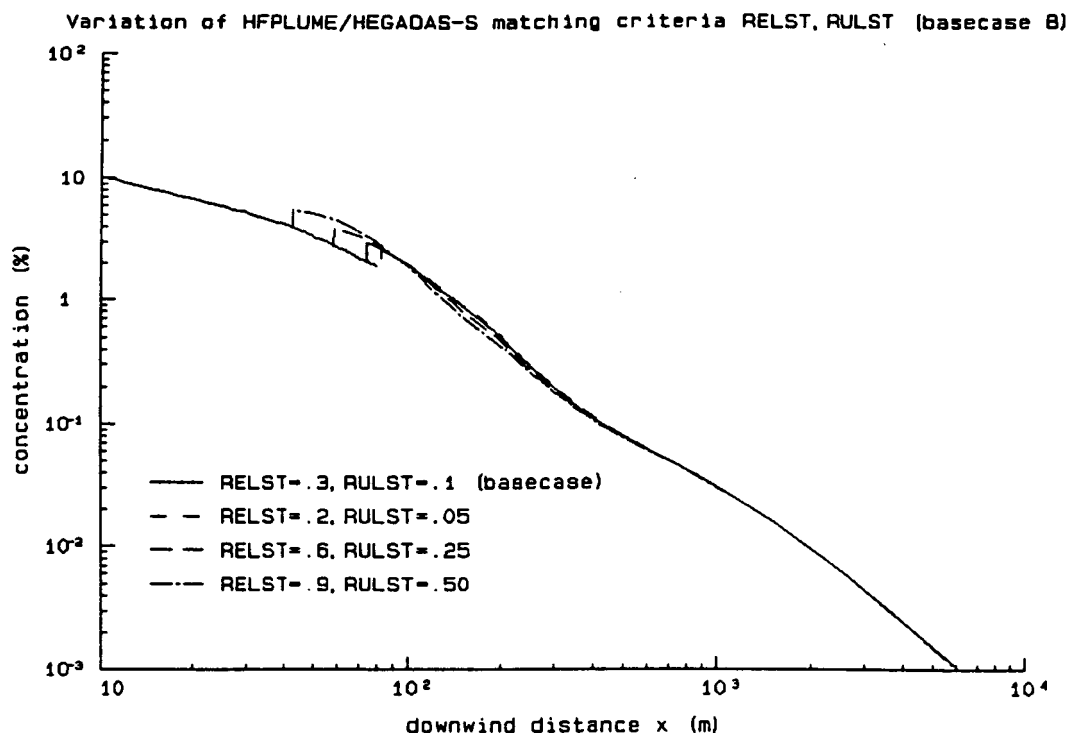


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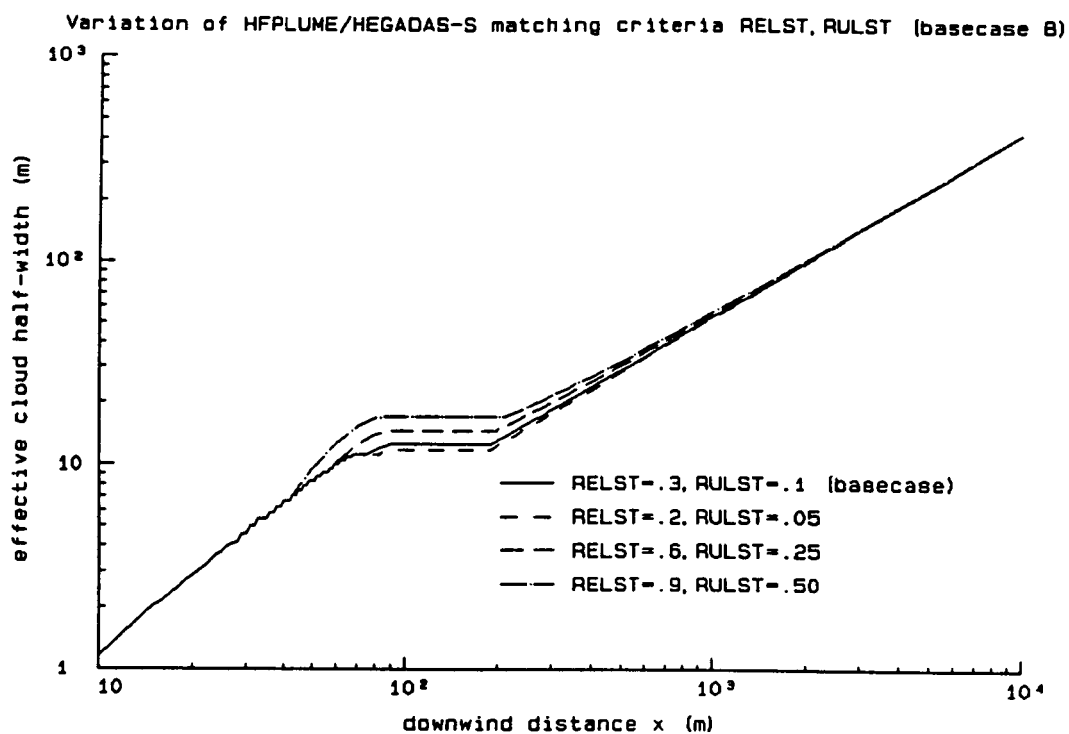


(b)

Fig. 10.31. Effect of variation of HFPLUME/HEGADAS-S transition criteria; HFPLUME/HEGADAS-S transition is made if the proportion of heavy gas entrainment in the total entrainment is larger than $(1-\text{RELST}) \times 100\%$ and the difference in plume speed and ambient speed is less than $\text{RULST} \times 100\%$; recommended and default values are $\text{RULST} = 0.3$, $\text{RELST} = 0.1$; base case A
 (a) centre-line concentration (% molar fraction; HFPLUME sectional-mean value and HEGADAS value at ground level)
 (b) effective half-width B_{eff} of cloud

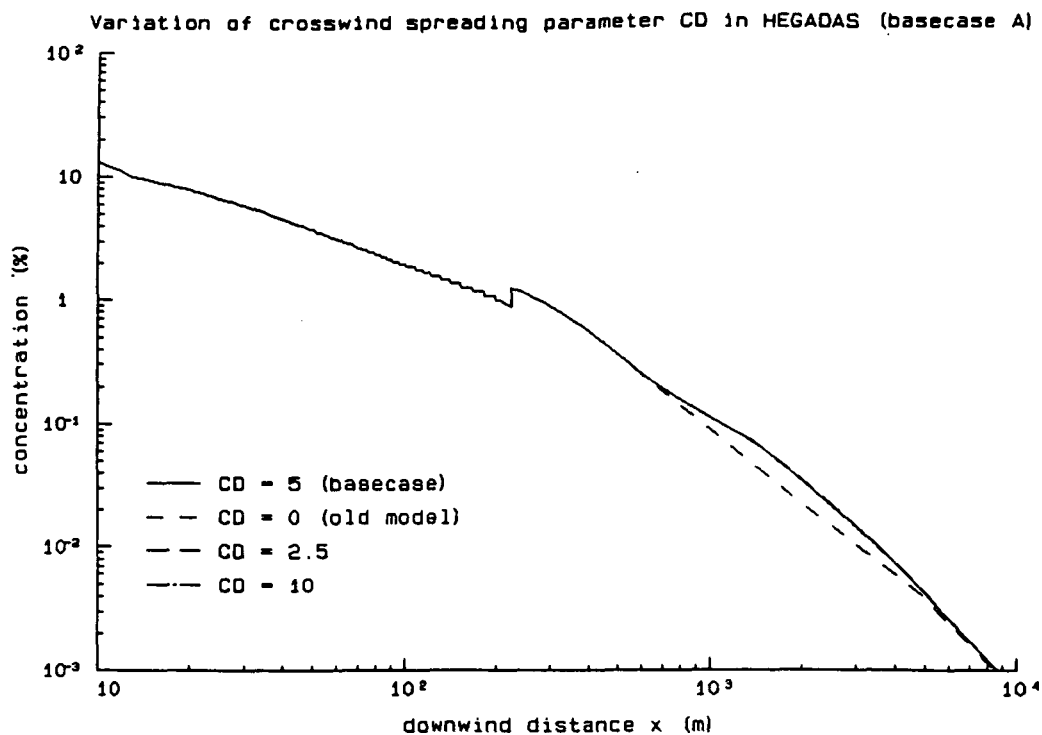


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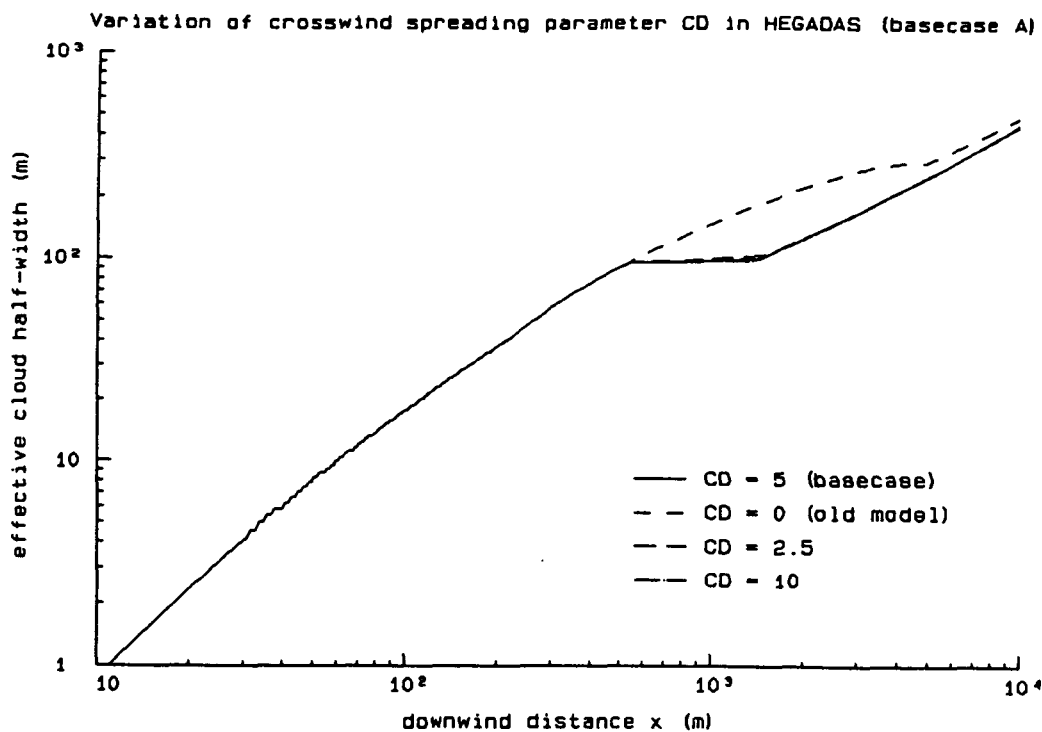


(b)

Fig. 10.32. Effect of variation of HFPLUME/HEGADAS-S transition criteria; HFPLUME/HEGADAS-S transition is made if the proportion of heavy gas entrainment in the total entrainment is larger than $(1-\text{RELST}) \times 100\%$ and the difference in plume speed and ambient speed is less than $\text{RULST} \times 100\%$; recommended and default values are $\text{RULST} = 0.3$, $\text{RELST} = 0.1$; base case B
 (a) centre-line concentration (% molar fraction; HFPLUME sectional-mean value and HEGADAS value at ground level)
 (b) effective half-width B_{eff} of cloud



(a)



(b)

Fig. 10.33. Effect of variation of crosswind spreading parameter CD in HEGADAS (base case A); original HEGADAS-4 formulation (C_E gravity-spreading law without collapse of gravitational spreading) and new HEGADAS-5 formulation (inclusion of effect of collapse; $C_D = 2.5, 5$ (default value) and 10); base case A
 (a) centre-line concentration (% molar fraction; HFPLUME sectional-mean value and HEGADAS value at ground level)
 (b) effective half-width B_{eff} of cloud

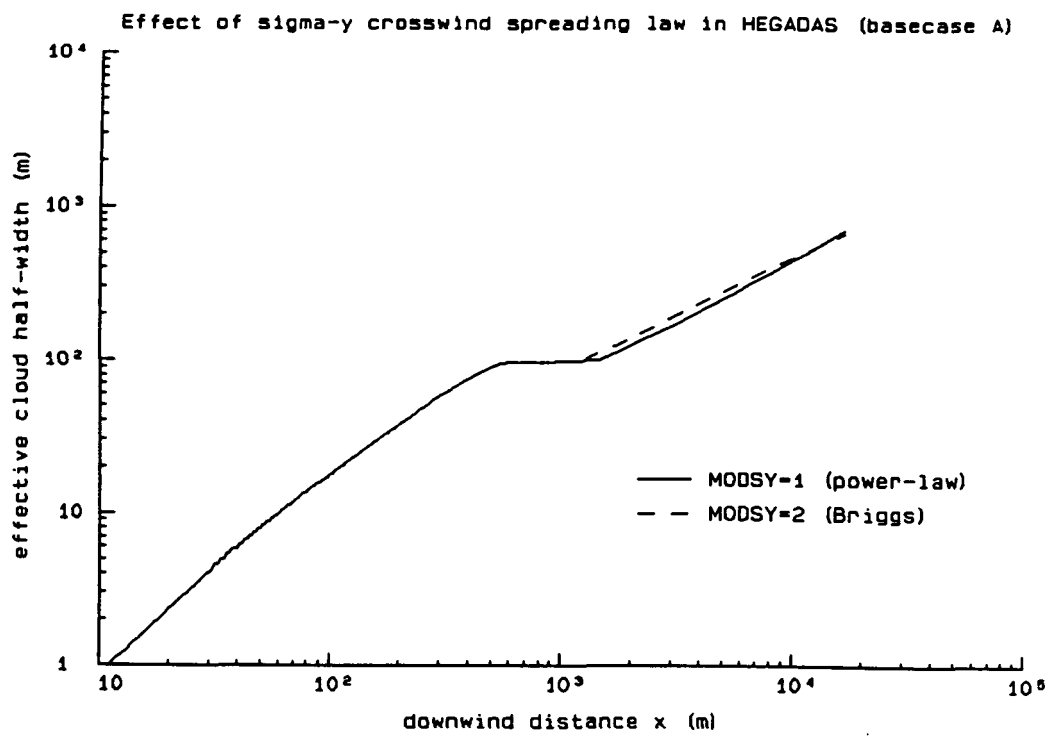
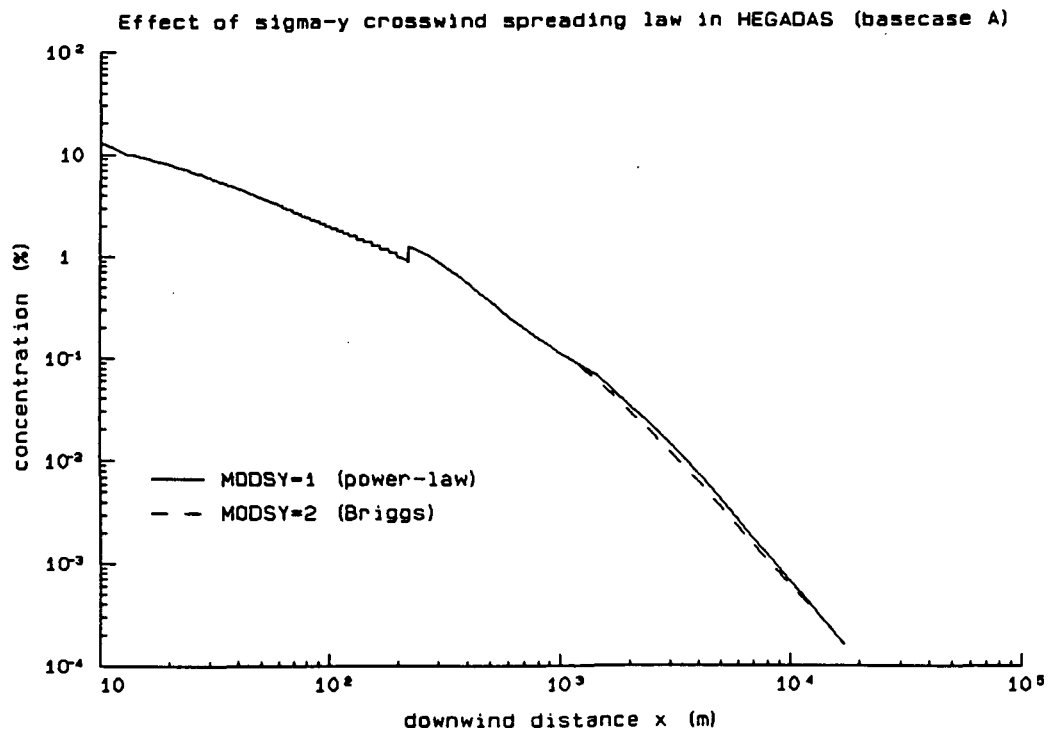
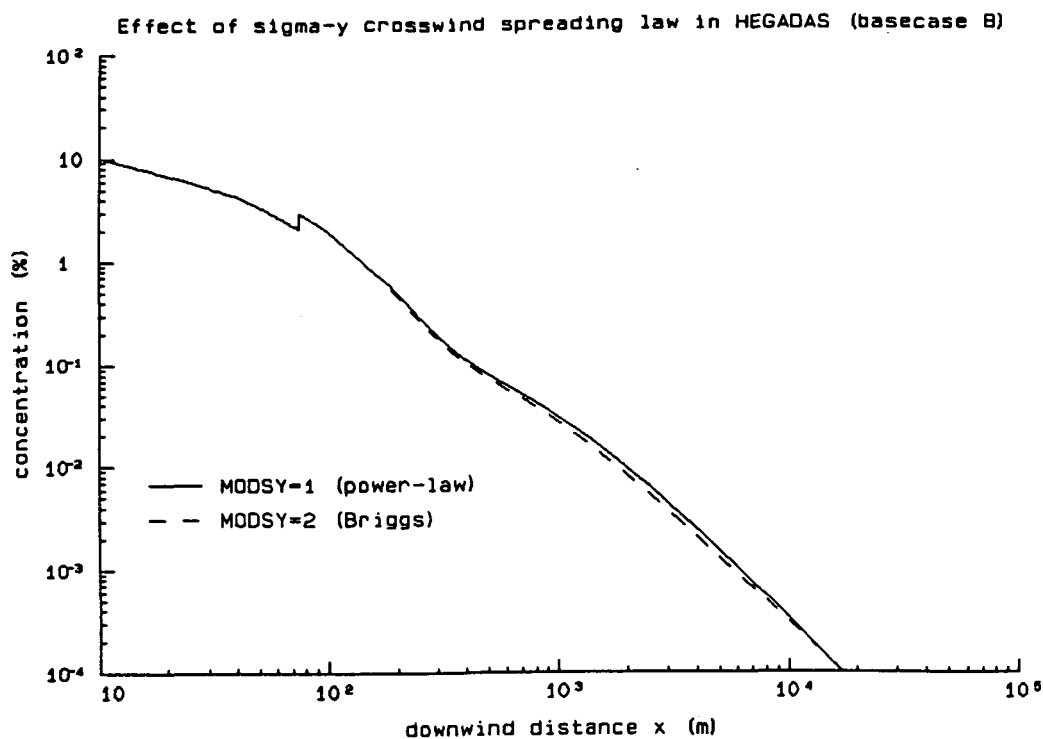
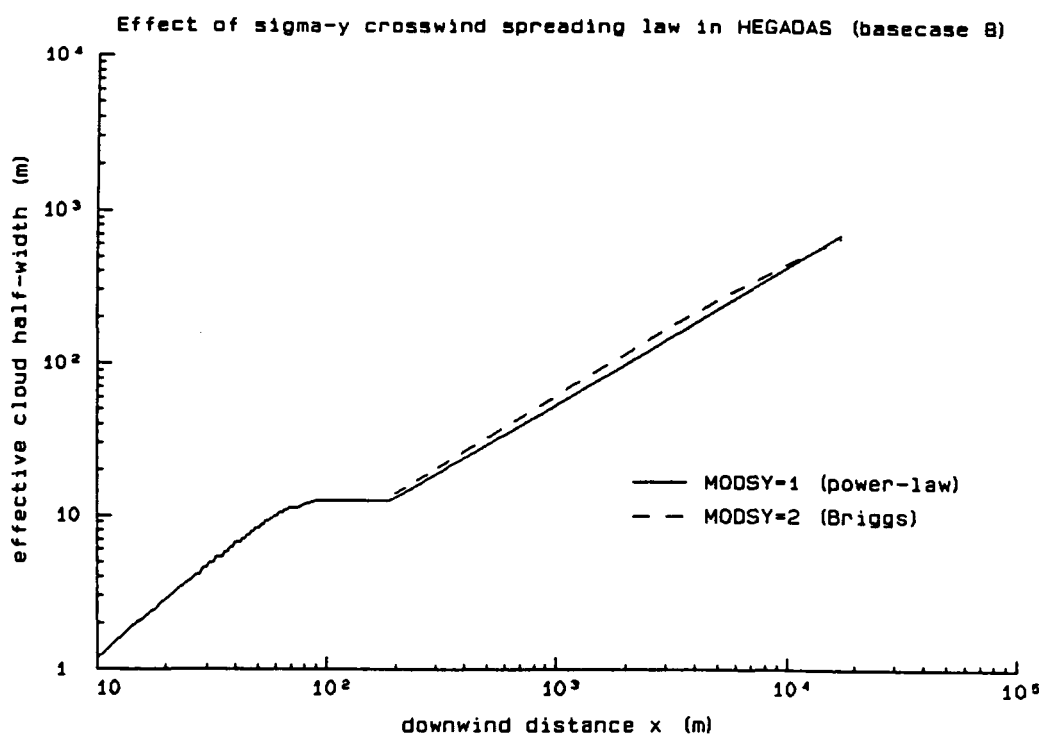


Fig. 10.34 Effect of type of σ_y crosswind spreading law in HEGADAS; MODSY=1 corresponds to the original HEGADAS-4 power-law for σ_y and MODSY=2 to the Briggs law for σ_y (new, default option in HEGADAS-5); base case A

- (a) centre-line concentration (% molar fraction; HFPLUME sectional-mean value and HEGADAS value at ground level)
- (b) effective half-width B_{eff} of cloud



(a)



(b)

Fig. 10.35 Effect of type of σ_y crosswind spreading law in HEGADAS; MODSY-1 corresponds to the original HEGADAS-4 power-law for σ_y and MODSY-2 to the Briggs law for σ_y (new, default option in HEGADAS-5); base case B

(a) centre-line concentration (% molar fraction; HFPLUME sectional-mean value and HEGADAS value at ground level)

(b) effective half-width B_{eff} of cloud

APPENDIX 1

DEVELOPMENT OF MODELS FOR FLASHING TWO-PHASE
JET RELEASES FROM PRESSURISED CONTAINMENT

by

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Paper presented at the ECMI Conference on the Application of
Mathematics in Industry, Strathclyde University, Glasgow,
Scotland, August 1988.

DEVELOPMENT OF MODELS FOR FLASHING TWO-PHASE
JET RELEASES FROM PRESSURISED CONTAINMENT

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§A1.1: Introduction:

Reliable assessment of the hazards associated with accidental releases of flammable or toxic gases is essential for the design and operation of chemical plant and storage facilities. Models are needed to predict the rate of formation and initial physical state of gas clouds (source models) and their subsequent transport and dilution (dispersion models). This paper summarises progress in modelling the accidental release from storage of a pressurized liquid-gas. The model need be no more complex than is required in context, should be of comparable accuracy to subsequent dispersion models, and should possess similar mathematical structure.

Previous work (Ooms 1972, Birch et al. 1984; van den Akker et al. 1983; Botterill et al. 1984; Wheatley 1987a, 1987b; Raj and Morris 1988) on dense and buoyant plumes, pressurized gas jets, and liquid-gas jets, supported the view that predictions accurate in context could be obtained by means of an essentially simple, one-dimensional, sectionally-averaged model.

§A1.2: Jet Development: A Control-Volume Analysis:

We regard the jet and ambient atmosphere as a single fluid (of variable composition) occupying the upper half-plane above a horizontal ground surface. The jet and ambient merge infinitesimally so that no jet "boundary" exists at finite distance from the jet-axis; entrainment occurs therefore "at infinity". The release and early jet development is presumed essentially horizontal, aligned with the ambient (horizontal) wind. No slip occurs amongst the constituent phases of the developing jet. Mean-flow within both ambient and jet is everywhere steady.

We begin by introducing a set of control-volumes $\tau(x)$, $x>0$, an analysis of which results in an integral-averaged description of jet development independent of detailed assumptions regarding induced and ambient turbulence.

The Control-Volume $\tau(x)$: First construct a vertical surface at such distance upwind of the release point that ambient flow is negligibly perturbed. Second, at arbitrary distance $x>0$ downwind of the release-point, construct a vertical "cross-section" $\Sigma(x)$ through the developing jet. Third link these (semi-infinite) planes by skirting the ground and pipework surfaces and passing through the jet at the plane of release. Finally construct a fourth bounding surface Σ_{∞} at great (notionally infinite) distance from the jet-axis such as to enclose the (infinite) volume $\tau(x)$. [See Figure A1.]

Integration of the basic equations of motion over such a control-volume results, given an assumed "thin" jet (Hinze 1959), in the integral forms:

$$\begin{aligned} \iint_{\Sigma} c u_{\infty} dA &= (c_{\square} / \rho_{\square}) dm/dt|_{\square} \\ \iint_{\Sigma} (\rho u - \rho_{\infty} u_{\infty})_{\square} dA &= dm/dt|_{\square} [1 - (\rho_{\infty} u_{\infty}) / (\rho_{\square} u_{\square})] - \iint_{\Sigma_{\infty}} \rho u_{\square} dA; \\ \iint_{\Sigma} [\rho u (u_x - u_{\infty}) + (p - p_{\infty}) e_x]_{\square} dA &= (u_x^{\square} - u_{\infty}^{\square}) dm/dt|_{\square} + (p_{\square} - p_{\infty}) A_{\square}; \\ \iint_{\Sigma} [\rho u (h + (1/2) u^2 - h_{\infty} - (1/2) u_{\infty}^2)]_{\square} dA &= (h_{\square} + (1/2) u_{\square}^2 - h_{\infty}^{\square} - (1/2) u_{\infty}^{\square 2}) dm/dt|_{\square}. \end{aligned}$$

[Notation: $dm/dt|_{\square}$, mass flow rate issuing from the release point (ρ, c, u, p, h), density, pollutant mass-concentration, velocity, absolute pressure, and specific enthalpy of the ensemble-averaged flow. The affix " $\square$ ", identifies conditions at the release-plane; the suffix " ∞ " conditions within the unperturbed atmosphere.

]

These equations express in integral form conservation of pollutant mass-flux, air entrainment, and excess above ambient of (horizontal) momentum and energy. They enable "matching" of conditions at the release orifice to conditions immediately following the external "flash".

§A1.3: Sectionally Averaged Jet Motion:

The above integral equations may be further simplified in the zone of approximately self-similar or established flow in order to provide a "top-hat" or sectionally averaged description of jet development. We replace the detailed but unknown variation within each "cross-section" of the jet velocity and density by a single value representative of the entire cross-section; and assign to the jet a notional "jet-width" beyond which the conditions revert to ambient. Substitution then yields a "top-hat" description comprising a single entrainment relationship in the form of a quadrature, together with the three first integrals:

$$\begin{aligned} d/dx[\pi/4D^2(\rho u - \rho_\infty u_\infty)] &= \text{Entr}_{\text{shear}}(D, u, \rho, c) ; \\ dm/dt|_{\square} &= \pi/4D^2 \rho u ; \text{Entr}_{\text{shear}} = d/dx \iint_{\Sigma_\infty} \rho_\infty u_\bullet dA ; \\ [u - u_\infty] / [u_\square - u_\infty + (p_\square - p_\infty) / \rho_\square / u_\square] &= (c/\rho) / (c_\square / \rho_\square) ; \\ (h + (1/2)u^2 - h_\infty - (1/2)u_\infty^2) / (h_\square + (1/2)u_\square^2 - h_\infty - (1/2)u_\infty^2) &= (c/\rho) / (c_\square / \rho_\square) . \end{aligned}$$

[Notation: D jet diameter, ρ section-mean density, c section-mean pollutant mass-concentration, u section-mean velocity, $dm/dt|_{\square}$ release mass flow-rate.]

These equations are closed by specifying the entrainment function $\text{Entr}_{\text{shear}}$. The jet pressure is essentially ambient throughout the developed region. Local thermodynamic equilibrium is assumed. This description of the development of a liquified gas jet is of limited scope: it enables a broad description of liquid

evaporation, temperature fall and recovery, and the reduction in flow-speed that accompanies air entrainment.

§A1.4: The Jet Cross-Section; Relationship to the "top-Hat" Description:

No information regarding the cross-sectional variation of such key parameters as contaminant concentration or jet temperature is provided, at any rate directly, by the simple "top-hat" description of jet development. However, the known point-local thermodynamic behaviour may be combined with empirically determined "self-similarity" profiles in order to deduce the sectional variation in, say, temperature consistent with the integral-averaged fluxes of released liquid-gas, momentum-excess, entrained air, and total-energy.

Introduce similarity profiles within the zone of established flow of the general form;

$$c/c_* = \phi_c(y/D_*, z/D_*; D_*; \chi^2); (u-u_\infty)/(u_*-u_\infty) = \phi_u(y/D_*, z/D_*; D_*);$$

in which $c_*(x)$ and $u_*(x)$ are the section-local and centre-line values of contaminant mass-concentration and flow-speed within the jet, $D_*(x)$ a representative "jet-width", and in which finally χ^2 is the turbulent Schmidt number measuring the relative diffusivities within the jet of momentum and concentration; ϕ_u and ϕ_c are universal functions independent of the downwind displacement $x > 0$.

Consistency then requires that the several physically meaningful fluxes be invariable amongst "top-hat" and each "cross-sectional" description; it results in the linking of jet "centre-line" (c_*, u_*, D_*) and "sectional-mean" (c, u, D) variables via the non-linear integral equations:

$$\begin{aligned} \iint_{\Sigma(x)} cu \, d\Sigma &= \pi/4D^2 cu; \\ \iint_{\Sigma(x)} (\rho u - \rho_{\infty} u_{\infty}) \, d\Sigma &= \pi/4D^2 (\rho u - \rho_{\infty} u_{\infty}); \\ \iint_{\Sigma(x)} \rho u(u - u_{\infty}) \, d\Sigma &= \pi/4D^2 \rho u(u - u_{\infty}). \end{aligned}$$

The notation is that the symbols of the integrands refer to turbulent-mean point-values within the chosen cross-section $\Sigma(x)$. The identical symbols of the right-hand sides refer to sectionally averaged values resulting from a "top-hat" model evaluation.

§A1.5: Jet Asymptotics; "Top-Hat" and "Gaussian" Descriptions:

It remains to determine an appropriate form for the "top-hat" entrainment function and for the self similarity functions that describe established (self-similar) flow. In the far-field the profile shapes and entrainment law are well established: profile shapes are (neglect ground effects) broadly Gaussian (List 1982, Abramovich 1963), so that

$$\phi_u(r/D_*) = \exp(-4r^2/D_*^2); \quad \phi_c(r/D_*) = \exp(-4r^2/\gamma^2/D_*^2); \quad 0 \leq r < \infty;$$

r being the radial displacement "off-axis" in the plane of the cross-section $\Sigma(x)$. It follows from the consistency equations that "top-hat" and "centre-line Gaussian" parameters are asymptotically related via the explicit forms (Compare Henderson-Sellers 1981, Davidson 1986).

$$\begin{aligned} (T_* - T_{\infty})/(T - T_{\infty}) &= (\rho_* - \rho_{\infty})/(\rho - \rho_{\infty}) = c_*/c = 2/\gamma^2; \\ (u_* - u_{\infty})/(u - u_{\infty}) &= (D/D_*)^2 = 2; \quad u_{\infty} \neq 0; \end{aligned}$$

results deduced for a trace (ideal) gas contaminant in possibly humid but not saturated air. Following temperature recovery therefore jet centre-line concentrations are deduced for much diluted jets by a simple scaling applied to the associated "top-hat" results: solution of a set of non-linear integral equations for the centre-line values is not required.

§A1.6: Jet Development: The "Top-Hat" Entrainment Function:

We return to the "classical" theory of jets and the theoretical analysis of Albertson (1948), Hinze (1959), or Abramovich (1963), all of which suggest that a simple "mixing-length" closure of the kinetic energy equation might provide an acceptable entrainment relationship. Consider the kinetic-energy equation when integrated over the standard control volume $\tau(x)$:

$$d/dx \iint_{\Sigma} \rho u ((1/2)u^2 - (1/2)u_{\infty}^2) d\Sigma = \iint_{\Sigma(x)} \Sigma_{xr}^{trb} \partial u / \partial r d\Sigma.$$

Σ_{rx}^{trb} is a Reynolds' stress. The Prandtl closure for neutrally buoyant jets has the simple form (Hinze 1959)

$$\Sigma_{xr}^{trb} = -\mu^2 \rho_{\infty} D_*^2 |\partial u / \partial r| \partial u / \partial r;$$

in which μ^2 is a constant. Presumption of a Gaussian form for the velocity profile and the auxiliary condition $\rho = \rho_{\infty}$ yields an entrainment function:

$$\text{Entr}_{\text{shear}} = 6\mu^2 \rho_{\infty} D_* (u_* - u_{\infty})^3 / u_* (u_* + 2u_{\infty}).$$

The equivalent "top-hat" representation is, in the far-field, simply

$$\text{Entr}_{\text{shear}} = e\pi\rho_{\infty}D(u-u_{\infty})^3/(u+(1/2)u_{\infty})/(u-(1/2)u_{\infty}); \mu^2 = 3e/\sqrt{\pi}.$$

The entrainment coefficient e has for the (neutral) far-field the well established value $e = 0.08$ (Morton, Taylor, Turner 1956, Ooms 1972, Petersen 1978, 1987).

Consider next the influence of density upon the "top-hat" entrainment function. Evidence indicates that the influence of (positive) density differences between gas jet and ambient is somewhat to reduce the degree of entrainment that would otherwise occur (Yoshinobu and Saima 1977, Resplandy 1969), and certainly this seems intuitively satisfactory, though at variance with the marginally dense jet results of Ricou and Spalding (1961), in which a slight increase in entrainment above neutral buoyancy was recorded. We assume that the effect of density differences upon the dominant Reynolds' stress is described by a multiplicative factor of the general form

$$\Sigma_{xr}^{\text{trb}} = -\rho\psi(\rho/\rho_{\infty})\mu^2D_{\star}^2|\partial u/\partial r|\partial u/\partial r; \psi(\rho/\rho_{\infty}) \rightarrow 1 \text{ as } \rho/\rho_{\infty} \rightarrow 1.$$

Consider further the asymptotic behaviour of the "Gaussian"-jet entrainment function under the assumption that velocity differences between jet and ambient wind are large. Reduction in entrainment with increasing density occurs only if the leading order expression of the densimetric correction to the dominant Reynolds' stress has the form $\psi(\rho/\rho_{\infty}) = \rho_{\infty}/\rho$. It follows that the (Gaussian) entrainment function has the asymptotic form

$$\begin{aligned} \text{Entr}_{\text{shear}} &= (1/\sqrt{2})e\pi D_{\star}u_{\star}\eta(\rho_{\star}/\rho_{\infty}); \Delta\rho_{\star} = \rho_{\star} - \rho_{\infty}; u_{\star}/u_{\infty}, \rho_{\star}/\rho_{\infty} \gg 1; \\ \eta(\rho_{\star}/\rho_{\infty}) &= [1 + 2\chi^2/(2\chi^2 + 1)\Delta\rho_{\star}/\rho_{\infty}]/[1 + 2\chi^2(3\chi^2 + 2)/(2\chi^2 + 1)/(3\chi^2 + 1)\Delta\rho_{\star}/\rho_{\infty}]; \end{aligned}$$

valid for isothermal gas jets (contaminant concentration proportional to the density difference between jet and ambient air). Further simplification requires

a value for the turbulent Schmidt number which in the far field is approximately 1.35 (Rouse, Yih, and Hyumphreys 1952) but which in the dense jet has a value near unity (Birch and Brown 1987). Setting therefore $\gamma^2=1$ we propose an equivalent "top-hat" entrainment function of the form

$$\text{Entr}_{\text{shear}} = \epsilon \pi D n (\rho/\rho_\infty) (u-u_\infty)^3 / (u+(1/2)u_\infty) / (u-(1/2)u_\infty); u > u_\infty;$$

$$n(\rho/\rho_\infty) = [1+4/3(\rho/\rho_\infty-1)] / [1+5/3(\rho/\rho_\infty-1)].$$

§A1.7: Jet Development: Theory versus Experiment:

We compare the above developed "top-hat" model with a programme of large-scale, pressurized, liquid-propane releases conducted jointly by Shell Research Ltd and by BP Research International (Cowley and Tam 1988). The experimental site was the (former) BP refinery at the Isle of Grain. We consider a subset (Table A1.1) of the eighty-four trials comprising steady, unignited, wind-aligned, "full-bore" (full pipe diameter) releases of liquid propane. These trials involved the discharge of tonne quantities of liquid propane via a 50mm diameter 100m long pipe placed parallel to and 1m above levelled ground. The data here summarised is this author's interpretation of very extensive, "instantaneous", sensor data: it is recognised that differing instrumental averaging times may affect somewhat the details of concentration/temperature correlations.

Considerable flashing was evident within the release pipe, with two-phase choked flow at the orifice. The steady release-rate and release (orifice) pressure were experimentally determined. Release-plane void-fraction is calculated upon the basis of assumed thermodynamic equilibrium and negligible inter-phase slip: temperatures recorded at the orifice are broadly consistent

with thermodynamic equilibrium at the choke-front. Energy losses within the release pipe due either to heat transfer to atmosphere or to wall friction are assumed negligible. Validation is little affected by uncertainties in the prediction of two-phase choked flow within pipes (van den Akker and Bond 1984).

Consider first the assumption of thermodynamic equilibrium (van den Akker, Spoelstra, and Snoey 1983). Figure A1.2 illustrates the degree of departure between local thermodynamic equilibrium and a set of (instantaneous) pairs of propane concentration and temperature measurements conducted both on- and off-axis at distances of 9 and 14 metres downwind of the release plane. Generally good agreement exists between the theoretical prediction of an essentially linear relationship between volumetric concentration (%) and temperature (C), and the mean trend of the experimental results. A large degree of scatter is however evident.

Consider next the performance of the "top-hat" entrainment function in reproducing the down-wind variation of temperature, and "volumetric" concentration of propane. The chosen value of γ^2 was precisely unity. Figures A1.3 through A1.8 illustrate the degree of agreement between theory and momentary point-local values plotted as a function of downwind distance and distance off-axis. As can be seen the general agreement between the simple "top-hat" model and data is reasonable as regards jet "width" and mean "subcooling" below ambient; whereas (clearly) the detailed prediction of centre-line concentration or temperature, or the displacement off-axis of (say) the flammability limits is beyond the model scope, there being generally large differences between sectional-mean and centre-line values of either temperature or concentration. Note, however, the sensitivity of predictions at distance off-axis to fluctuations in the ambient wind-direction (resulting in greater scatter and inaccuracy at the jet "edge").

Finally contrast the predictions of the point-local concentration and temperature profiles deduced from the sectionally averaged values given assumed Gaussian velocity and (mass) concentration profiles with the experimental data of Figures A1.3 through A1.8 ($\chi^2 = 1.35$). Generally the centre-line variation is well captured, though some systematic underprediction of values significantly off-axis is evident.

§A1.8: Conclusions:

A simple but effective model has been developed describing the steady release to coflowing ambient of a pressurised liquid-gas. Several features of the analysis appear new or at least new in this context: in particular the derivation of shear entrainment function for a neutrally buoyant jet via (Prandtl) "mixing-length" closure of the kinetic-energy equation; and the associated derivation and functional form of the densimetric correction $\eta(\rho/\rho_\infty)$ (§A1.6). Focus upon shear entrainment permits (§A1.6) the derivation of point-local from sectional-mean predictions given only self-similarity and an assumed "profile" form, and in addition allows the straightforward analysis of jet "asymptotics" (§A1.5). The model structure allows successive estimation of "sectional-mean" or "top-hat" properties and of point-local predictions conditional upon an assumed self-similar "profile" form; and has merit in permitting step-by-step tuning to experimental data.

Novel experimental data on the large-scale release of liquidified propane have been presented. These show good agreement with theoretical prediction.

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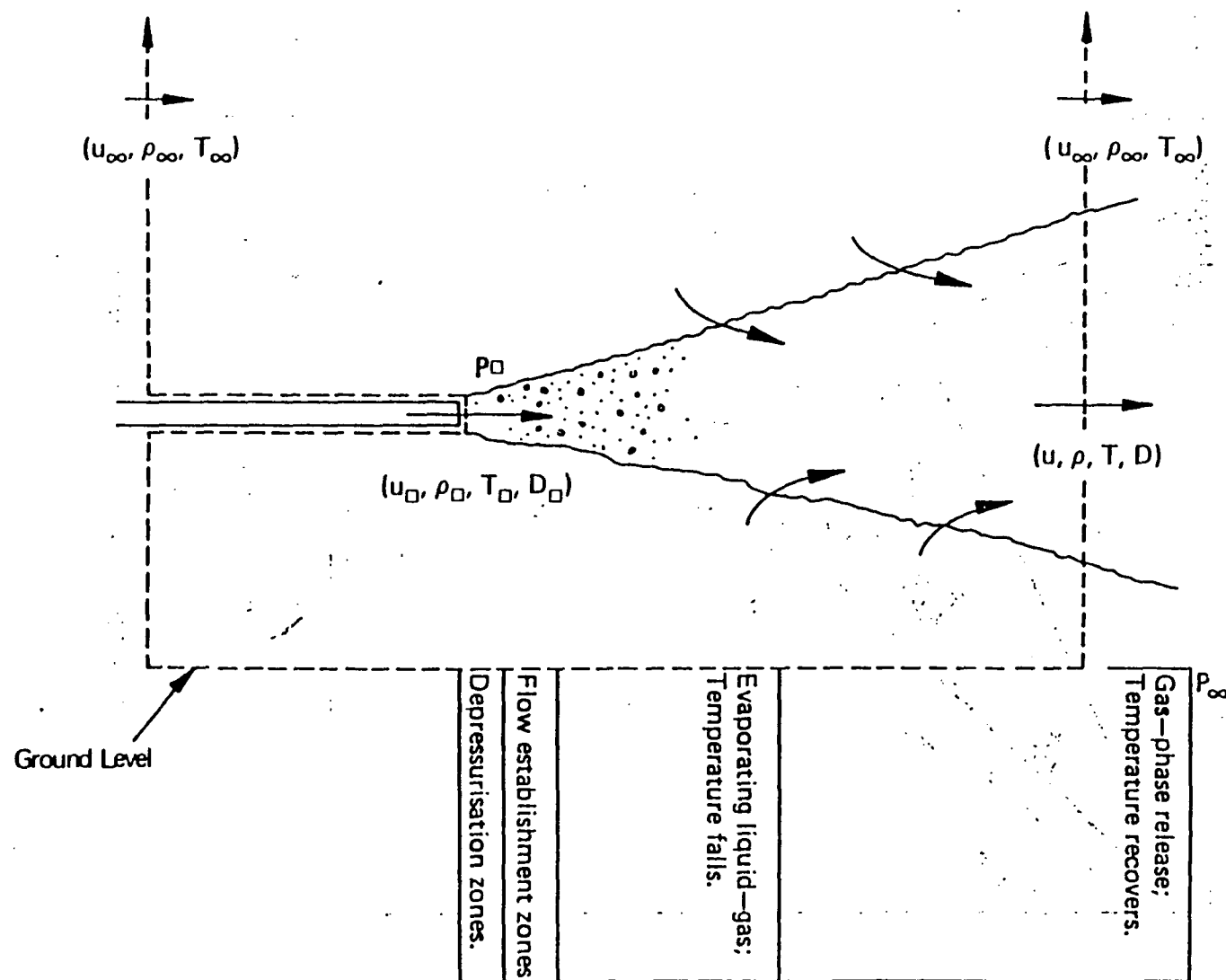


FIG A1.1 Jet release: cross-section through a typical control volume.

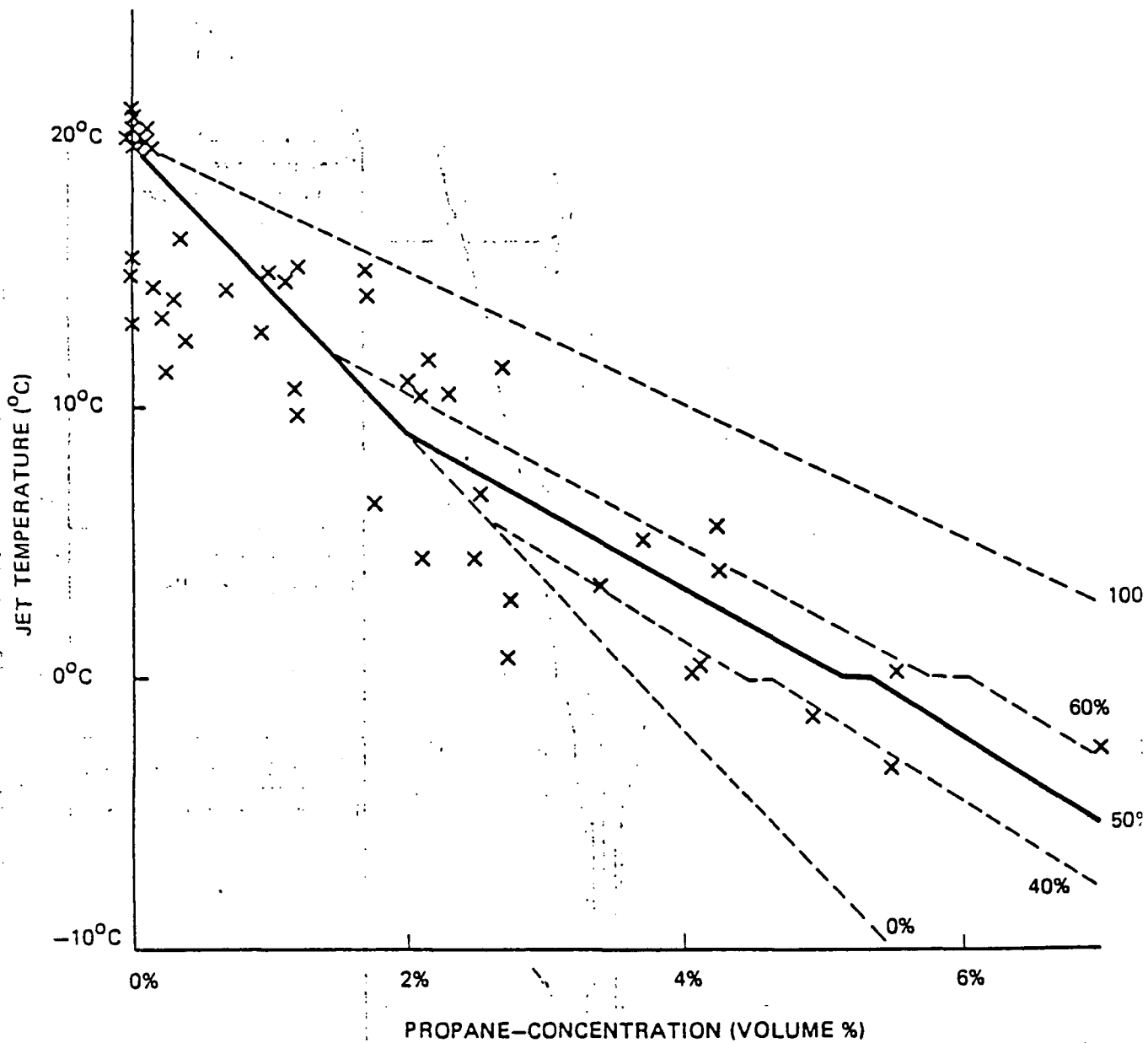


FIG A1.2(a) Isle of Grain Trial P25. Measured jet temperatures and concentrations, and equilibrium values for given humidity levels.

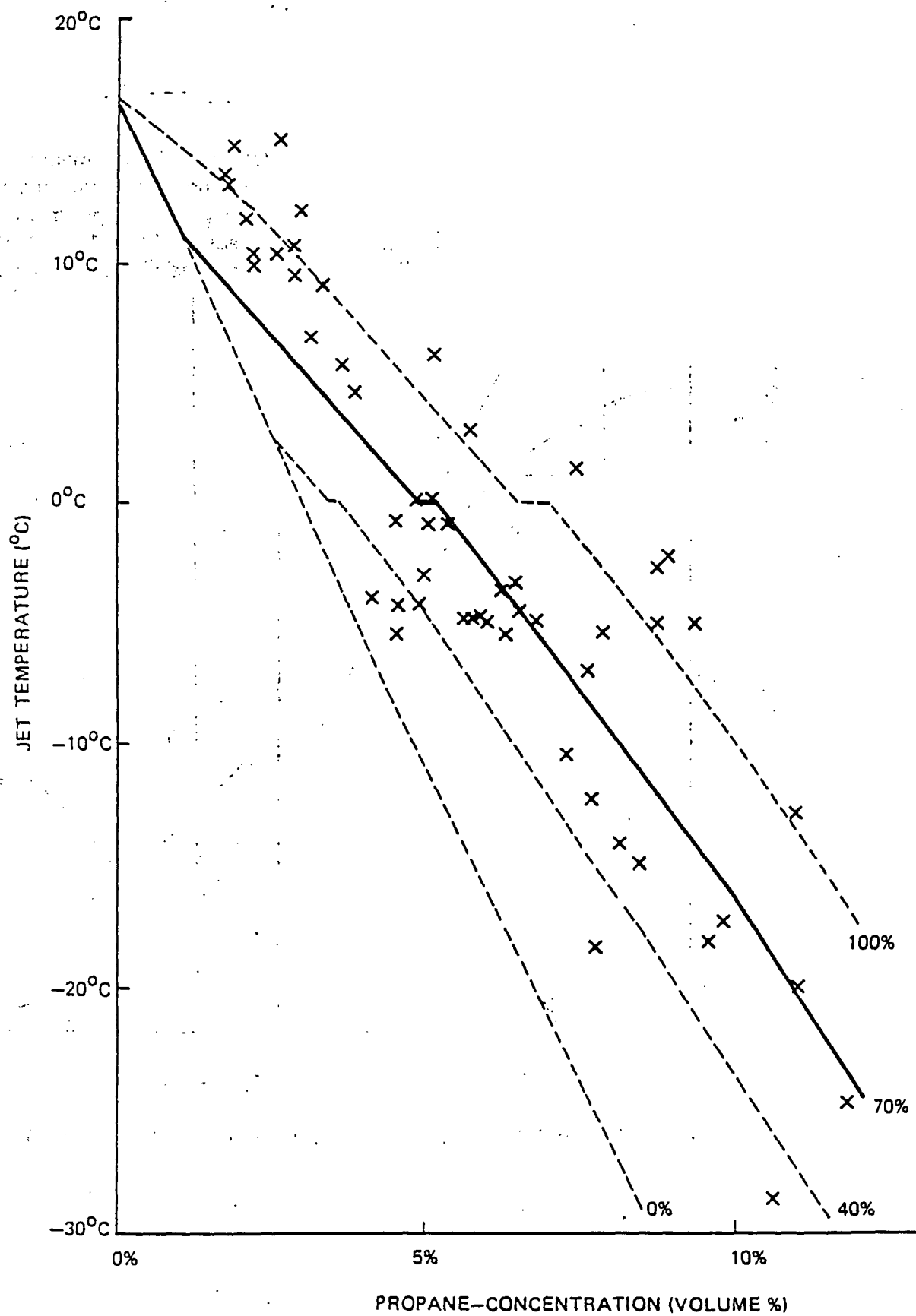


FIG A1.2(b) Isle of Grain Trial P29. Measured jet temperatures and concentrations, and equilibrium values for given humidity levels.

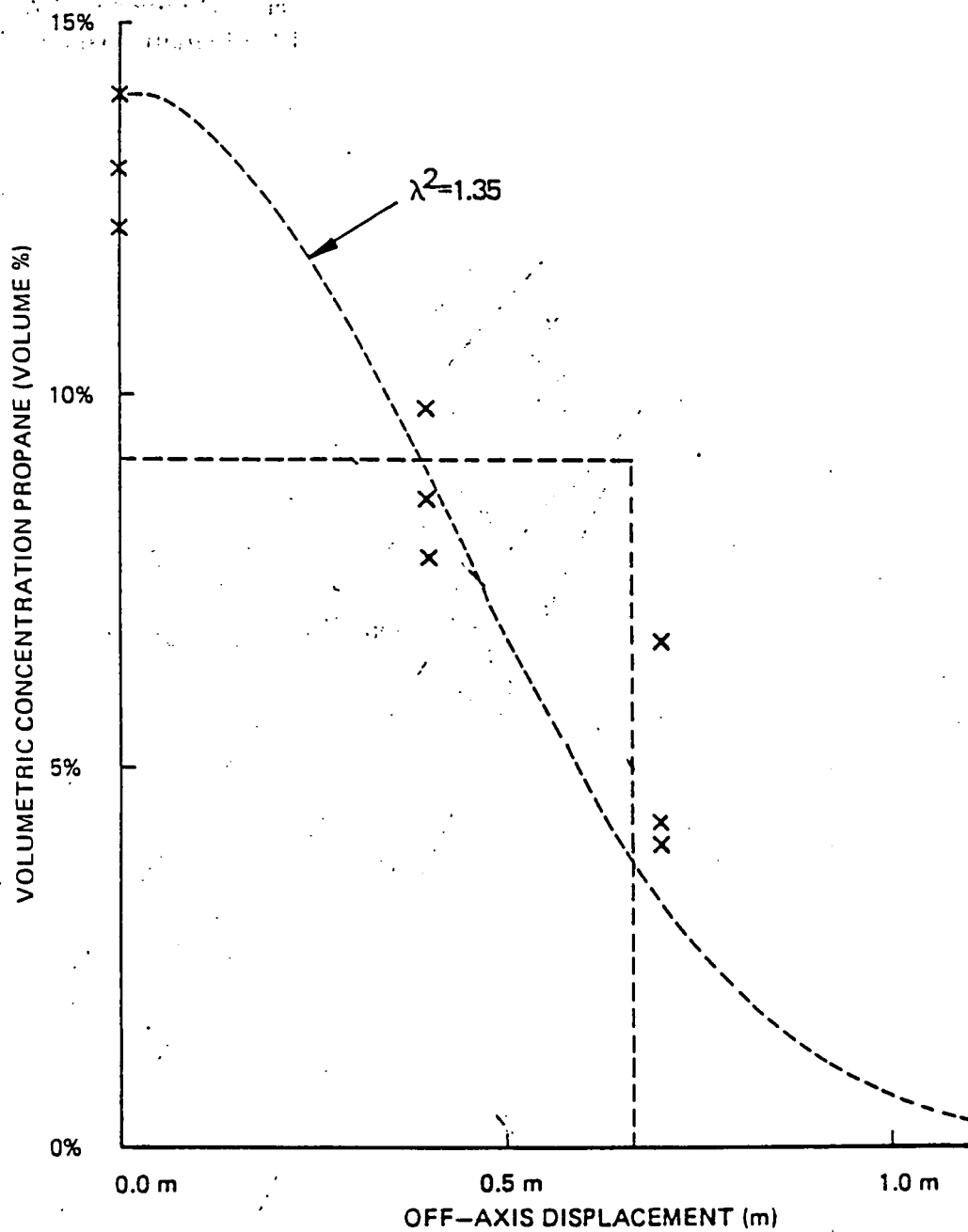
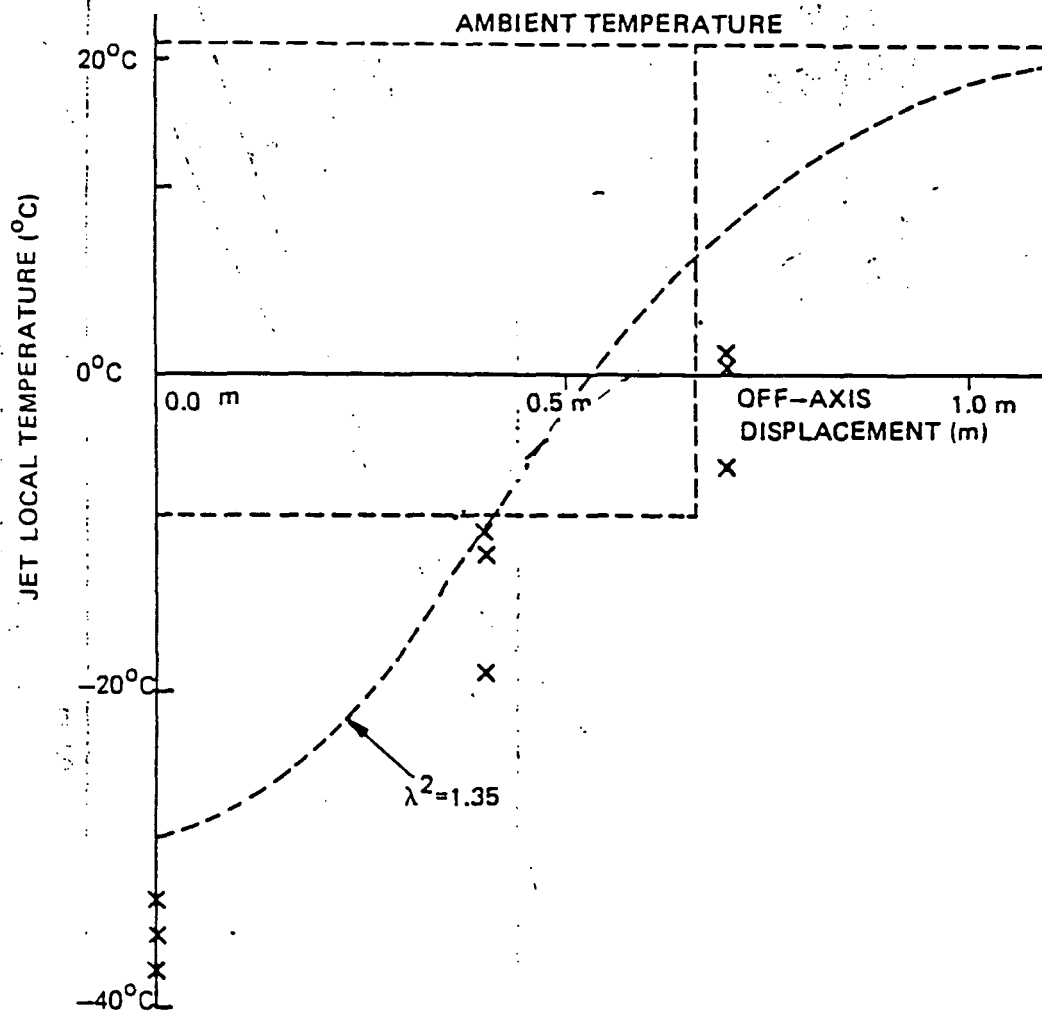


FIG A1.3 Isle of Grain Trial P26. Propane concentration profiles. Experimental values 9.0 m from release point: Gaussian and top-hat predictions at 9.1m.



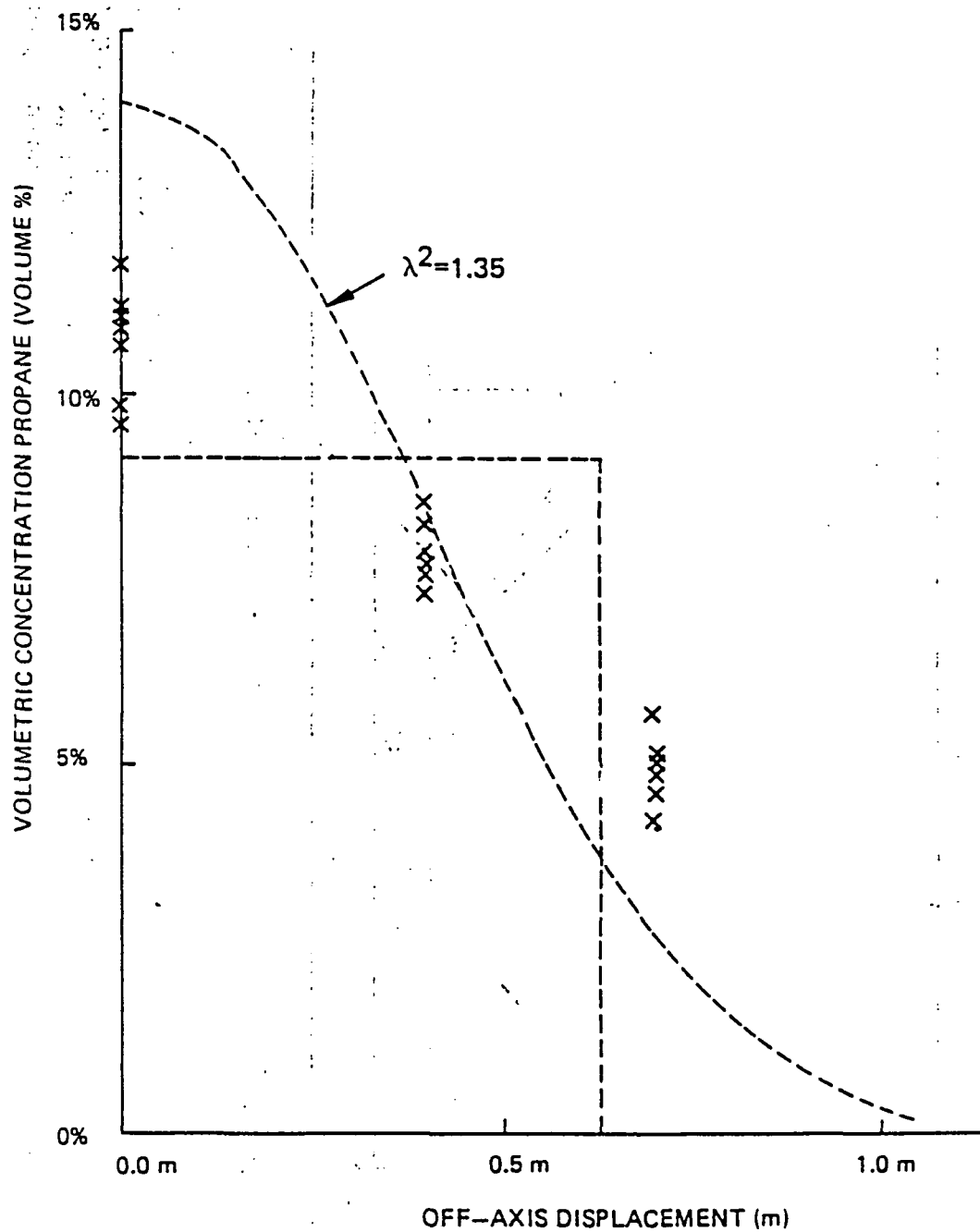


FIG A1.5 Isle of Grain Trial P29. Propane concentration profiles. Experimental values 9.0 m from release point: Gaussian and top-hat predictions at 9.1m.

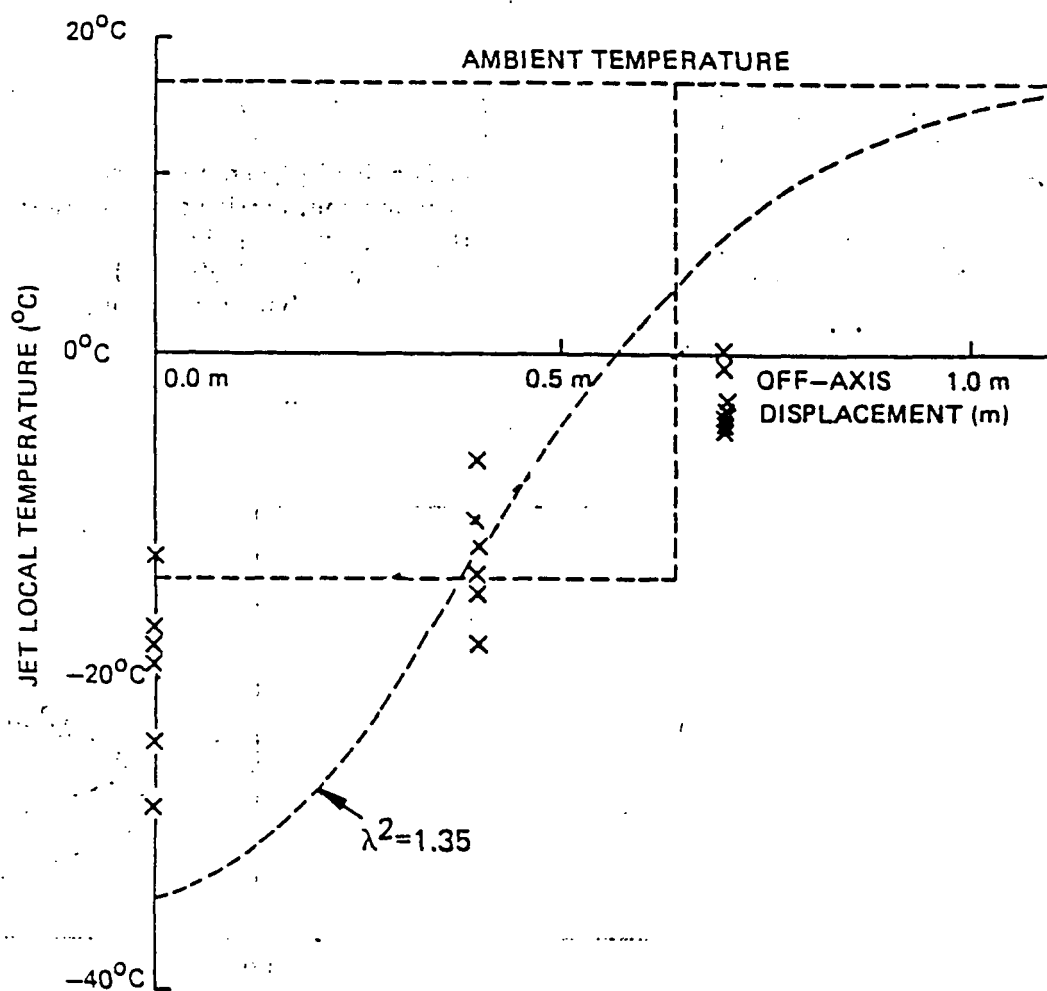


FIG A1.6 Isle of Grain Trial P29. Jet temperature profiles. Experimental values 9.0 m from release point: Gaussian and top-hat predictions at 9.1 m.

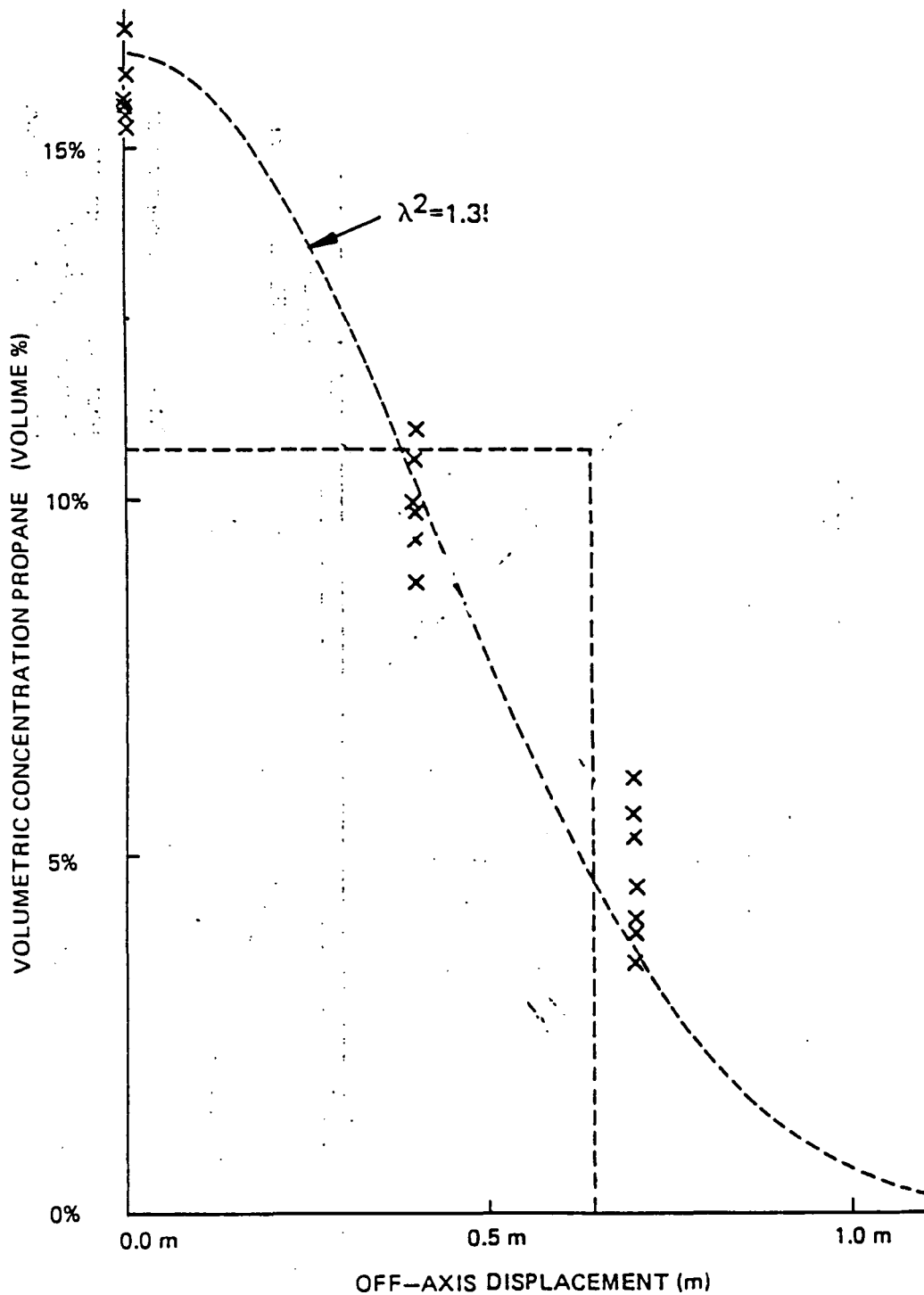


FIG A1.7 Isle of Grain Trial P30. Propane concentration profiles. Experimental values 9.0 m from release point: Gaussian and top-hat predictions at 9.1m.

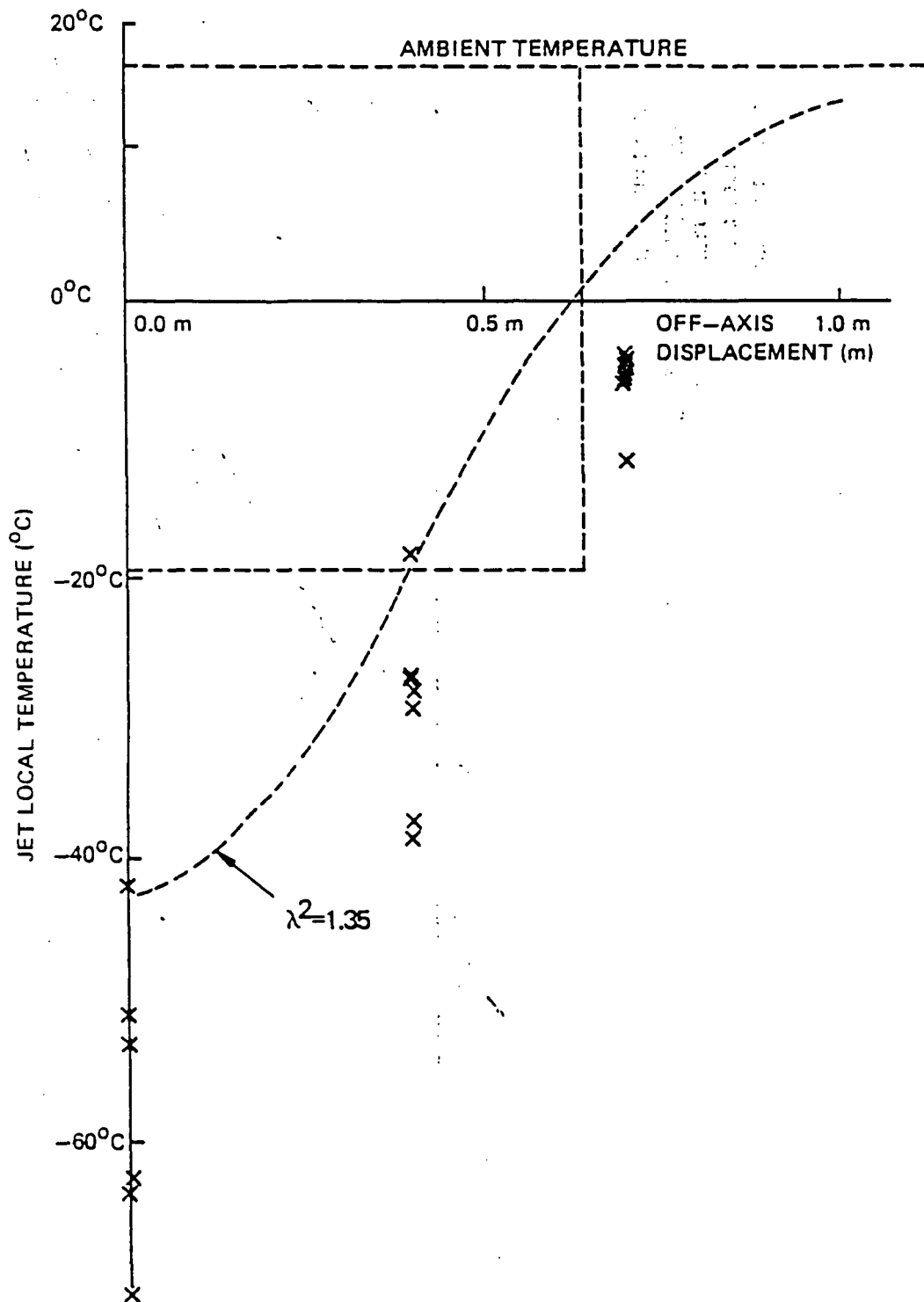


FIG A1.8 Isle of Grain Trial P30. Jet temperature profiles. Experimental values 9.0 m from release point: Gaussian and top-hat predictions at 9.1 m.

APPENDIX 2. DEVELOPMENT OF MODELS FOR PASSIVE ENTRAINMENT

WITHIN THE ATMOSPHERE SURFACE LAYER

Contents

A2.1: Introduction

A2.2: The Atmosphere Surface Layer

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A2.5: Disselhorst's Analysis: Comparison with experimental correlations of Singer and Smith

A2.6: Conclusions

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§A2.1: Introduction

Near to the point of release plume development is principally governed by source buoyancy, release momentum, and the influence of chemical reaction. Wind-shear and ambient density gradients may also be significant. In the far-field by contrast dispersion is largely governed by the diffusion by ambient turbulence of a passive contaminant.

Near the source, therefore, there is no need for a passive dispersion model; far from the source such a model determines plume evolution. Inasmuch as the far-field is to be determined by asymptotic matching of a near-field ("top-hat") and a far-field (Pasquill/Gifford) model, accurate representation of passive (ambient turbulence driven) entrainment within the near-field model HFPLUME is unnecessary. If such passive entrainment is represented, its role is as a (typically small) correction to entrainment dominated by the mechanisms near release.

Passive entrainment can be given within HFPLUME an (essentially) qualitative treatment based upon an understanding of surface layer scaling, and the inter-relation of ambient conditions, surface layer parameters, and the relationship between turbulence and diffusion.

This Appendix is based upon, but differs somewhat from, an analysis by Disselhorst (1984): First surface layer structure is elucidated; next an analysis is made of the origin and asymptotics of passive entrainment; finally the correlation of Disselhorst is presented and a brief comparison made with experiment. This area is still the subject of research. It seems rather likely that Disselhorst's correlation for (ambient turbulence) entrainment is of sufficient accuracy for our present (limited) purpose.

§A2.2: The Atmosphere Surface Layer

The surface layer is that atmosphere layer immediately adjacent to the Earth's surface and of a depth very much less than the local boundary layer thickness. The basic parameters describing the surface layer (over level horizontally uniform terrain) are as follows (Hanna 1982): $z_r > 0$, the surface roughness $h \gg z_r$, the boundary layer thickness u_* , the friction velocity L , the Monin-Obukhov length; w_* , the convective velocity. The Monin-Obukhov length, and convective velocity w_* have the definitions:

$$L = (T_\infty u_*^3) / (g \kappa u_* T_*), \quad w_* = -u_* (h / \kappa L)^{1/3}.$$

[Notation: κ von Karman's constant, g acceleration due to gravity, $u_* T_*$ surface to air heat-flux, T_∞ atmosphere (absolute) temperature.]

The wind and temperature profiles are related to the friction velocity and Monin-Obukhov length via the standard description (Wieringa 1980, Hanna 1982, Randerson 1984):

$$[\kappa(z+z_r)/u_*] du_\infty/dz = \psi_u(\zeta);$$

$$\psi_u(\zeta) = (1-22\zeta)^{-1/4}, \quad \zeta < 0,$$

$$\psi_u(\zeta) = 1+6.9\zeta, \quad \zeta \geq 0,$$

$$\zeta = (z+z_r)/L, \quad L = u_*^3 / \kappa / (g/T_\infty) / (u_* T_*), \quad z/h \ll 1.$$

These forms may be explicitly integrated (Randerson 1984, Raj and Morris 1988) to yield a standard set of velocity profiles determined by Monin-Obukhov length, surface roughness, and reference wind-speed at a user-specified height.

The temperature profile is conventionally expressed as a gradient of "potential" temperature, that is the difference between an adiabatic lapse rate and that observed (correlated) for a given surface roughness and Monin-Obukhov length. This distinction is in practice negligible, the dry adiabatic lapse rate being typically 9.7C/km. Reference to standard literature correlations (Arya 1982, Wieringa 1980) yields the forms (surface layer),

$$[\kappa(z+z_r)/T_*]dT_{\infty}^{\text{pot}}/dz = \psi_T(\zeta);$$

$$\psi_T(\zeta) = 1/\sqrt{1-13\zeta}, \quad \zeta < 0,$$

$$\psi_T(\zeta) = 1+9.2\zeta, \quad \zeta \geq 0.$$

$$\zeta = (z+z_r)/L, \quad L = u_*^3/\kappa/(g/T_{\infty})/(u_*T_*) \quad , \quad z/h \ll 1.$$

These differential forms may be explicitly integrated (Raj and Morris 1988, Nieuwstad and van Dop 1982) to yield a complete temperature profile $T_{\infty}(z)$ as a function of Monin-Obukhov length, surface roughness, and a single reference temperature at known height.

It remains to determine the Monin-Obukhov length L in terms of the Pasquill/Gifford (P/G) classification (Hanna 1982; Stern, Boubel, Turner and Fox 1984) and surface roughness z_r . The correlation is that of Colenbrander (1985), after Irwin (1979), and has the range of validity $1\text{mm} \leq z_r \leq 2\text{m}$:

$$L(z_r, P/G) = \begin{cases} -10.99z_r^{0.0993}, & P/G = \text{"A"}, \\ -13.44z_r^{0.1631}, & P/G = \text{"B"}, \\ -113.5z_r^{0.2946}, & P/G = \text{"C"}, \\ \infty, & P/G = \text{"D"}, \\ 125z_r^{0.3090}, & P/G = \text{"E"}, \\ 26.12z_r^{0.1667}, & P/G = \text{"F"} \end{cases}$$

Thus, given surface roughness and P/G category, we may deduce the Monin-Obukhov length, and hence, given the observed temperature and wind-speed at some reference height (typically 10m) above the ground surface, we may deduce the friction velocity u_* , the temperature fluctuation scale T_* (which may be negative), and hence the air temperature at the roughness height and the induced ground-to-air heat flux $u_* T_*$. This last provides a consistency check upon the combination of observed temperature, wind-speed, and P/G category, in that the flux $u_* T_*$ cannot plausibly exceed insolation levels at the release site.

§A2.3: Atmosphere Entrainment: Discussion

We seek to introduce a set of correlations based upon Monin-Obukhov similarity in the surface layer, such as will allow an approximate description of air entrainment for passive dispersion. This entrainment is in addition to that attributed to source momentum or buoyancy, and is **dominant** only in the far-field. For the integral averaged model HFPLUME we deduce the asymptotic form

$$\rho_\infty u_\infty d/dx[(\pi/4)D^2] = \text{Entr}_{\text{turb}}^{\text{amb}},$$

valid in the limit of passive dispersion. Comparison with the model PLUMEPATH (Ooms 1972; Ooms and Duijm 1984), suggests that dispersion due to ambient turbulence is reasonably described, at any rate for moderate downwind distances, by the form

$$\text{Entr}_{\text{turb}}^{\text{amb}} = 2^{-1/3} \pi e_{\text{turb}}^{\text{amb}} \rho_\infty (\varepsilon D^4)^{1/3}.$$

D is the effective diameter, ε the (integral averaged) turbulent dissipation, and ρ_∞ the atmosphere density. This results in the asymptotic growth of order $x^{3/2}$

as a function of downwind distance x . By contrast the expected far-field dispersion is governed by a constant eddy diffusivities with plume area increasing linearly with distance downwind.

Substitution in the (turbulent) diffusion equation of the standard Gaussian plume/image-plume model (Hanna 1982) yields for **constant** horizontal and vertical diffusivities the asymptotic forms

$$d\sigma_y/dx = K_y/(u_\infty \sigma_y), \quad d\sigma_z/dx = K_z/(u_\infty \sigma_z).$$

[Notation: x horizontal distance downwind of release, u_∞ mean wind-speed, (K_y, K_z) horizontal/vertical (eddy) diffusivity, (σ_y, σ_z) horizontal/vertical standard deviation.]

The expected asymptotic behaviour is, therefore,

$$\text{Entr}_{\text{turb}}^{\text{amb}} = (4\pi/\chi^2) \rho_\infty [K_y(\sigma_z/\sigma_y) + K_z(\sigma_y/\sigma_z)],$$

in which note the dependence on the plume aspect ratio; χ^2 is the turbulent Schmidt number.

Further, reference to Lagrangian statistic theories of horizontally and vertically homogeneous turbulence yields (Taylor 1921, Hanna 1982, Kao 1982), the relationships,

$$\sigma_y^2 = \langle u'_y u'_y \rangle T_y(x/u_\infty), \quad \sigma_z^2 = \langle u'_z u'_z \rangle T_z(x/u_\infty), \quad x/u_\infty \gg \max(T_y, T_z);$$

$$\sigma_y^2 = \langle u'_y u'_y \rangle (x/u_\infty)^2, \quad \sigma_z^2 = \langle u'_z u'_z \rangle (x/u_\infty)^2, \quad x/u_\infty \ll \min(T_y, T_z).$$

[Notation $x>0$ downwind displacement, u_∞ mean wind-speed, (T_y, T_z) twice the horizontal/vertical Lagrangian timescale, (σ_y, σ_z) horizontal/vertical standard deviation, $(\sqrt{\langle u'_y u'_y \rangle}, \sqrt{\langle u'_z u'_z \rangle})$ horizontal/vertical root mean square ambient wind-speed fluctuations.]

These results may be matched to span the entire range $x>0$ by extrapolating the initially linear plume expansion until it intersects the (far field) asymptote. The plume horizontal and vertical standard deviations at this (mid range) transition satisfy (upon elimination of the Lagrangian timescales) the equations,

$$\ell_y = 2K_y / \sqrt{\langle u'_y u'_y \rangle}, \quad \ell_z = 2K_z / \sqrt{\langle u'_z u'_z \rangle}.$$

The length scales ℓ_y and ℓ_z are by construction of a magnitude corresponding to the "collapse" of turbulent air entrainment associated with the growth of plume width. The mechanism of entrainment is driven by motions associated with the most energetic eddies, with entrainment "strong" for plume widths less than the eddy length scale, and weak thereafter. This suggests that the Lagrangian scales ℓ_y and ℓ_z are representative of the length scales of turbulent kinetic energy dissipation as the result of horizontal and vertical motions.

We introduce, therefore, the dissipation parameters ϵ_y and ϵ_z which (analogous to Arya 1982) defined as follows:

$$\epsilon_y = \langle u'_y u'_y \rangle^{3/2} / \ell_y, \quad \epsilon_z = \langle u'_z u'_z \rangle^{3/2} / \ell_z.$$

Substitution of these results and definitions into the asymptotic entrainment equation yields, in the far field,

$$\text{Entr}_{\text{turb}}^{\text{amb}} = (4\pi/\gamma^2) \rho_{\infty} (\ell_y \ell_z)^{2/3} [\epsilon_y^{1/3} (\ell_y/\ell_z)^{1/6} + \epsilon_z^{1/3} (\ell_z/\ell_y)^{1/6}].$$

Comparison of this formula with the near-field form suggests that the aspect ratio weighted term may be identified with the cube root of the dissipation of turbulent kinetic energy, resulting in an asymptotic form proportional to the product $(\ell_y \ell_z)^{2/3} \epsilon^{1/3}$.

Consider next the coupling of this far-field result to the near-field form proposed by Briggs (1965) and later Ooms (1972). Asymptotic analysis for the typical case of "momentum deficit" matching far from the ground surface yields (Chapter 4) the asymptotic form $D = (4/\gamma) \sqrt{(\sigma_y \sigma_z)}$, provided that the **averaging times** are chosen appropriately. Reference to Hanna (1982) yields that the contribution to diffusion of eddies of frequency $1/t$ is negligible for (Lagrangian) times from release of order t . The transition to the entrainment form $(\ell_y \ell_z)^{2/3} \epsilon^{1/3}$ occurs at notional time $\max(T_y, T_z)$ so that the Lagrangian picture is reproduced by an Eulerian plume the averaging time of which is comparable to the Lagrangian time-scale $\max(T_y, T_z)$. Further for elevated plumes the relationship between (Eulerian) averaging time and plume width is (Hanna 1982) proportional to the 0.2 power of the averaging time. This results, for an early plume assigned an "instantaneous" averaging time $\tau \approx 19s$ (TNO 1989, Chapter 4), in the "transition widths"

$$D_y = (\tau/T_y)^{1/5} (4\ell_y/\gamma), \quad \langle u'_y u'_y \rangle_{T_y} = \ell_y^2, \quad T_y > 0,$$

$$D_z = (\tau/T_z)^{1/5} (4\ell_z/\gamma), \quad \langle u'_z u'_z \rangle_{T_z} = \ell_z^2, \quad T_z > 0.$$

Continuity then suggests that the entrainment function throughout the downwind range might be represented by the formula

$$\text{Entr}_{\text{turb}}^{\text{amb}} = \pi \phi_{yz} \tau \rho_{\infty} [\max(D, D_y) \max(D, D_z)]^{2/3} \epsilon^{1/3};$$

$$\phi_{yz}^{\tau} = 2^{-2/3} \gamma [\tau^2 / (T_y T_z)]^{-2/5} [(\ell_y / \ell_z)^{1/6} + (\ell_z / \ell_y)^{1/6}].$$

This recognizes that the distribution of eddies in horizontal and vertical senses differ markedly, and that the the plume "diameter" may exceed the characteristic vertical scale D_z much before its horizontal counterpart D_y .

Inasmuch as the eddy dissipation ϵ differs somewhat from the weighted average of the scales ϵ_y and ϵ_z , we would not expect this formula to be **exact**, but rather to reflect the functional form and proportionality. Comparison with the near-field suggestion of Ooms (1972) and Disselhorst (1984), yields that ϕ_{yz}^{τ} is of approximate magnitude $2^{-1/3} e_{\text{turb}} \approx 0.79$, $e_{\text{turb}} = 1.0$. In addition the transition from near-field $D^{4/3}$ entrainment to that (constant) appropriate to the far-field is somewhat uncertain: D_y and D_z as represented above **are** representative magnitudes; however experimental fitting is necessary to determine the **precise** location of the transition.

§A2.4: Surface Layer Correlations

The eddy diffusivity in the surface layer has the standard form (Arya 1982)

$$K_z = \gamma^2 \kappa u_* (z + z_r) / \psi_u(\zeta),$$

$$\zeta = (z + z_r) / L, \quad L = u_*^3 / \kappa (g / T_{\infty}) / (u_* T_*), \quad z/h \ll 1;$$

in which $\gamma^2 \approx 1.35$, the turbulent Schmidt number, has been introduced to reflect the different diffusivities of (horizontal) momentum and concentration. The correlation $\langle u'_z u'_z \rangle$ is correlated in the surface layer by the form (Nieuwstad and van Dop 1982),

$$\sqrt{(\langle u'_z u'_z \rangle)}/u_* = 1.3 \psi_{\langle u'_z u'_z \rangle}(\zeta), \quad \psi_{\langle u'_z u'_z \rangle} = \{1 + 3 \min[0, (z+z_r)/L]\}^{1/3}.$$

It follows that the vertical length-scale ℓ_z satisfies the (dimensionless) relation,

$$\ell_z/(z+z_r) = (1.52 \chi^2 \kappa) / [\psi_u(\zeta) \psi_{\langle u'_z u'_z \rangle}(\zeta)],$$

or in the case of neutral stability $\ell_z/(z+z_r) \approx 0.83$. Further the horizontal standard deviation $\sqrt{(\langle u'_y u'_y \rangle)}$ is well correlated (Panofsky, Tennekes, Lenschow and Wyngaard 1977) by means of the formula,

$$\sqrt{(\langle u'_y u'_y \rangle)}/u_* = 12^{1/3} \psi_{\langle u'_y u'_y \rangle}; \quad \psi_{\langle u'_y u'_y \rangle} = \{1 + (1/6) \min[0, (z+z_r)/L]\}^{1/3};$$

whereas the horizontal diffusivity K_y is some ten times its vertical counterpart K_z (Kao 1982). This results in the horizontal length scale

$$\ell_y/(z+z_r) = (8.7 \chi^2 \kappa) / [\psi_u(\zeta) \psi_{\langle u'_y u'_y \rangle}(\zeta)],$$

or in the case of neutral stability $\ell_y/(z+z_r) \approx 4.7$. The eddy dissipation rate is, following Disselhorst (1984),

$$\varepsilon = u_*^3 / \kappa / (z+z_r) \psi_\varepsilon; \quad \psi_\varepsilon = 1 + 4\zeta, \quad \zeta \geq 0; \quad \psi_\varepsilon = 1 - 2\zeta, \quad \zeta < 0.$$

§A2.5: Disselhorst's Analysis

Disselhorst (1984) proposed a somewhat different formulation; again based on an analysis of the eddy length scales in horizontal and vertical directions.

His proposals covered the entire boundary layer, and not just the near surface fraction. However, for the surface layer his proposals reduce to the formulae,

$$\text{Entr}_{\text{turb}}^{\text{amb}} = \pi e_{\text{turb}}^{\text{amb}} \rho_{\infty}(\varepsilon)^{1/3} [\ell_y^{4/3} + \ell_z^{4/3}];$$

$$\begin{aligned} \ell_y = & \begin{cases} \min[D/2, 0.88(1-7.4\kappa\zeta)(1-5\kappa\zeta)^{-1}(z+z_r)], & \text{P/G= \{"A","B","C"\},} \\ \min[D/2, 0.88(z+z_r)] & , \text{P/G= \{"D"\},} \\ \min[D/2, 0.88(z+z_r)/(1+0.1\zeta)] & , \text{P/G= \{"E","F"\},} \end{cases} \end{aligned}$$

$$\begin{aligned} \ell_z = & \begin{cases} \min[D/2, 0.88(1-7.4\kappa\zeta)(1-5\kappa\zeta)^{-1}(z+z_r)], & \text{P/G= \{"A","B","C"\},} \\ \min[D/2, 0.88(z+z_r)] & , \text{P/G= \{"D"\},} \\ \min[D/2, 0.88(z+z_r)/(1+4\zeta)], & , \text{P/G= \{"E","F"\},} \end{cases} \end{aligned}$$

$$\begin{aligned} \varepsilon = & \begin{cases} (1-5\kappa\zeta)u_*^3/\kappa/(z+z_r) & , \text{P/G= \{"A","B","C"\},} \\ u_*^3/\kappa/(z+z_r) & , \text{P/G= \{"D"\},} \\ (1+4\zeta)u_*^3/\kappa/(z+z_r) & , \text{P/G= \{"E","F"\},} \end{cases} \end{aligned}$$

$$e_{\text{amb}}^{\text{turb}} = 1.0, \quad \zeta = (z+z_r)/L, \quad z/h < 0.02, \quad L = u_*^3/\kappa/(g/T_{\infty})/(u_*T_*).$$

[Notation: z_r surface roughness, L Monin/Obukhov length, u_* friction velocity, κ von Karman's constant, T_{∞} atmosphere (absolute) temperature, u_*T_* surface/air heat-flux, h boundary layer depth, ε dissipation rate of turbulent kinetic energy, (ℓ_y, ℓ_z) turbulent (transverse horizontal, vertical) eddy length-scales; D plume diameter, z centroid height; P/G Pasquill/Gifford class.]

In this analysis for convective conditions the difference between horizontal and vertical length scales is replaced by "neutral" and convective scales which play analogous roles in the representation of the passive entrainment. This

explains the identity of the expressions for ℓ_y and ℓ_z for Pasquill stability classes "A" through "C".

In addition to air entrainment the aspect ratio of the developing plume is modified in response to the ambient turbulence, in a manner compatible with the observed Pasquill/Gifford ratio σ_y and σ_z . Inasmuch as this analysis will complicate transition from an airborne to a touchdown plume, and exerts little influence on integral average fluxes of buoyancy and momentum, we have neglected this effect in the transcription to the model HFPLUME.

For "instantaneous" conditions the plume width and height are represented by scale $D_y/2$ and $D_z/2$ whereas for long averaging time the corresponding standard deviations are $\sqrt{(D_y^2/4 + \sigma_{y,c}^2)}$ and $\sqrt{(D_z^2/4 + \sigma_{z,c}^2)}$ in which the deviations $\sigma_{y,c}$ and $\sigma_{z,c}$ relate to plume meander. This component of the analysis is not required in the context of the computer model HFPLUME.

Finally Disselhorst's formula presumes an arithmetical rather than harmonic averaging of entrainment due to horizontal and vertical diffusion. Disselhorst did not distinguish K_y and K_z for far-field diffusion. This difference has some influence upon entrainment for intermediate plume widths, but is asymptotically unimportant. The functional form suggests a harmonic mean, but certainly does not exclude the simpler algebraic form.

Disselhorst compares his theoretical results with a set of empirical correlations developed at Brookhaven National Laboratory by Singer and Smith (1964). A series of calculations were performed for various wind-speeds and stability classes for a dense gas release from a large chimney. Full details of the (comparison) release are as follows:

Release Conditions:

mass flux released: 19.2kg/s;	gas molecular weight: 42.1g/mol;
release temperature: 31C;	gas (isobaric) specific heat: 1.0kJ.kg/K;
stack height: 50m;	stack diameter: 41cm;
surface roughness: 30cm;	wind-speed reference height: 20m.

Figure A2.1 illustrates the agreement between the predictions of the above model and the correlation of Singer and Smith (1985) in respect of the maximum ground level concentration. The product of maximum ground level concentration and wind-speed is plotted against wind-speed. The stability classes for a neutral atmosphere are, according to Singer and Smith, " B_1 " for wind-speeds less than 5.5m/s and "C" otherwise. Generally the agreement is fair (but note the logarithmic scale). Figure A2.2 contrasts the predicted displacement of maximum ground-level concentration as a function of wind-speed for neutral stability. Agreement is again satisfactory, though for neutral stability an improvement in predictive accuracy over that achieved by the Ooms' model PLUMEPATH is not apparent. Figures A2.3 and A2.4 illustrate similarly the predictions of maximum ground-level concentration and its downwind displacement for stable (Singer and Smith class "D") and unstable (Singer and Smith class " B_2 ") conditions. Clearly trends are correctly reproduced, whereas predictive accuracy is but fair.

§A2.5: Conclusions

The formulation of Disselhorst has modest success in predicting entrainment and plume path for systems dominated by ambient turbulence, and is of comparable accuracy to the prototype plume model PLUMEPATH on which it is based. It seems likely that improved accuracy can be achieved by fitting the several estimated coefficients to dispersion data. Inasmuch as ambient turbulence is regarded within

HFPLUME as a minor contributor to the plume entrainment high accuracy is not needed. It is sufficient, in this context, to reproduce the order of magnitude and stability trends of ambient turbulence driven entrainment.

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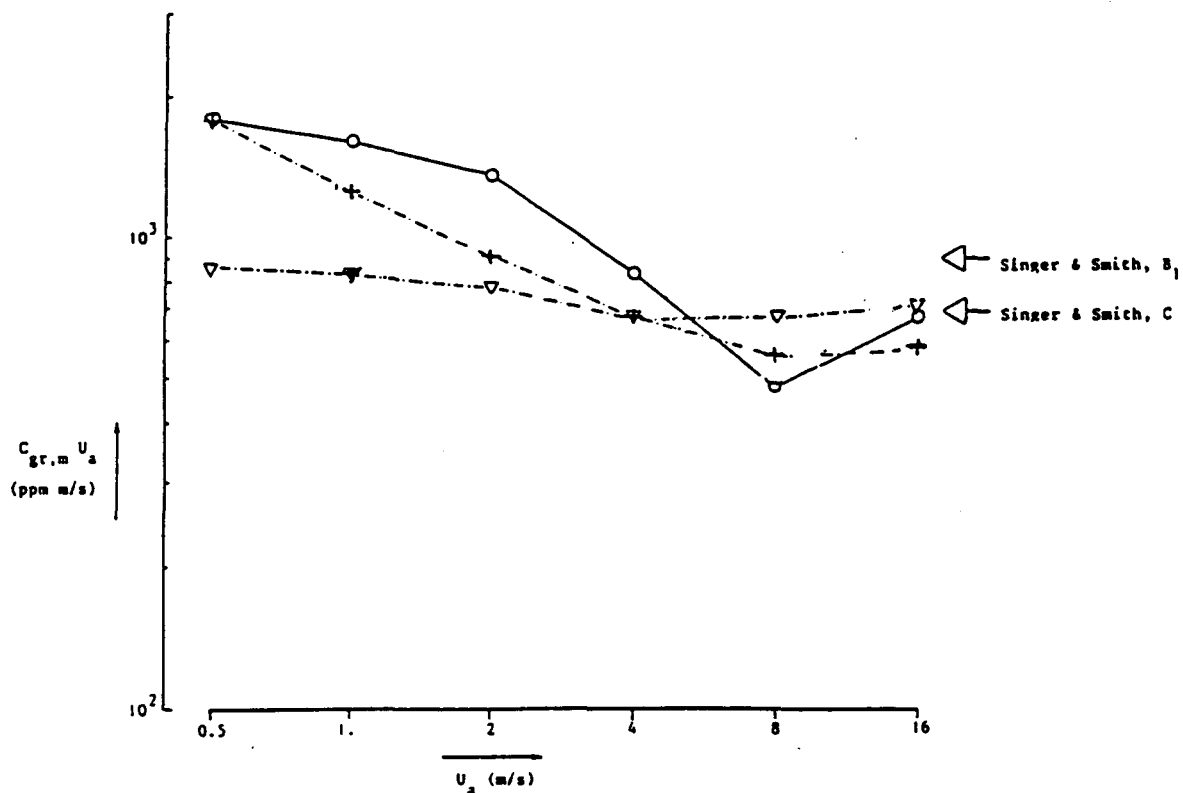


Fig. A2.1. Maximum ground-level concentration versus wind speed: theory (Disselhorst, 1984) versus experiment (Singer and Smith, 1966)

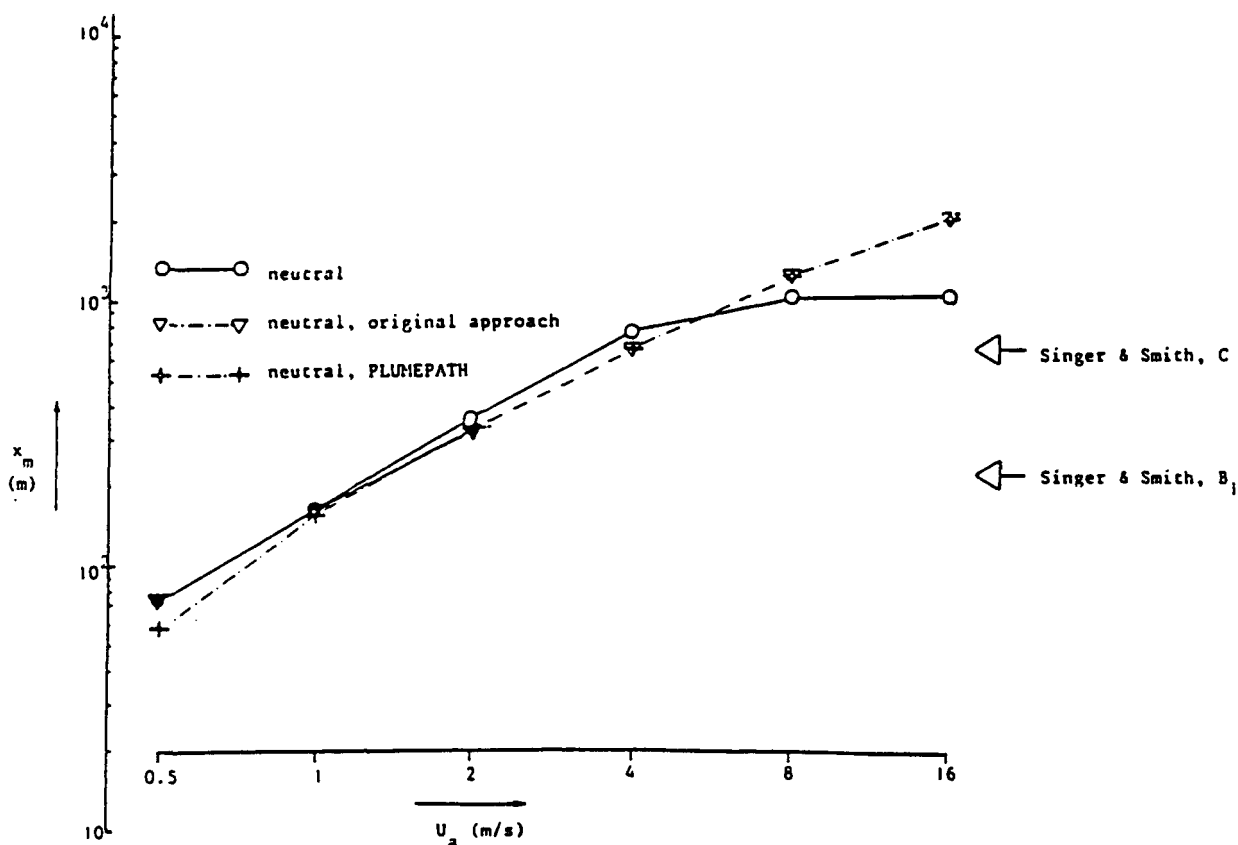


Fig. A2.2. Distance to ground-level maximum versus wind speed: theory (Disselhorst, 1984) versus experiment (Singer and Smith, 1966) [Note: the 'original' approach is for passive dispersion proportional to $(\epsilon D^4)^{1/3}$ without the eddy-scale "cut-off" at l_y or l_z . Aspect ratio effects are also neglected]

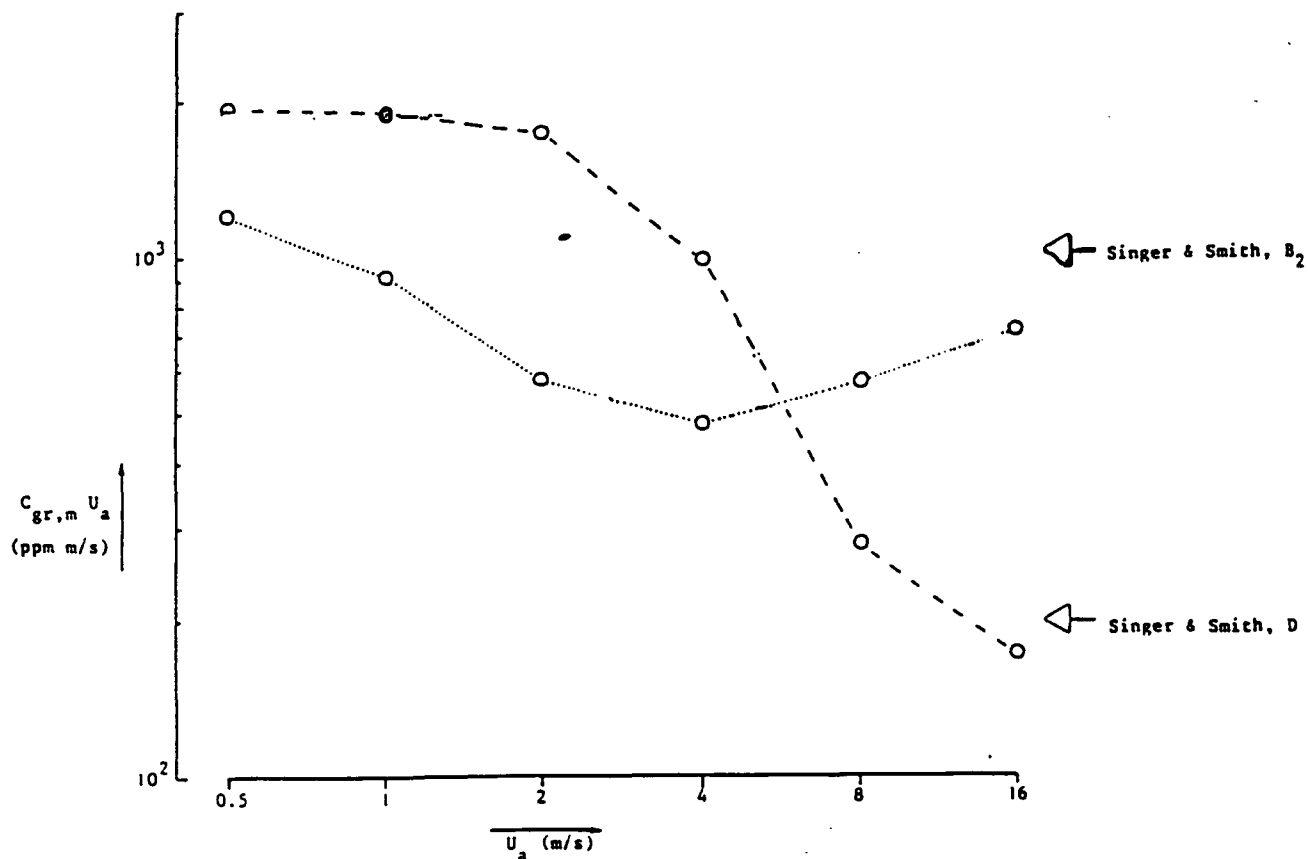


Fig. A2.3. Maximum ground-level concentration versus wind speed: theory (Disselhorst, 1984) versus experiment (Singer and Smith, 1966)

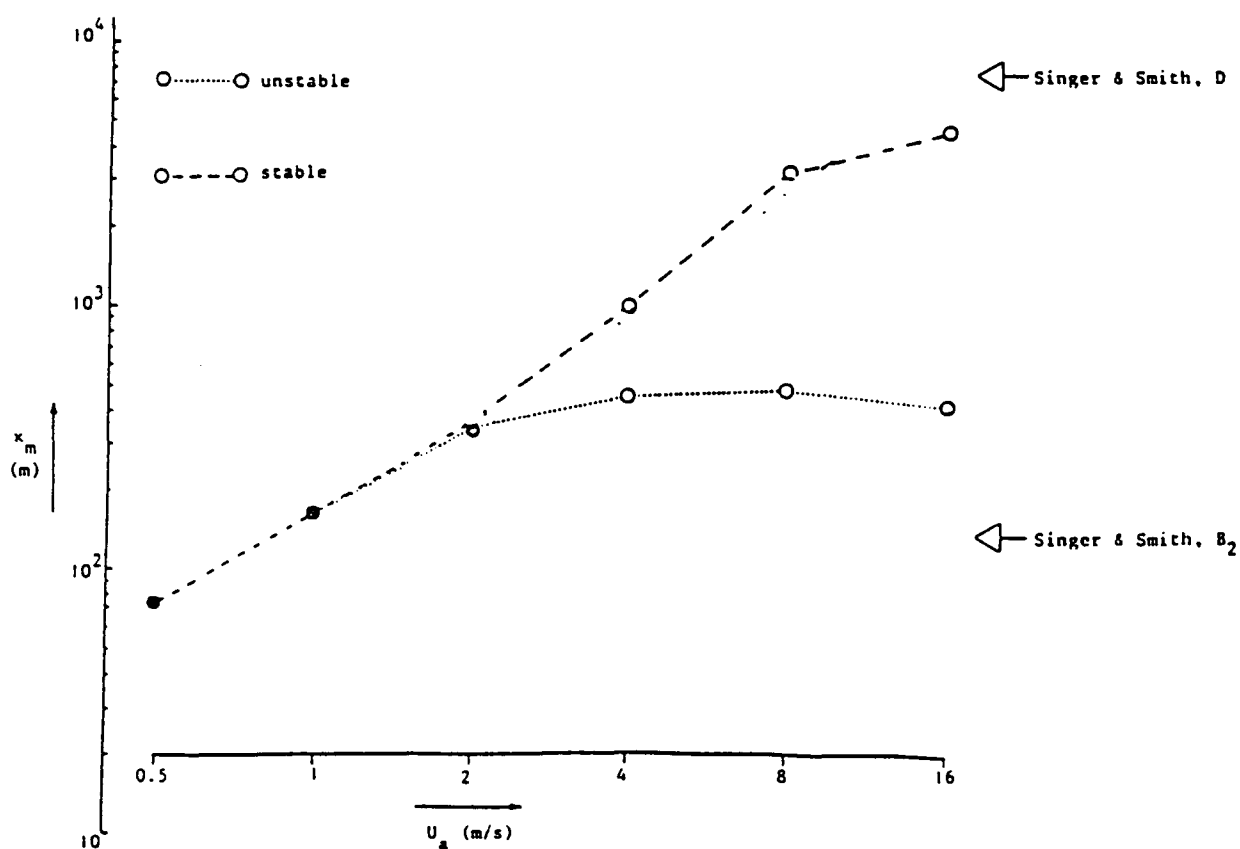


Fig. A2.4. Distance to ground-level maximum versus wind speed: theory (Disselhorst, 1984) versus experiment (Singer and Smith, 1966) [Note: the comparison is of 'stable' (Singer and Smith class D) and 'unstable' (Singer and Smith class B_2) conditions. The wind speed is that at 20 m above groundlevel]

APPENDIX 3

DISPERSION OF RELEASES OF DENSE GAS:
DEVELOPMENT OF THE HEGADAS-4 MODEL.

by

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Notation

For each item we give the symbol, followed where appropriate by its functional dependence (on e.g. x or t or c), and then the meaning of the symbol and the number of the equation where it is defined or the section in which it is introduced.

a	Constant in convective entrainment formulation.	equ.(5.19)
a_x	Coefficient in expression for σ_x	equ.(6.11)
A_i	Secondary source area seen by observer i (time-dependent model)	sec. 6.2
b $b(x)$	Half-width of mid part of crosswind concentration profile	equ.(2.2)
b_x	Exponent in expression for σ_x	equ.(6.11)
B	Source half-width used in dispersion calculation	sec. 4.2
B_{eff}	Effective half-width of the plume	equ.(3.14)
B_i, B'_i	Source half-width seen by observer i (time-dependent model)	sec. 6.2
B_p	Primary source half-width	sec. 4.2
c $c(x,y,z)$	Gas concentration	sec. 2
c_A $c_A(x)$	Ground-level centreline concentration	equ.(2.2)
c'_A	c_A after longitudinal diffusion correction (time-dependent model)	sec. 6.3
C	Constant in plume width growth rate	equ.(4.10)
C_0	Constant in observer velocity calculation	app. B
C_E	Lateral gravitational spreading constant	equ.(4.8)
C_f	Friction factor, used in forced convection heat transfer	sec. 5.1
C_{pm}	Specific heat capacity of gas-air mixture	sec. 5.1
D	Added heat per mole of gas-air mixture	sec. 5.1
D^*	Dimensionless parameter in water vapour transfer	equ.(5.13)
e	Release quantity of gas (per unit crosswind width) in tracer experiments	sec. 6.3
E	Flux of gas from the source	sec. 4.2

H	Gas layer height defined by Britter	equ.(3.15)
H_{eff}	Effective plume height	equ.(3.6)
H_g	Gas blanket height (time-dependent model)	sec. 6.1
k	von Karman constant (=0.41)	sec. 3.1
K_y	Lateral turbulent diffusivity	sec. 4.1
K_z	Vertical turbulent diffusivity	sec. 3.1
L	Source length used in dispersion calculation	sec. 4.2
L_c, L'_c, L_c^*	see appendix C	
L_i	Secondary source length seen by observer i (time-dependent model)	sec. 6.2
L_p	Primary source length	sec. 4.2
L^*	Dimensionless parameter in water vapour transfer	equ.(5.13)
M	Molecular weight	sec. 5.1
N	Parameter in water vapour transfer formulation	equ.(5.13)
N^*	Dimensionless parameter in water vapour transfer	equ.(5.13)
P_{wv}	Vapour pressure of water	sec. 5.2
P	Pressure	
q_E	Source strength in McQuaid experiments	sec. 3.2
Q_p	Flux of gas (mass per unit area) from primary source of gas Steady state: sec. 4.2, Time dependent $Q_p(t)$: sec. 6.1	
$Q_{max}^*, Q_{max}^*(L)$	Maximum take-up flux of gas from source into the atmosphere	equ.(4.15), equ.(4.16)
Q^*	Flux of gas from primary or secondary source used in dispersion calculations Steady state: sec. 4.2, Time dependent $Q^*(t)$: sec. 6.1	
$Q_{H,f}, Q_{H,n}$	Forced and natural convection heat flux from the surface	sec. 5.1
Q_{wv}	Water vapour flux from surface	sec. 5.2
R	Gas constant	sec. 5.1
R, R(t)	Secondary source radius (time-dependent model)	sec. 6.1

R_1	$R_1(t)$	Primary source radius (time-dependent model)	sec. 6.1
R_g	$R_g(t)$	Gas blanket radius (time-dependent model)	sec. 6.1
Ri_*	Ri_T	Bulk Richardson number	equ.(3.5)
Ri_B		Bulk Richardson number defined by Britter	sec. 3.2
R_{max}		Maximum radius of secondary source (time-dependent model)	app. B
S_{crit}		Critical supersaturation of water	sec. 5.2
S_y	$S_y(x)$	Crosswind dispersion coefficient	equ.(2.2), sec. 4.1
S_z	$S_z(x)$	Vertical dispersion coefficient	equ.(2.2)
$S, S^*, S_i^*, S_{yi}, S'_{yi}$		see appendix C	
t		Time	
t_{1i}, t_{2i}		Times at which observer i encounters the upwind and downwind edges of the secondary source	sec. 6.1
T		Temperature	
T_m		Temperature of gas-air mixture	sec. 5.1
T_s		Temperature of surface	sec. 5.1
u		Mean wind-tunnel velocity (McQuaid experiments)	sec. 3.2
u_*		Friction velocity (defined by $\tau = -\rho_a u_*^2$, calculated in the model from equ. (3.5))	sec. 3.1
u_0		Wind velocity at height z_0	sec. 3.1
u_e		Entrainment velocity, Volume of air entrained through top of cloud per unit area	sec. 3.1
u_{eff}	$u_{eff}(x)$	Effective velocity, the mean horizontal transport velocity of gas passing x	equ.(3.9)
u_i	$u_i(x,t)$	Velocity of travel of observer i (time-dependent model)	sec. 6.2
u_T		Velocity scale for entrainment including convective entrainment	sec. 5.3
u_x	$u_x(z)$	Wind velocity in the atmosphere	sec. 3.1
V_0, V_m		Specific molar volume of air, of gas-air mixture	sec. 5.1
w_*		Free convection velocity scale	equ.(5.18)

W	Half-width of concentration profile in crosswind dispersion discussion	sec. 4.1
W_c, W_c', W_c^*	see appendix C	
x	Distance downwind from source centre	
x_i $x_i(t)$	Location of observer i at time t (time-dependent model)	sec. 6.2
x_p	Used in discussion of dispersion in the wind direction (time-dependent model)	sec. 6.3
x_t	Downwind distance at which the half-width of the middle part of the concentration profile, b , becomes zero	sec. 4.1
x_v	Constant included in equ. 4.12 to ensure continuity of S_y across transition where b becomes zero	sec. 4.1
y	Crosswind distance from plume centreline	
y_{w3}	Molar fraction of picked-up water vapour in the cloud; see also appendix A	sec. 5.2
z	Vertical distance from (level) surface	
z_0	Reference height at which wind speed is specified	sec. 3.1
z_R	Roughness length, a parameter related to the roughness of the ground surface	sec. 3.1
α	Exponent in the wind velocity profile	equ.(2.1)
α_T	Thermal diffusivity	sec. 5.1
β	Exponent in expression for σ_y	equ.(4.2)
γ	Used in derivation of S_y formulation	sec. 4.1
Γ	Gamma function: see standard mathematical tables	
δ	Coefficient in expression for σ_y	equ.(4.2)
δ_ξ	Reduced boundary layer thickness in water vapour transfer formulation	equ.(5.12)
Δ	Dimensionless form of δ_ξ	equ.(5.12)
ζ	$-- \frac{1}{\rho} \left(\frac{\partial \rho}{\partial T} \right)_p$, so for an ideal gas $\zeta = 1/T$.	sec. 5.1

λ		The Monin-Obukhov length, related to the stability of the atmospheric boundary layer ($\lambda < 0$ for unstable, $\lambda > 0$ for stable, infinite for neutral)	sec. 3.1
ν		Kinematic viscosity	sec. 5.1
ρ		Density	
ρ_a	$\rho_a(z)$	Density of ambient air	sec. 3.1
ρ_m	$\rho_m(c)$	Density of the gas-air mixture in the cloud	sec. 3.1
ρ_E		Density of the gas emitted from the source	sec. 4.2
$\Delta\rho$		Density difference between the cloud and the ambient air at $z=H_{eff}$	equ.(3.7)
$\Delta\rho_0$		Initial density difference in KPA experiments	sec. 3.3
σ_x		Longitudinal dispersion coefficient	sec. 6.3
σ_y		Crosswind dispersion coefficient for neutral density point source releases	equ.(4.1)
τ		Shear stress	sec. 3.3
Φ	$\Phi(Ri_*)$	Dimensionless function describing the influence of density stratification on vertical diffusion (entrainment)	sec. 3.1
Ψ_1		Function giving influence of stability on wind velocity profile	equ.(B.1), equ.(3.4)
ξ		Integration variable	equ.(6.13)

DISPERSION OF RELEASES OF DENSE GAS:
DEVELOPMENT OF THE HEGADAS-4 MODEL

1. INTRODUCTION

In assessing the potential hazards associated with industrial installations, it is often necessary to consider the possible consequences of the accidental release of flammable or toxic gases. As part of this assessment, calculations of their dilution in the atmosphere are required. Mathematical models of gas dispersion are used for the calculations. Many such gases, either by virtue of their molecular weight or low temperature, are denser than air when released. The dispersion of such dense clouds is qualitatively, as well as quantitatively, different from the behaviour of neutrally buoyant releases. Hence there has been considerable interest in recent years in the development of our understanding of dense gas dispersion, and of models for this process.

Dense-gas dispersion models tend to fall into two categories (although there are a few with an intermediate status). Most complex are three-dimensional grid solutions of sets of partial differential equations which represent, at some level of turbulence closure, approximations to the averaged Navier-Stokes equations. These models have the prospect of eventually being able to deal with such complexities as flow around obstacles. However, their application to such flows is still under development and is likely to require larger-scale computing facilities than are generally available today. The other main category comprises integral models, which take assumed profile shapes and solve ordinary differential equations for such parameters as height and width of the cloud. Some empirical input is required, for example, to determine relations for the

entrainment of air into the cloud. It seems that the best of such models can predict dispersion over flat surfaces at least as well as the more complex models, and at much lower computational cost.

The model HEGADAS is an example of the latter type. It uses forms of concentration profile that can be used without a need for sudden change into the region of passive dispersion. The basic model (HEGADAS-2) was described by Colenbrander(1980). Since then a number of changes have been made to HEGADAS. Some, such as heat transfer, were clearly necessary additions for the proper description of dispersion of materials such as LNG. The need for inclusion of water vapour transfer, by contrast, only becomes clear as a result of the analysis of field data. Some further changes have been made as a result of a better understanding of laboratory experiments.

This report contains a full description of the formulation of HEGADAS, with these changes included. The validation of the model against field data is the subject of a number of papers (Puttock et al., 1982, 1984, Colenbrander and Puttock, 1984, Puttock, 1987).

This technical description corresponds to the implementations of the model in the programs HEGADAS-S and HEGADAS-T that have been made available on public release through the U.S. National Technical Information Service. This version of the HEGADAS programs is now referred to as HEGADAS-4. The NTIS reference number for the program diskettes and the Users Guide is PB89-164552.

2. SIMILARITY PROFILES

It is the basis of such a model that assumptions are made about the shape of (horizontal and vertical) profiles of quantities such as concentration and velocity. These profile shapes are chosen to be a reasonably simple representation of the experimentally observed behaviour of such clouds.

For a steady plume of dense gas, the following similarity profiles are used in HEGADAS for the time-mean wind velocity u_x in the atmospheric surface layer and for the vapour concentration c :

$$u_x = u_o \left(\frac{z}{z_o} \right)^\alpha \quad \dots (2.1)$$

$$c(x,y,z) = c_A(x) \exp \left[- \left(\frac{|y| - b(x)}{S_y(x)} \right)^2 - \left(\frac{z}{S_z(x)} \right)^{1+\alpha} \right] \text{ for } |y| > b \quad \dots (2.2)$$

$$c(x,y,z) = c_A(x) \exp \left[- \left(\frac{z}{S_z(x)} \right)^{1+\alpha} \right] \quad \text{for } |y| < b$$

The x-direction in the Cartesian coordinate system coincides with the wind direction (see Figure 1); the y and z directions are the horizontal and vertical crosswind directions respectively. The $z = 0$ plane represents the earth's surface and the $y = 0$ plane is the plane of symmetry of the vapour plume. z_o is an arbitrary reference height at which the velocity is u_o . The method of deriving the wind profile exponent α is given in appendix B. The similarity profiles used are illustrated in Figure 1.

There are four variables which need to be determined in order that the concentration at any point is determined by (2.2). These four

variables all depend on the downwind distance x only. They are c_A , the ground-level centreline concentration, S_z , a plume height parameter, b , the half-width of the middle part of the crosswind concentration profile, and S_y , the width of the gaussian edges of the crosswind concentration profile. Equations must be derived for the change of these variables with distance. Solution of the model then requires only the numerical solution of ordinary differential equations for these four variables, and for the heat and water vapour content of the plume, which can also be important.

3. VERTICAL MIXING

3.1 The vertical dispersion coefficient S_z

If the plume were two-dimensional (i.e. no variation in the y-direction), the vertical concentration distribution

$$c(x,z) = c_A(x) \exp \left[- \left(\frac{z}{S_z(x)} \right)^{1+\alpha} \right] \quad \dots(3.1)$$

should satisfy the simple two-dimensional diffusion equation

$$u_x \frac{\partial c}{\partial x} = \frac{\partial}{\partial z} \left(K_z \frac{\partial c}{\partial z} \right) \quad \dots(3.2)$$

where we take the turbulent diffusivity K_z to be given by

$$K_z = \frac{k u_* z}{\Phi(Ri_*)} \quad \dots(3.3)$$

In this expression the variable u_* is the friction velocity, which is formally defined in terms of the surface shear-stress; however, the ratio $\frac{u_*}{u_o}$ can be obtained from the logarithmic wind velocity profile

(Businger, 1973):

$$\frac{u_*}{u_o} = k \left[\ln \left(\frac{z_o + z_R}{z_R} \right) - \Psi_1 \left(\frac{z_o}{\lambda} \right) \right]^{-1} \quad \dots(3.4)$$

where Ψ_1 is defined in Appendix B and $k = 0.41$ is the von Karman constant. For a given reference height z_o this ratio depends on the two length scales z_R , the roughness length, which is determined by the roughness of the

ground, and λ , the Monin-Obukhov length, which is dependent on the stability of the atmosphere.

Ri_* is a bulk Richardson number, which gives a measure of the extent of the influence of the gas density. It can be defined as follows:

$$Ri_* = g \frac{\Delta\rho}{\rho_a(z=0)} \frac{H_{eff}}{u_*^2} \quad \dots(3.5)$$

where g is the gravitational acceleration, $\rho_a(z=0)$ the air density at ground level, $\Delta\rho$ is a characteristic density difference between the plume and the surrounding air, and H_{eff} is the effective height of the plume, which can be defined by

$$H_{eff} = \frac{1}{c_A} \int_0^\infty c dz = \frac{\Gamma(\frac{1}{1+\alpha})}{1+\alpha} S_z \quad \dots(3.6)$$

The density difference $\Delta\rho$ is defined as:

$$\Delta\rho = \rho_m(c=c_A) - \rho_a(z=H_{eff}) \quad \dots(3.7)$$

where the expression $\rho_m(c=c_A)$ denotes the density of a mixture of gas with concentration c_A and ambient air. The density difference takes account of changes due to both the presence of the gas mixture and to atmospheric stratification. (Note that the temperature of the air which is entrained to be incorporated in this mixture is taken to be that at height $z=H_{eff}/2$. See discussion in Puttock, 1987, section 2.3.)

The function $\Phi(Ri_*)$ in equation (3.2) describes the influence of the density stratification on the diffusion in the vertical direction and is obtained from experimental data as we will show later in sections 3.2 - 3.6.

We can obtain an equation for S_z in the two dimensional case by substituting equations (2.1), (3.1) and (3.3) into equation (3.2), and

making use of the conservation of mass flux ($\int_0^\infty cu_x dz = \text{constant}$). We then find that the dispersion coefficient $\dot{S}_z(x)$ can be determined from the following ordinary differential equation:

$$\frac{d}{dx} \left(\frac{S_z}{z_0} \right)^{1+\alpha} = - \frac{k}{z_0} \frac{u_*}{u_0} (1+\alpha)^2 / \Phi(Ri_*) \quad \dots(3.8)$$

It is now convenient to define the horizontal transport velocity of the emitted gas in the plume, averaged over the plume height, which is given by:

$$u_{eff} = \frac{\int_0^\infty u_x c dz}{\int_0^\infty c dz} \quad \dots(3.9)$$

Using for u_x and c expressions (2.1) and (2.2b) we find:

$$u_{eff} = \left(\frac{S_z}{z_0} \right)^\alpha \frac{1}{\Gamma \left(\frac{1}{1+\alpha} \right)} u_0 \quad \dots(3.10)$$

The entrainment velocity is defined for a plume with well-defined edges as the rate of mixing of air into the plume per unit surface area per unit time. In this case we can define an analogous entrainment velocity u_e by:

$$u_e = \frac{d}{dx} (u_{eff} H_{eff}) \quad \dots(3.11)$$

which, using expressions (3.6) and (3.10) for H_{eff} and u_{eff} , can be expressed as:

$$u_e = \frac{u_0}{z_0^\alpha (1+\alpha)} \frac{d}{dx} S_z^{1+\alpha}$$

and, making use of Equation (3.8) we find :

$$u_e = (1+\alpha) k u_* / \Phi(Ri_*) \quad \dots(3.12)$$

Equation (3.8) describes the entrainment of air into the plume if the plume width is constant, so that the problem is two-dimensional. This condition does not hold for a dense vapour plume, which will spread laterally due to the density difference with the surrounding air. For this case, Equation (3.8) has been generalised into

$$\frac{d}{dx} \left[B_{eff} \left(\frac{S_z}{z_o} \right)^{1+\alpha} \right] = \frac{k}{z_o} \frac{u_*}{u_o} (1+\alpha)^2 B_{eff} / \Phi(Ri_*) \quad \dots(3.13)$$

The variable B_{eff} is the effective half-width of the plume, defined by

$$B_{eff} = b + \frac{\sqrt{\pi}}{2} S_y \quad \dots(3.14)$$

This definition has been chosen because integration of the similarity profile for the concentration (Equation 2.2) in the y-direction gives

$$\int_0^\infty c(x,y,z) dy = c_A \left(b + \frac{\sqrt{\pi}}{2} S_y \right) \exp \left[- \left(\frac{z}{S_z} \right)^{1+\alpha} \right]$$

The crosswind gravity-spreading of the plume is discussed in Section 4.

3.2 Entrainment rates determined in a wind tunnel

The dilution of the gas is effected by vertical mixing of air into the plume. This is determined by the entrainment function $\Phi(Ri_*)$. The form of $\Phi(Ri_*)$ is derived from laboratory data. A variety of laboratory experiments on entrainment through density interfaces have been performed which appear to be relevant. However, they give contradictory results. Further study has shown that the flow in some apparently simple experiments is much more complex than assumed; consequently, the data from these experiments must be discounted. Because of the importance of the vertical mixing in the dispersion, the next few sections comprise a discussion of the experimental data, leading to the formulation of the expression for $\Phi(Ri_*)$ used in HEGADAS.

Britter (1980) analysed the experiments carried out by McQuaid (1976) in a 29 m long wind tunnel with a width of 0.3 m. Dense carbon dioxide gas was introduced 16 m from the entrance at the bottom of the tunnel through a 0.3 x 0.05 m porous plate. Measurements of velocity and concentration were made up to 5 m downwind of the centreline of the source. From a measured ground level concentration c_A , Britter defined the local heavy gas layer height H as:

$$H = \frac{\rho_E q_E}{c_A u} \quad \dots(3.15)$$

where ρ_E is the density of the emitted carbon dioxide and q_E the source strength (in m^3/s per meter tunnel width) and u is the mean velocity in the tunnel ($\approx 0.8 u_{\text{max}}$). When ρ and ρ_a are the densities of the gas mixture and air, respectively, we can write:

$$\rho = c_A + \left(1 - \frac{c_A}{\rho_E}\right) \rho_a \quad \dots(3.16)$$

and

$$\Delta\rho = \rho - \rho_a = c_A \frac{\rho_E - \rho_a}{\rho_E} = c_A \frac{\Delta\rho_o}{\rho_E} \quad \dots(3.17)$$

The bulk Richardson number derived from these parameters is $Ri_B = g \frac{\Delta\rho}{\rho_a} \frac{H}{u^2}$,

in which we substitute Equations (3.15) and (3.17) for H and $\Delta\rho$ to obtain:

$$Ri_B = g \frac{\Delta\rho_o}{\rho_a} \frac{q_E}{u^3} = \text{constant} \quad \dots(3.18)$$

From the experimental data Britter determined the entrainment rate u_e/u as a function of this bulk Richardson number, Ri_B . McQuaid gives

$(u_*/u)^2 = 1.7 \times 10^{-3}$ in the working section of the tunnel in the absence of any dense fluid and hence we find: $Ri_* = Ri_B/0.0017$ and

$u_e/u_* = 24.3 \times (u_e/u)$. This dimensionless entrainment rate u_e/u_* as a function of Ri_* is given in Figure 2 (McQuaid data points).

3.3 Annular entrainment studies in the laboratory

In several publications results are given of experiments on interfacial mixing between a heavy fluid layer and a light fluid layer on top of it. The best resemblance with atmospheric dispersion under stably stratified conditions with wind is observed in experiments where the turbulence is supported by a shear flow. Such a flow is generated either by a surface stress acting on the upper layer (Kantha et al., 1977, Kato and Phillips, 1969) or by horizontal jets, either in the top layer (Ellison and Turner, 1959) or in the bottom layer (Lofquist, 1960, Moore and Long, 1971). The experimental results on interfacial mixing are presented in the form of a non-dimensional entrainment velocity as function of a bulk Richardson number.

The experiments of Kantha, Phillips and Azad (1977) (hereafter KPA) were conducted in an annular tank. A constant stress $\tau = \rho u_*^2$ was applied by a rotating screen at the surface of a stratified fluid consisting of a light upper layer and a heavy bottom layer. The depth H of the mixed upper layer and the screen velocity were observed in time.

The initial condition consisted of two layers with uniform densities and a density difference $\Delta\rho_0$. During an experiment the density of the upper layer appeared to remain uniform and increased with increasing layer depth H ; the density of the bottom layer remained at its initial value. The bulk Richardson number Ri_* remained constant during an experimental run, and the entrainment velocity u_e was derived from the observations of the rate of change of H .

The entrainment relation used originally in HEGADAS was based in part on the KPA data. However, further experiments with annular tanks have shown that the results are not directly applicable. Scranton and Lindberg (1983) used density and velocity probes to study in more detail flow patterns and entrainment in rotating screen experiments. They found an extremely inhomogeneous distribution of turbulence energy over the radius of the annulus with very high turbulence levels close to the outer wall. From their observations they derived a conceptual flow model as given in Figure 3. They concluded that these experiments show a complex three-dimensional, nonhomogeneous flow with secondary motions due to channel curvature. Entrainment was observed to occur only in the outer portion of the interface. Figure 4 indicates the experimental variability in annular entrainment studies. Although it is a simplistic representation of the experiments, involving many parameters, it serves as an illustration that results differ widely depending on experimental details.

3.4 Entrainment rates determined in a wind flume

Kranenburg (1984) studied entrainment rates between stably stratified water layers in a wind flume. The flume contained two water layers: a dense bottom layer and a light top layer of fresh tap water. The relative density difference, varying from 0.005 to 0.039 was obtained by sodium chloride, dissolved in the bottom layer. The initial depth of the upper layer was 0.10 m in all experiments. A fan sucked air through an air intake constructed at the upstream end wall. The air velocities at 0.1 m above the water surface varied from 4 to 11 m/s. The shear stress exerted by the air flow on the water surface was determined from measured velocity profiles in air and water and from pressure-difference measurements in the

air. The three methods produced consistent values of u_* . The presence of the end walls limits the duration of an experiment since the surface shear stress generates an accelerating mean flow in the wind direction in the top layer and a flow against the wind in the bottom layer. It was necessary to extend the duration of the experiments at larger values of Ri_* since the time for the entrainment process to become fully developed increases, and the entrainment rate decreases, as Ri_* increases. In the larger Ri_* experiments the water transported in the upper layer was selectively withdrawn with an adjustable skimmer valve at the downstream end, pumped back and discharged smoothly at the upstream end. Kranenburg corrected the results of the entrainment experiments for some additional mixing caused by this procedure.

Entrainment rates u_e of dense fluid into the top layer were determined from the rate of increase of the top layer depth H , read from filmed shadowgraph images: $u_e = dH/dt$. In the fully developed entrainment

process the Richardson number $g \frac{\Delta \rho}{\rho} \frac{H}{u_*^2}$ is constant and hence the

entrainment rate is also constant. The dimensionless entrainment rates u_e/u_* measured by Kranenburg are given in Figure 2.

3.5 The Entrainment relation used in HEGADAS for stable stratification

For entrainment of air into a heavy gas layer at ground level we return to Equation (3.12).

$$u_e = (1+\alpha) k u_* / \Phi(Ri_*)$$

For the determination of the function $\Phi(Ri_*)$ we have used the experimental data of McQuaid and Kranenburg discussed above. The geometry of the McQuaid experiments very well simulated atmospheric plume

dispersion, but the Richardson numbers in large heavy gas emissions at low wind speed conditions may exceed the range of these experiments. For high Richardson numbers we fitted our entrainment relation to the Kranenburg data, which agree well with McQuaid's data for overlapping Richardson numbers. For large values of Ri_* the entrainment rates measured by Kranenburg are substantially larger than the data from the annular entrainment experiments discussed in Section 3.3. However, Price (1979) and Thompson (1979) extrapolated the KPA results to zero aspect ratio and found $u_e/u_* = (0.8 \pm 0.1) Ri_*^{-1/2}$. This $Ri_*^{-1/2}$ behaviour was also predicted by several numerical models (Kranenburg, 1984) and is in good agreement with the Kranenburg data. In view of the large uncertainties associated with the annular entrainment experiments due to curvature, the former HEGADAS entrainment relation, which was based for high Ri_* on KPA, has been replaced by one based on the Kranenburg data .

The Φ - function now reads:

$$\Phi(Ri_*) = (1.0 + 0.8 Ri_*)^{1/2} \text{ for } Ri_* > 0 \quad \dots(3.19)$$

Graphical representations of u_e/u_* , expressed in equations (3.12) and (3.19), are given in Figure 2 for $\alpha = 0.1$ and 0.7 . In theory the value of α may vary between zero and one but in almost all applications of the model the possible range will be from 0.1 (very low surface roughness; neutral atmospheric stability) to 0.7 (high surface roughness; stable atmosphere).

As a consequence of the definition of $\Delta\rho$, the formulation is equally applicable to the dispersion of a trace gas in a stable ambient atmosphere, where $\Delta\rho > 0$ owing to the ambient density gradient. It remains

to be seen whether it provides a good description of such dispersion with Φ given by (3.19). This is covered in Section 3.6 below.

Two comments can be made in relation to the adoption of equation (3.19). First, it is more conventional to use an expression where $\Phi \sim Ri_*^{-1}$ for large Ri_* , rather than $\Phi \sim Ri_*^{-\frac{1}{2}}$. However, most of the experiments which have been used to support Ri_*^{-1} have been experiments without mean shear (e.g. Turner, 1968), or those, such as KPA, where the initial simple interpretation has been shown to be inappropriate. As emphasised by Britter (1988) the mechanisms of entrainment through strong density gradient can be different when driven by mean shear rather than by external turbulence. In the same paper, Britter suggests that even the McQuaid data are approaching a Ri_*^{-1} asymptote at the largest Ri_* ; however, the data in fact fit the $Ri_*^{-\frac{1}{2}}$ asymptote of Equation (3.19) just as well, if not better.

Second, we agree with the contention of Britter (1988) that dense gas releases, when not constrained laterally, spread so that Ri_* very rapidly reaches the range of the McQuaid data. Thus the form of the Φ function for larger values of Ri_* may be almost irrelevant in practical terms. This is consistent with our observation that changing to equation (3.19) from the previous relation based on KPA has made very little difference to practical dispersion predictions.

3.6 Vertical dispersion in an unstable atmosphere

For non-neutral atmospheric stability the value of $\rho_a(z = H_{eff})$ in Equation (3.8) is obtained from Businger's (1975) relation for the potential temperature in the atmospheric surface layer, given the roughness length z_R , the Monin-Okubkhov length λ , the friction velocity u_* and the

air temperature at ground level. For unstably stratified conditions ($Ri_* < 0$), we have arranged $\Phi(Ri_*)$ to be compatible with the results of the Prairie Grass tracer dispersion experiments.

In the Prairie Grass Project, sulphur dioxide was released as a tracer from a steady-state point source at a height of 0.46 m. Concentrations were measured at a height of 1.5 m along arcs at distances of 50 m, 100 m, 400 m and 800 m from the source. We used the experimental data presented by Horst (1979). He calculated a normalised concentration $u_* \chi / E$ by dividing the crosswind-integrated concentration $\chi(z=1.5m)$ by the source strength E , and multiplying it by the friction velocity u_* . The experimental values as a function of $1/\lambda$ are shown as dots in Figure 5. Positive values of λ correspond to stable atmospheric conditions, negative values of λ to unstable ones. Horst used Businger's (1973) relations for the vertical profiles of wind velocity and temperature and fitted them to the observed profiles to estimate the Monin-Obukov length λ for a height of 2 m and the friction velocity u_* for each diffusion experiment; the roughness length he used was $z_R = 0.6$ cm.

The open symbols in Figure 5 denote cases where the computed λ varied by more than a factor of 2 between heights of 1 m and 4 m. This indicates that Businger's relations were not compatible with the observed profiles of wind velocity and temperature.

By choosing

$$\Phi(Ri_*) = (1 - 0.6 Ri_*)^{-0.5} \quad \dots (3.20)$$

for unstable conditions (Ri_* and $\lambda < 0$) a good fit between the HEGADAS calculations and the Prairie Grass data was obtained, as is shown by the

curve in Figure 5. Figure 5 also shows that the data for stable conditions are well predicted using Φ as in Equation (3.19).

Expression (3.20) is used in the model calculations whenever Ri_* becomes negative, irrespective of whether it is due to cloud buoyancy or to unstable atmospheric stratification.

4. GRAVITY SPREAD AND LATERAL MIXING

4.1 The cross-wind dispersion coefficient S_y

[Note further discussion of this topic in the main report section 5.3]

The crosswind dispersion coefficient S_y is determined in a way very similar to the method described by te Riele (1977). Consider first the widely used crosswind concentration distribution

$$c = c_A \exp \left\{ -\frac{1}{2} \left(\frac{y}{\sigma_y} \right)^2 \right\} \quad \dots(4.1)$$

Experimental data on crosswind dispersion from ground level point sources have been collected in the Gifford-Pasquill system (Turner, 1969), this giving the crosswind dispersion coefficient σ_y as a function of the downwind distance.

This dependence may be well approximated by a power law.

$$\sigma_y = \delta x^\beta \quad \dots(4.2)$$

To extend this to our similarity profile with uniform mid-part, we assume that the turbulent crosswind diffusion coefficient K_y is directly proportional to the wind velocity u_x and the half-width of the concentration profile W (to be defined later) to some power γ , such that

$$K_y = K_o u_x W^\gamma, \quad \dots(4.3)$$

Making use of the conservation of mass flux ($\int_0^\infty c u_x dz = \text{constant}$) it is now easily shown that (4.1), with $2^{-\frac{1}{2}} \sigma_y$ replaced by S_y , satisfies the simple two-dimensional diffusion equation

$$u_x \frac{\partial c}{\partial x} = \frac{\partial}{\partial y} \left(K_y \frac{\partial c}{\partial y} \right)$$

provided that

$$\sigma_y \frac{d\sigma_y}{dx} = K_o W^\gamma \quad \dots(4.4)$$

Taking W to be the half-width of an equivalent top-hat profile (i.e. a profile with the same centreline value and area) gives

$$W = (\pi/2)^{1/2} \sigma_y \quad \dots(4.5)$$

we then find from equation (4.4) that $\gamma = 2 - \frac{1}{\beta}$ and $K_o = \frac{2\beta}{\pi} \{\delta\sqrt{\pi}/\sqrt{2}\}^{1/\beta}$

If the middle part b in the similarity profile for the concentration (Equation (2.2)) is zero, Equation (4.4) is equivalent to

$$S_y \frac{dS_y}{dx} = \frac{4\beta}{\pi} W^2 \left[\frac{\delta\sqrt{\pi}}{W/2} \right]^{1/\beta} \quad \dots(4.6)$$

where

$$W = \frac{\sqrt{\pi}}{2} S_y$$

In the heavy gas dispersion model we assume that equation (4.6) also holds true if b is not zero. For this case we define the profile half-width W as

$$W = b + \frac{\sqrt{\pi}}{2} S_y \quad \dots(4.7)$$

A dense vapour plume will spread laterally due to the difference in density between it and the surrounding air. This gravitational spreading is taken into account with the simple spreading law.

$$\frac{dB_{eff}}{dt} = C_E \left[gH_{eff} \left(1 - \frac{\rho_a(z=0)}{\rho_m(c=c_A)} \right) \right]^{1/2} \quad \dots(4.8)$$

where C_E is the spreading constant; we now use $C_E = 1.15$, following the data analysis of van Ulden (1984).

By using the definitions of H_{eff} and u_{eff} , we obtain:

$$\frac{dB_{eff}}{dx} = \frac{1}{u_{eff}} \frac{dB_{eff}}{dt} = C \left[1 - \frac{\rho_a(z=0)}{\rho_m(c=c_A)} \right]^{\frac{1}{2}} \left[\frac{S_z}{z_o} \right]^{\frac{1}{2}-\alpha} \quad \dots (4.10)$$

with

$$C = C_E \frac{(gz_o)^{\frac{1}{2}}}{u_o} \left[\Gamma \left(\frac{1}{1+\alpha} \right) \right]^{\frac{3}{2}} (1+\alpha)^{-\frac{1}{2}} \quad \dots (4.11)$$

With B_{eff} determined by Equation (4.10) and S_y by Equation (4.6) the crosswind width b follows from Equation (3.14).

Above the source we neglect gravitational spreading ($B_{eff} = B$) and crosswind dispersion of the plume ($S_y = 0$; $b = B$). At some distance downwind, x_t , the half-width of the middle part of the concentration profile b becomes zero and downwind of this position the crosswind profile is completely Gaussian, with S_y given by:

$$S_y = \sqrt{2} \delta(x + x_v)^\beta \quad \dots (4.12)$$

where x_v can be determined from $S_y(x_t) = \sqrt{2} \delta(x_t + x_v)^\beta$.

At $x = x_t$ we assume that the lateral gravitational spreading of the plume terminates.

4.2 The ground level centreline concentration c_A

Downwind of the area source the concentration c_A can be determined from the integral mass balance

$$E = \int_0^\infty \int_{-\infty}^\infty c u_x dy dz \quad \dots (4.13)$$

where E is the source strength. Substituting in this expression the similarity profiles for c and u_x , equations (2.1) and (2.2), we find:

$$c_A = \frac{E(1+\alpha)z_o^\alpha}{2u_o S_z^{1+\alpha} (b + \frac{\sqrt{\pi}}{2} S_y)} \quad \dots (4.14)$$

Above the area source the ground level concentration is taken to be a constant.

Here we distinguish between two cases:

1. The vertical vapour mass flux Q_p is greater than the maximum vapour flux that can be taken up into the atmosphere, Q_{max}^* .

For a source of length L_p we determine Q_{max}^* as follows: above the source we take the vapour concentration to be 100 %, i.e. $c_A = \rho_E$, the 100 % gas density at emission conditions, and define Q_{max}^* by:

$$Q_{max}^* (L_p) = \frac{\rho_E}{L_p} \int_0^\infty \exp \left[- \left(\frac{z}{S_z (x=0.5 L_p)} \right)^{1+\alpha} \right] u_x dz = \frac{\rho_E u_o S_z^{1+\alpha} (x=0.5 L_p)}{(1+\alpha) z_o^\alpha L_p} \quad \dots (4.15)$$

This means that we neglect the crosswind gravitational spreading and the crosswind dispersion of the plume above the source, so then the problem is two-dimensional and Q_{max}^* does not depend on the width of the source. If now $Q_p > Q_{max}^* (L_p)$, the emitted gas cannot be directly taken up into the atmospheric wind field and a 100 % vapour blanket forms above the source. This vapour blanket is heavier than air and spreads due to gravitational forces. For the steady-state situation the gas blanket length L , half-width B , and vapour mass flux $Q^* = Q_{max}^* (L)$ must be such that the take-up rate into the atmosphere $Q^* . L . B$ is the same as the gas production rate $Q_p . L_p . B_p$. In the steady-state model we can only deal with rectangular sources of length L_p , Q_{max}^* and half-width B_p . Analogous to equation (4.15), $Q_{max}^* (L)$ can be determined from:

$$Q_{\max}^* (L) = \frac{\rho_E u_o S_z^{1+\alpha} (x=0.5 L)}{(1+\alpha) z_o^\alpha L} \quad \dots (4.16)$$

and then L and B can be calculated iteratively from the identity

$$Q_{\max}^* (L) \cdot L \cdot B = Q_p \cdot L_p \cdot B_p, \text{ assuming that } \frac{L}{L_p} = \frac{B}{B_p}.$$

In the dispersion calculation we now introduce a source length L and half-width B with a ground level concentration $c_A = \rho_E$.

2. If $Q_p \leq Q_{\max}^* (L_p)$, the emitted gas can be directly taken up into the atmosphere and no 100 % vapour blanket forms.

The source length L and half-width B for the dispersion calculation are now the same as the primary source length L_p and half-width B_p and the constant ground level concentration c_A above the source is determined iteratively in such a way that

$$\begin{aligned} Q^* &= Q_p = \frac{c_A}{L_p} \int_0^\infty \exp - \left[\frac{z}{S_z (x=0.5 L_p)} \right]^{1+\alpha} u_x dz \\ &= \frac{c_A u_o S_z^{1+\alpha} (x=0.5 L_p)}{(1+\alpha) z_o^\alpha L_p} \quad \dots (4.17) \end{aligned}$$

If the source is not rectangular we treat it as a rectangular one of the same surface area.

5. THERMAL EFFECTS

The thermodynamics of the mixing of the dense gas with ambient air are calculated in a subroutine (THERMO). It is assumed that the gas, air and water vapour behave as ideal gases with constant specific heats. For cold gas releases, the condensation of water can have a significant effect, owing to the heat of condensation liberated, and there is a smaller effect from its freezing. For gases with more complex properties (such as reaction with water), a specific subroutine to calculate the special thermodynamics in that case can easily be substituted for THERMO.

One input parameter supplied to THERMO by the model is the additional heat transferred to the cloud by heat transfer. Variation of this parameter can also make allowance for varying temperatures of entrained air. It was also found necessary, for LNG releases on the sea, to allow for variation in the water content of the cloud due to vapour transfer from the surface. The modelling of these processes is described below.

5.1 Heat transfer from the surface

5.1.1 Theory

Heat transfer from the substrate to the cold vapour cloud is described by the following expressions for forced (Holman, 1981) and natural (McAdams, 1954) convection heat flux:

$$Q_{H,f} = \frac{1}{2} \left(\frac{\alpha_T}{\nu} \right)^{2/3} C_f \rho_m C_{pm} u (T_s - T_m) \quad \dots (5.1)$$

$$\text{and} \quad Q_{H,n} = 0.14 \left[\frac{\alpha_T^2 \zeta g}{\nu} (\rho C_{pg})^3 \right]^{1/3} (T_s - T_m)^{4/3} \quad \dots (5.2)$$

where C_f is the friction factor, u the gas velocity (m/s), T_s and T_m the temperatures of substrate and mixture (K), C_{pm} the specific heat of the mixture (J/kg/K), ρ the density (kg/m³) and g the gravitational acceleration (m/s²). The expressions contain the following gas properties: α_T the thermal diffusivity (m²/s), ν the kinematic viscosity (m²/s), and C_{pg} the specific heat (J/kg/K). The parameter $\zeta = -\rho^{-1}(\partial\rho/\partial T)_p$, so for an ideal gas $\zeta = 1/T$. The friction factor $C_f = 2 (u_*/u)^2$, where u_* is the friction velocity (m/s). For methane $\alpha_T/\nu = 1.35$; for other gases this ratio is only slightly different. For u we take the logarithmic wind velocity at 10 m height, u_{10} . Thus expression (5.1) for forced convection heat flux can be written as

$$Q_{H,f} = 1.22 \frac{u_*^2}{u_{10}} \rho C_{pm} (T_s - T_m) \quad \dots (5.3)$$

For ρ , C_{pm} and T_m we take the gas mixture properties corresponding with the ground-level centre line concentration c_A . Using the ideal gas law

$P = \frac{R}{M} \rho T$, expression (5.2) for natural convection may be rewritten as:

$$Q_{H,n} = 0.14 g^{1/3} \frac{P}{R} \left[\left[\frac{\alpha_T}{\nu} \right]^2 \frac{\nu}{T^2} (M C_{pg})^3 \right]^{1/3} \left[\frac{(T_s - T_m)^2}{T} \right]^{2/3} \quad (5.4)$$

For methane, propane and air the value of the group

$$\left[\left[\frac{\alpha_T}{\nu} \right]^2 \frac{\nu}{T^2} (M C_{pg})^3 \right]^{1/3} \text{ is } 24, 29 \text{ and } 20 \text{ m}^{-2/3} \text{s}^{-1/3} \text{K}^{-5/3} \text{kmole}^{-1} \text{J, resp.}$$

If the value of this combination of constants is not specified in the input data for a model run, the methane value 24 is used.

For T in expression (5.4) we take the mean temperature $(T_s + T_m)/2$, where T_m is the gas mixture temperature corresponding to the ground-level centre-line concentration c_A . In HEGADAS the pressure P is taken to be the standard atmospheric pressure (760 mm Hg).

The approach adopted in the calculation sequence of HEGADAS is to compute the heat fluxes for both free and forced convection. For $T_s > T_m$, the maximum value of the two is selected as the heat flux from the substrate, i.e. $Q_H = \max(Q_{H,f}, Q_{H,n})$. For $T_s < T_m$, $Q_H = Q_{H,f}$ is chosen. The heat flow picked up from the substrate can be written as $(D/V_m) u_{eff} B_{eff} H_{eff}$, where D is the added heat per mole of mixture and V_m is the specific molar volume of the mixture. To take heat transfer into account, the following equation is now added to the set given in Sections 3 and 4:

$$\frac{d}{dx} \left[\frac{D}{V_m} u_{eff} B_{eff} H_{eff} \right] = Q_H B_{eff}, \quad \dots(5.6)$$

For places where the middle part of the concentration profile has disappeared ($b = 0$), we take:

$$\frac{d}{dx} \left[\frac{D}{V_m} u_{eff} H_{eff} \right] = Q_H \quad \dots(5.7)$$

The temperature T_m and density ρ of the gas/air mixture and the specific molar volume V_m are computed in the thermodynamic subroutine for a given mole fraction of the emitted gas and a given amount of added heat D . This subroutine of the HEGADAS programme also takes into account the latent heat of condensation and of freezing of water vapour present in the air;

see Appendix A. The original formulation of vertical dispersion (equation 3.13) can be written as

$$\frac{d}{dx} \begin{bmatrix} U_{eff} & B_{eff} & H_{eff} \end{bmatrix} = ku_* (1+\alpha) B_{eff} / \Phi(Ri_*); \quad \dots(5.8)$$

If the gas cloud temperature differs from ambient, relation (5.8) is not correct. For, in this case, the change in volume flow $u_{eff} B_{eff} H_{eff}$ is not affected by entrainment alone, but also by changes in the specific molar volume V_m due to heat transfer from the substrate and mixing with air of a different temperature. These effects have been taken into account by formulating the entrainment relation in terms of mole flow:

$$\frac{d}{dx} \begin{bmatrix} u_{eff} & B_{eff} & H_{eff} / V_m \end{bmatrix} = ku_* (1+\alpha) B_{eff} / (V_o \Phi(Ri_*)) \quad \dots(5.9)$$

with V_o the molar volume of air. If the constant middle part of the concentration profile has disappeared ($b = 0$), we now use:

$$\frac{d}{dx} \begin{bmatrix} u_{eff} & H_{eff} / V_m \end{bmatrix} = ku_* (1+\alpha) / (V_o \Phi(Ri_*)). \quad \dots(5.10)$$

5.1.2 Experimental test

In order to study the processes of heat transfer, water vapour transfer and convective entrainment in dense gas clouds, a series of laboratory experiments involving cold nitrogen flowing across a water surface were conducted. These are described by Colenbrander and Puttock (1984) and in Appendix D. The results of series 3 of the experiments (heat

transfer without water vapour transfer) were used to test this heat transfer relation.

The natural convection heat flux is calculated for the conditions at the middle of the box (location B) during the series 3 experiment. For the vapour temperature we found $T_g = 161.4$ K and for the oil surface temperature we take $T_s = 286$ K.

Hence we find

$$Q_{H,n} = 75 \times 16.9 \text{ Wm}^{-2} = 1270 \text{ Wm}^{-2} \quad (5.11)$$

The forced convection heat flux was calculated with equation (5.1), using $\alpha_T/\nu = 1.35$ and $C_f = 0.005$. For u in equation (5.1) we took the bulk velocity of the vapour stream, which was calculated from the nitrogen flow rate and the estimated height of the vapour stream as outlined below.

The nitrogen release rate was taken to be 83 kg/h, i.e. the rate at 700s from the start of the release. At a temperature of 161.4 K we find a density of 2.1 kg/m^3 and hence a volume flow rate of $0.011 \text{ m}^3/\text{s}$. From the temperature profiles we determined the height of the vapour stream to be 0.06 m. Since the width of the box was 1 m we then arrived at a bulk velocity $u = 0.18 \text{ m/s}$. Equation (5.1) then gives $Q_{H,f} = 150 \text{ Wm}^{-2}$ which is almost an order of magnitude smaller than the calculated free convection heat flux.

The calculated free convection heat flux $Q_{H,n} = 1270 \text{ Wm}^{-2}$ is some 20% lower than the heat flux, calculated from the measured temperature increase.

We also used HEGADAS to calculate the temperature increase between location A and C. As gas emission temperature we took 140.6 K, the measured temperature at location A. The nitrogen release rate was

83 kg/h. The "wind velocity" was taken to be 0.18 m/s at a reference height of 0.01 m. The roughness length was chosen to be 10^{-5} , giving $u_* = 0.01$ m/s. The gravitational spreading and dispersion in the crosswind direction were set to zero and the plume width was taken constant.

Figure 6 shows the HEGADAS calculation of the heat transfer rate, compared with observations. The calculation gives an air concentration increase of 1.3% per 0.5 m, in agreement with the experimental findings. Air entrainment is further discussed in Section 5.3.

5.2 Transfer of water vapour from a water surface into the cloud

The mechanism by which condensation within the thermal boundary layer can increase the rate of evaporation from a liquid surface has been described by Turkdogan (1964) and Rosner (1967). In the following, we take the theoretical approach of Rosner (1967).

Figure 7 shows schematically vapour pressure profiles immediately above the surface of a liquid evaporating into a colder gas. It is assumed (and confirmed *a posteriori*) that the condensation does not significantly change the temperature profile across the boundary layer. Curve A shows the vapour pressure profile in the absence of any condensation. If there were condensed water present at all levels in the boundary layer, then the vapour pressure profile would be curve B, which is the equilibrium vapour pressure corresponding to the local temperature at each level. In fact, provided foreign nuclei are not available in this region, condensation cannot begin until the vapour pressure reaches critical supersaturation s_{crit} , which is again a function of the local temperature, and is indicated as curve C. The actual vapour pressure profile, therefore, must intersect

curve C. It can be shown that the stable solution is the one in which the profile is tangential to curve C, i.e. curve D.

Rosner presents solutions of the transcendental equation for the dimensionless form Δ of the reduced boundary layer thickness δ_n , where

$$\Delta \equiv \frac{\delta_n}{T_s} \left[- \frac{\partial T}{\partial z} \right]_{z=0}, \quad \delta_n \equiv p_{wv}(0) / \left[- \frac{\partial p_{wv}}{\partial z} \right]_{z=0} \quad (5.12)$$

Δ is a function of three dimensionless parameters

$$N^* \equiv \frac{N}{R T_s}, \text{ where } N \equiv R \left[\frac{d(\ln s_{crit})}{d(1/T)} \right]_{T=T_s} \approx \text{const.}, \quad (5.13)$$

$$L^* \equiv \frac{c_p}{R T_s}, \quad D^* \equiv s_{crit}(T_s).$$

For water, N/R is approximately 1200 K (Derived from data in Figure 7-4 of Pruppacher and Klett, 1978). With the use also of values of L^* and D^* appropriate to water, Rosner's plotted results then give values of Δ which are in the range 0.20 ± 0.01 for $0^\circ\text{C} \leq T_s \leq 30^\circ\text{C}$. We therefore use the value 0.20 for Δ .

The water vapour flux from the surface is then

$$Q_{wv} = \frac{1}{\Delta} \frac{(p_{wv}(T_s) - p_{wv}(T_m))}{C_{pm} T_s p} Q_H \quad \dots(5.14)$$

In this expression we substitute for Q_H the heat flux calculated as described in section 5.1. For C_{pm} we take the gas mixture properties corresponding with the ground-level centre line concentration C_A .

The transfer of water vapour from the surface is then taken into account in HEGADAS by adding a further differential equation:

$$\frac{d}{dx} \left[y_{w3} u_{eff} B_{eff} H_{eff} / V_m \right] = Q_{wv} B_{eff}$$

or

...(5.15)

$$\frac{d}{dx} \left[y_{w3} u_{eff} H_{eff} / V_m \right] = Q_{wv}$$

if the middle part of the concentration profile has disappeared ($b = 0$).

In these expressions y_{w3} is the molar fraction of picked-up water vapour in the cloud.

The picked-up water vapour also contributes to the total molar flow in the cloud and we therefore extend the entrainment relations (5.9) and (5.10) to, respectively.

$$\frac{d}{dx} \left[u_{eff} B_{eff} H_{eff} / V_m \right] = \left[k u_* (1 + \alpha) / (V_o \Phi(Ri_*)) + Q_{wv} \right] B_{eff} \quad (5.16)$$

and, if $b=0$,

$$\frac{d}{dx} \left[u_{eff} H_{eff} / V_m \right] = k u_* (1 + \alpha) / (V_o \Phi(Ri_*)) + Q_{wv} \quad (5.17)$$

Solution of the set of differential equations by HEGADAS gives y_{w3} as a function of downwind distance x . Given y_{w3} , the thermal effects are automatically taken into account in the THERMO subroutine.

The predictions of this model can be tested against the nitrogen-box experiments. In Figure 8, the observations of the increase in water content between locations A and C in the series 2 experiments are shown. The predictions of HEGADAS are in good agreement with these

observations. In Figure 9, the predicted temperature increase with distance for the series 2 experiments is plotted together with the experimental data. Incorporation of water vapour pick-up gives very good agreement.

5.3 Convective entrainment

The objective of the laboratory experiments described in Appendix D was to study air entrainment caused by convective advection due to the temperature difference between the substrate and a cold vapour cloud.

To characterise the turbulence in a free convection layer a velocity scale w_* has been defined

$$w_* \equiv \left[\frac{g Q_H H_{eff}}{T_m \rho_m C_{pm}} \right]^{1/3} \quad \dots(5.18)$$

where H_{eff} is the layer height.

We estimated the heat flux Q_H at location B in the series 3 experiments to be 1.6 kW/m^2 . The height of the vapour stream for these experiments was found to be 0.06 m and $M C_p = 29.3 \text{ kJ/kmole}$ for nitrogen vapour. Using the numerical values of g , R and the atmospheric pressure p , we find $w_* = 0.14 \text{ m/s}$. This value is an order of magnitude larger than the estimated value for u_* : 0.01 m/s .

Several proposals have been made for model formulations to describe convective entrainment (Eidsvik, 1980; Zeman, 1982; Jensen and Mikkelsen, 1984). We follow the simple approach of Eidsvik by taking

$$u_T \equiv [u_*^2 + (a w_*)^2]^{1/2} \quad \dots(5.19)$$

as the velocity scale determining the turbulent entrainment rate. The constant a is determined experimentally as shown below. The full mathematical representation of vertical entrainment in HEGADAS is now obtained by replacing u_* with u_T in relation (5.16)

$$\frac{d}{dx} \left[u_{eff} B_{eff} H_{eff} / V_m \right] = \left[k u_T (1 + \alpha) / (V_o \Phi(Ri_T)) + Q_{wv} \right] B_{eff} \quad (5.20)$$

where Ri_T is given by equation (3.5) with u_* replaced by u_T .

After incorporation of the model formulation for convective entrainment HEGADAS calculations were done for the conditions during the series 2 experiments. The value of the constant a was chosen to fit the experimental data on air entrainment. Good agreement was obtained for $a = 0.2$ (Figure 10) so

$$u_T = [u_*^2 + (0.2 w_*)^2]^{1/2} \quad \dots(5.21)$$

6. THE TIME-DEPENDENT MODEL

The formulation described above provides the steady state version of the HEGADAS model. The time-dependent version of the model is capable of dealing with arbitrary time variation of the release rate of gas at the source, such as might be derived from an evaporating liquid pool.

6.1 Sources with time-dependent vapour emission rate and/or dimensions

As an example of a source with time-dependent vapour emission rate, a stationary, boiling liquefied gas pool in a diked area will be suitable. Here, as the ground cools down, the heat flux to the boiling pool decreases, resulting in a decreasing boil-off flux with time. For a spreading liquefied gas pool on land not only is the evaporation flux time-dependent but also the dimensions of the pool.

For use in the time-dependent dispersion model we assume the source to be circular with a radius $R_p(t)$, given as a function of the time t . If the source has another shape, it is represented as a circular one of the same surface area. In addition to $R_p(t)$, the vapour production rate $E(t)$ must be specified as a function of the time. We assume that the vertical vapour flux Q_p from the source is uniform over the source, so:

$$Q_p(t) = E(t)/(\pi R_p^2(t)) \quad \dots (6.1)$$

If this vertical vapour flux $Q_p(t)$ is less than the maximum flux that can be taken into the atmospheric flow field, Q_{max}^* , the gas is directly taken up by the wind.

The value of $Q_{\max}^*$ is calculated with the steady-state model and since we can only handle rectangular sources in the steady-state dispersion calculations, a circular source is treated as a square source of side $L = \sqrt{\pi} R_p(t)$ and for this source length the maximum take-up flux $Q_{\max}^*$ ($L = \sqrt{\pi} R_p(t)$) is calculated.

If $Q_p(t) > Q_{\max}^*$ ($L = \sqrt{\pi} R_p(t)$), the emitted gas cannot be directly taken up into the atmospheric wind field and a 100 % dense vapour blanket forms above the source. This gas blanket is taken to have a flat cylindrical shape of radius $R_g(t)$ and height $H_g(t)$. At the bottom of the blanket, gas is supplied from the source at a rate $E(t)$, while from the top, gas is taken up into the wind field at a rate $\pi R_g^2(t) Q_{\max}^*$ ($L = \sqrt{\pi} R_g(t)$), so that the mass balance for the gas blanket reads:

$$\frac{d}{dt} \left[\pi \rho_E R_g^2(t) H_g(t) \right] = E(t) - \pi R_g^2(t) Q_{\max}^* (L = \sqrt{\pi} R_g(t)) \dots (6.2)$$

It is assumed that the centre of the gas blanket remains stationary at $x = 0$. This assumption introduces relatively small errors, firstly because the height of the gas blanket is small and the wind velocity close to the earth's surface is low. Approximate calculations indicate that if the blanket were to travel with the wind, the distance travelled downwind by the blanket until it had been taken up completely would be very short. Secondly, a considerable mass has to be accelerated to the wind velocity; this reducing the travelled distance even more.

Owing to the density difference with the surrounding air, the blanket will slump and spread laterally. In order to describe this gravitational spreading we use the simple spreading law

$$\frac{d R_g(t)}{dt} = C_E \left[g H_g(t) \left(1 - \frac{\rho_a(z=0)}{\rho_E} \right) \right]^{\frac{1}{2}} \dots (6.3)$$

analogous to equation (4.8) describing the crosswind gravitational spreading of the plume. Given $E(t)$ and the appropriate initial conditions we can now solve the radius $R_g(t)$ and height $H_g(t)$ of the gas blanket as functions of time. If it appears that the radius of the source $R_p(t)$ is greater than $R_g(t)$, we put $R_g(t) = R_p(t)$ and adapt the calculated value of $H_g(t)$ accordingly. Thus the radius of the gas blanket is then always equal to or greater than the radius of the source.

If a gas blanket is present, the take-up flux into the atmosphere $Q^*(t)$ is taken to be $Q_{max}^* (L - \sqrt{\pi} R_g(t))$, so the take-up is no longer dependent on $Q_p(t)$. We therefore introduce here the concept of a secondary source of radius $R(t) = R_g(t)$ and take-up flux $Q^*(t) = Q_{max}^* (L - \sqrt{\pi} R_g(t))$. If no gas blanket is present the take-up flux $Q^*(t)$ is $Q_p(t)$ and we define the secondary source radius to be the same as that of the real source:

$$R(t) = R_p(t)$$

Summarising, we have defined the secondary source parameters as follows:

$$R(t) = R_g(t)$$

if a gas blanket is present

$$Q^*(t) = Q_{max}^* (L - \sqrt{\pi} R_g(t))$$

and

$$R(t) = R_p(t)$$

if no gas blanket is present.

$$Q^*(t) = Q_p(t)$$

... (6.4)

6.2 The transient dispersion model

In order to visualise the quasi-steady-state description of the transient behaviour of dense vapour clouds, we will follow observer "i", one of a number of observers travelling at a regular time interval Δt over the source. The subscript i refers to quantities associated with observer i.

The velocity $u_i(t)$ of observer i is time-dependent; the way in which it is related to the wind velocity u_x is described in Appendix A. The observer velocity increases with downwind distance and for all observers their velocity at a given location x is the same ($u_i(x) = u_{i+1}(x)$). This implies that at a given time t the velocity of observer i is greater than the velocity of the following observer ($u_i(t) > u_{i+1}(t)$).

Let observer i encounter the upwind edge of the secondary source at $t = t_{1i}$ and the downwind edge at $t = t_{2i}$ (see Fig. 11) and let $x_i(t)$ be the location of this observer at time t. As can be seen from Fig. 11 the local secondary half-width of the source $B'_i(t)$ observed at time t is given by:

$$B'_i(t) = \sqrt{R^2(t) - x_i^2(t)} \quad \dots (6.5)$$

The secondary source area A_i seen by observer i is found by evaluating the integral

$$A_i = \int_{t_{1i}}^{t_{2i}} 2 u_i(t) B'_i(t) dt \quad \dots (6.6)$$

The secondary source length L_i as seen by observer i is given by:

$$L_i = x_i(t_{2i}) - x_i(t_{1i}) \quad \dots (6.7)$$

and thus we find an average observed secondary half-width of the source

$$B_i = A_i/2L_i \quad \dots (6.8)$$

Similarly, the average take-up flux Q_i^* of observer i may be found from:

$$Q_i^* B_i L_i = \int_{t_{1i}}^{t_{2i}} Q^*(t) B'_i(t) u_i(t) dt \quad \dots (6.9)$$

In this way we can determine, for each of the n observers travelling over the source ($i = 1, n$), the observed dimensions L_i and B_i , the locations $x_i(t_{1i})$ and $x_i(t_{2i})$ of, respectively, the upwind and the downwind edge of the secondary source and the average take-up flux Q_i^* . From these the concentration distribution in the cloud can be determined at a specified time t_s .

To this end the location $x_i(t_s)$ of each observer at time t_s is calculated and for each observer a steady-state calculation is done, using the pertinent parameters L_i, B_i, Q_i^* and $x_i(t_{2i})$. Thus the concentration distribution parameters $c_A(x_i(t_s)), S_y(x_i(t_s)), b(x_i(t_s)), S_z(x_i(t_s))$ are determined for $i = 1, n$ and thus the concentration distribution $c(x_i(t_s), y, z)$, given by equation (2.1).

It will be clear that in this quasi-steady state approach the gravitational spreading of the cloud in the wind direction cannot be taken into account, unlike in heavier gas dispersion model for strictly instantaneous vapour releases, see Cox and Roe (1977) and Germeles and Drake (1975). Thus, the width of the cloud calculated with the model

presented here will be somewhat too large and the length too small, especially at very low wind velocities. In the calculated concentration levels in the bulk of the cloud we only introduce second order errors with this approach. We find the alternative, a model for an instantaneous release, less useful, since a spill will only occasionally result in a strictly instantaneous vapour release. (However, see section 6.5 below.) Some spreading in the wind direction is introduced in the gas blanket calculation, where we can use a radial spreading law because the centre of the gas blanket is assumed to remain stationary above the source at $x = 0$. In addition, a correction algorithm has been devised for use at the end of the calculation, which redistributes part of the lateral gravity spread to longitudinal spreading (see Appendix C). An input parameter determines whether this correction is applied.

For releases of short duration, dispersion in the wind direction may have a significant influence on the concentration level in the cloud. Accordingly, the calculated concentrations are adjusted to take account of this dispersion in the x-direction. The method followed is described in the next section.

6.3 Dispersion in the wind direction

[Note further discussion of this topic in the main report section 7.4]

Experiments have shown that the ground level gas concentration distribution due to an instantaneous release of $e \text{ kg/m}^2$ tracer gas from an infinite crosswind plane source at $x = 0$ can be reasonably well described by:

$$c(x; x_o) = \frac{e}{\sigma_x(x_o)(2\pi)^{\frac{1}{2}}} \exp \left[- \frac{(x - x_o)^2}{2\sigma_x^2(x_o)} \right] \quad \dots (6.10)$$

In this expression x_0 represents the location of the centre of gravity of the puff and is a function of the time elapsed since the release because the puff travels with the wind.

Literature data on σ_x as function of the downwind distance are scarce and not very well established see Beals (1971), Davies and Shair (1974), Suffman (1962), Tyldesley and Willington (1965) and Chatwin (1968). These data have been partly obtained from theoretical considerations and partly from experiments. On the basis of these data we have taken

$$\sigma_x(x_0) = a_x x_0^{b_x} \quad \dots (6.11)$$

for all atmospheric stability classes.

Let $c_A(x)$ be the ground level axis concentration of the plume, calculated as described earlier. We consider this concentration distribution as being due to the release of successive puffs of varying quantity $c_A(x_p) dx$ without dispersion in the x direction (see Fig. 12). Analogous to equation (40), the dispersion in the x -direction is taken into account by replacing an element of the concentration distribution of height $c_A(x_p)$ and width dx by an element with a Gaussian distribution

$$c'_A(x; x_p) = \frac{c_A(x_p) dx}{\sigma_x(x_p) (2\pi)^{\frac{1}{2}}} \exp \left[- \frac{(x - x_p)^2}{2\sigma_x^2(x_p)} \right] \quad \dots (6.12)$$

having the same area $c_A(x_p) dx$ (see Fig. 3).

The concentration distribution, corrected for dispersion in the x -direction, $c'_A(x)$ is then found by adding up the contributions to the concentration at point x of all the Gaussian distributed elements:

$$c'_A(x) = \frac{1}{(2\pi)^{\frac{1}{2}}} \int_0^\infty \frac{C_A(\xi)}{\sigma_x(\xi)} \exp \left[- \frac{(x-\xi)^2}{2\sigma_x^2(\xi)} \right] d\xi \quad \dots (6.13)$$

The only variable in the spatial concentration distribution, equation (2.2), which is corrected for this dispersion is the cloud axis concentration c_A . Even in a non-instantaneously released, but neutrally buoyant cloud, this correction would not be strictly rigorous for locations off the cloud axis since the variables S_y , b and S_z depend on the x -location in the cloud. This applies more to a heavy gas cloud where the growth of S_y , b and S_z with the downwind distance x depends on the local gas concentration. It does not seem possible, however, to apply a more rigorous correction for dispersion in the x -direction without moving away from the basic concepts of the discussed model.

6.4 Solution of the equations

The equations describing the time-dependent heavy gas dispersion problem given in the preceding sections are solved in a computer program written in Fortran 77. As input for this dispersion program, HEGADAS (heavy gas dispersion from area sources), the vapour production rate and source radius have to be given as functions of time. In addition, HEGADAS requires the atmospheric flow field parameters ρ_a ($z = 0$), u_o , z_o , z_R , λ , the point source dispersion parameters δ and β , the spreading constant C_E and the gas density ρ_E .

The program calculates the value of α and the dispersion parameters $c_A(x)$, $S_z(x)$, $S_y(x)$ and $b(x)$ at fixed distance intervals Δx and at specified times. Then the spatial concentration distribution at a specified time is given by relation (2.2). The program also evaluates the coordinates of concentration isopleths in the $y = 0$ and $z = 0$ planes at a given time for two specified concentration values c_u and c_L . Further, it calculates the vapour mass and the volume of those parts of the cloud where the concentration is $\geq c_L$ and $\geq c_u$. The latter feature enables us to

determine, for example, the cloud content between the flammability limits c_{UFL} and the iso-concentration contours for these concentration levels at specified times in the case of a flammable gas release.

6.5 Instantaneous gas release

For an instantaneous release of gas, or in very low winds, gravity spreading of the cloud in all directions, rather than just laterally, is important. For these circumstances, the model "HEGABOX" has been developed which treats the cloud as an expanding cylinder in its early stages (Puttock, 1988a). It has a smooth transition into HEGADAS for calculation of the dispersion further downwind, if required.

7. COMPARISON WITH EXPERIMENT

In the development of the model, the empirical input has been derived from laboratory experiments which, as far as possible, isolate the various physical mechanisms being considered. Comparison of model predictions with field data are then a validation of the model, rather than "calibration". (In the case of water vapour transfer, initial comparison showed that a significant mechanism was missing from the model, which was subsequently quantified in laboratory experiments.) The principal source of data for the validation of HEGADAS in the steady state has been the series of liquefied gas releases at Maplin Sands. These included steady releases of propane and LNG. The LNG plumes were affected significantly by surface heat transfer and water vapour transfer; indeed, the need to take water vapour transfer into account was deduced from analysis of the LNG experiments. For propane, however, these additional effects were not significant. Results of the comparison of predictions by HEGADAS and the field observations are given in a series of papers (Puttock et al., 1982, 1984, Colenbrander and Puttock, 1984). Good overall agreement is obtained for propane releases, and equally satisfactory agreement is obtained for LNG provided both surface heat transfer and water vapour transfer are taken into account.

Comparisons of HEGABOX/HEGADAS predictions with observations at Thorney Island are given by Puttock (1987).

8. CONCLUSIONS

1. An integral model for the dispersion of an initially dense gas has been formulated, using similarity profiles for the concentration in the vertical and crosswind directions.
2. Vertical mixing is based on wind tunnel and water channel experiments. It appears that practical calculations are unlikely to be affected by the form of the entrainment relation beyond the limits of the wind tunnel data, which have the most direct relevance to atmospheric dispersion.
3. The cloud spreads laterally owing to gravity, and also the edges diffuse. Atmospheric correlations for the lateral dispersion coefficient S_y are extended to infer the development of a profile with a uniform mid-part and diffuse edges.
4. Laboratory experiments with a layer of cold nitrogen flowing over water have confirmed the adequacy of three aspects of the model: (a) standard free-convection heat transfer at low velocities, (b) a formulation for water vapour transfer based on the critical supersaturation approximation for condensation within the thermal boundary layer, and (c) a convective entrainment formulation.
5. Comparison of model predictions against field data, presented in other papers, shows good agreement with observations, and demonstrates, for LNG releases on the sea, the necessity of taking into account both heat transfer and water vapour transfer to the gas clouds.
6. The model description corresponds to the implementations in the programs HEGADAS-S and HEGADAS-T that are available on public release through the U.S. National Technical Information Service.

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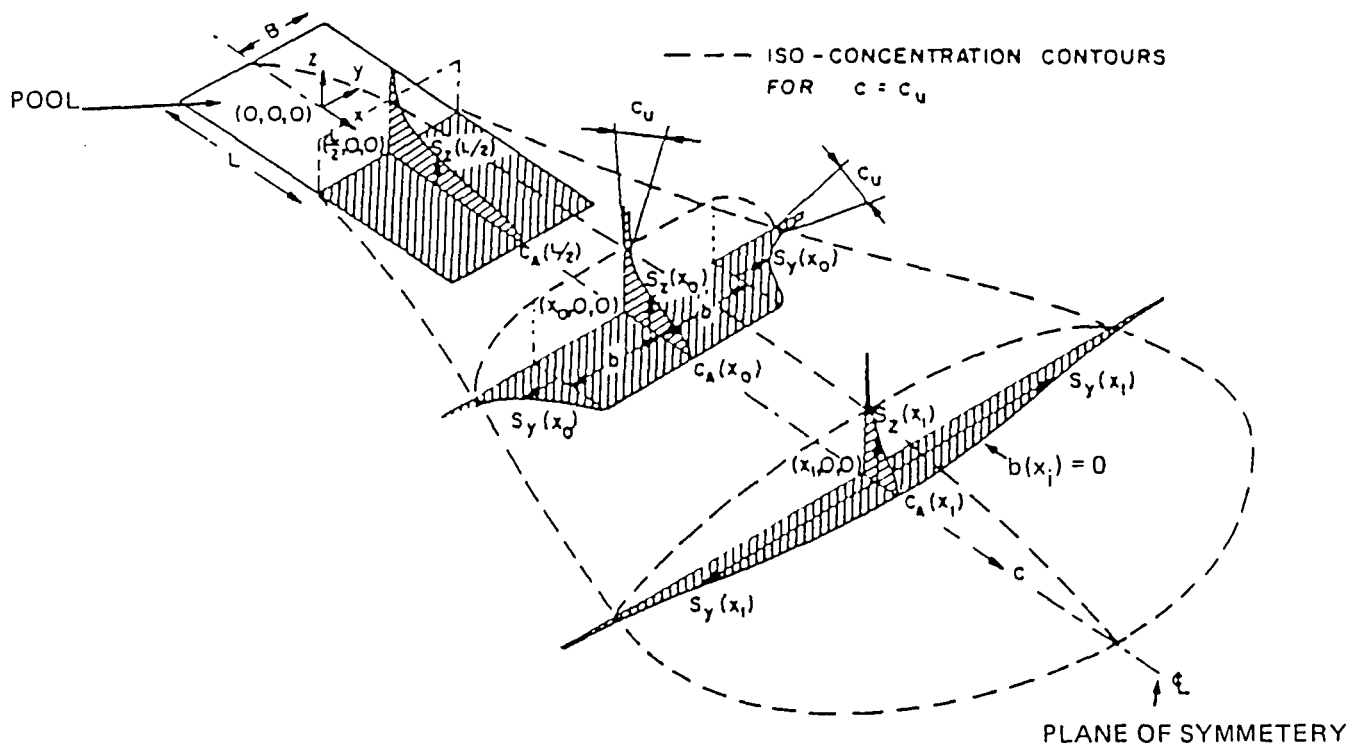


FIG. 1 — The similarity profiles for the concentration and iso-concentration contours in the planes $y = 0$, $z = 0$, $x = L/2$, $x = x_0$ and $x = x_1$

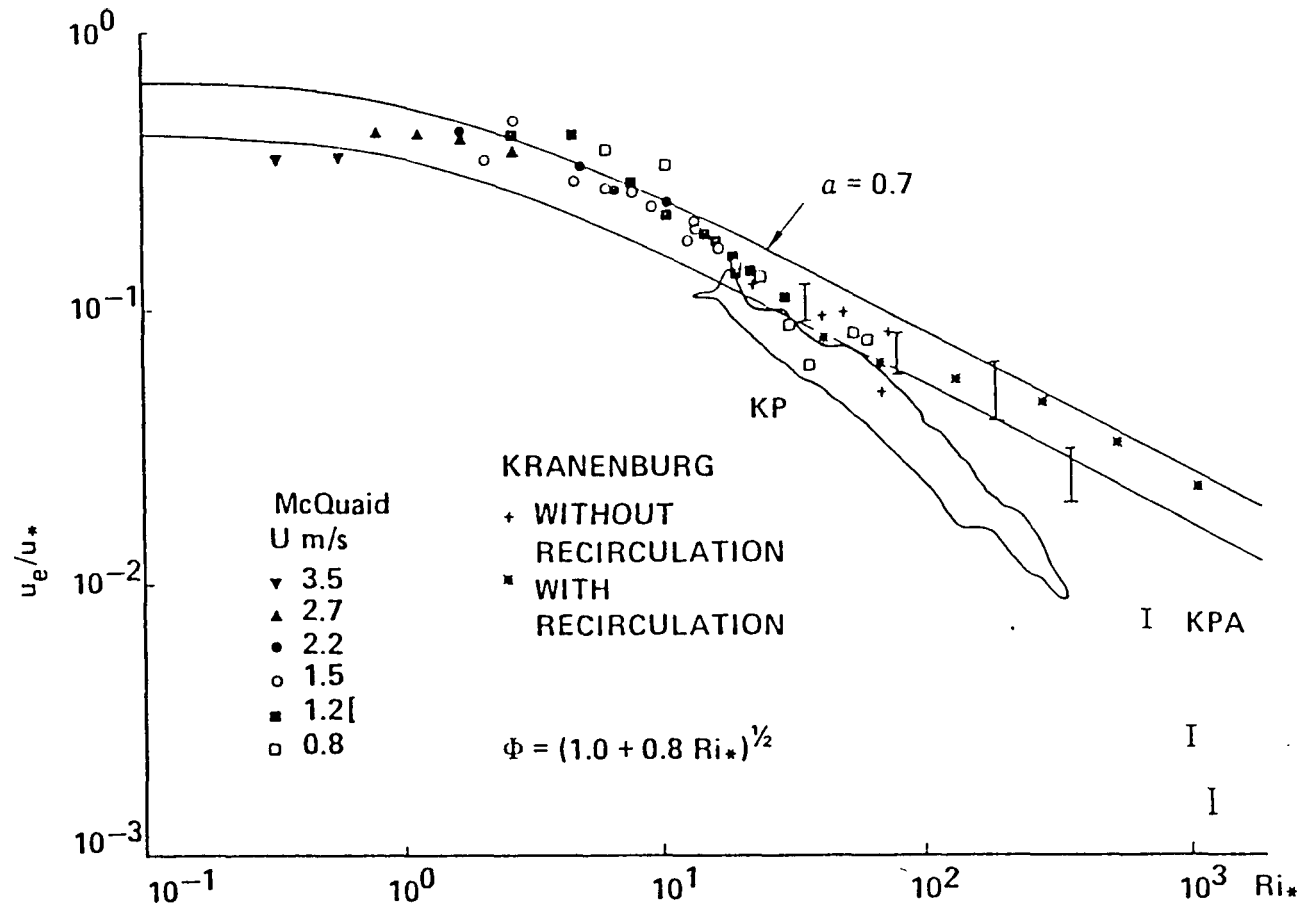


FIG. 2 — Dimensionless entrainment velocity u_e/u_* as a function of the bulk Richardson number Ri_* . The error bars indicate the results of the KPA experiments, corrected for side-wall drag ($H/W \rightarrow 0$). The KP data are continuously distributed within the cloud outlined in this Figure; these data are for $H/W \leq 0.6$. The solid lines represent our fit to the Kranenburg and McQuaid data: $u_e/u_* = 0.41 (1+\alpha)/\Phi(Ri_*)$

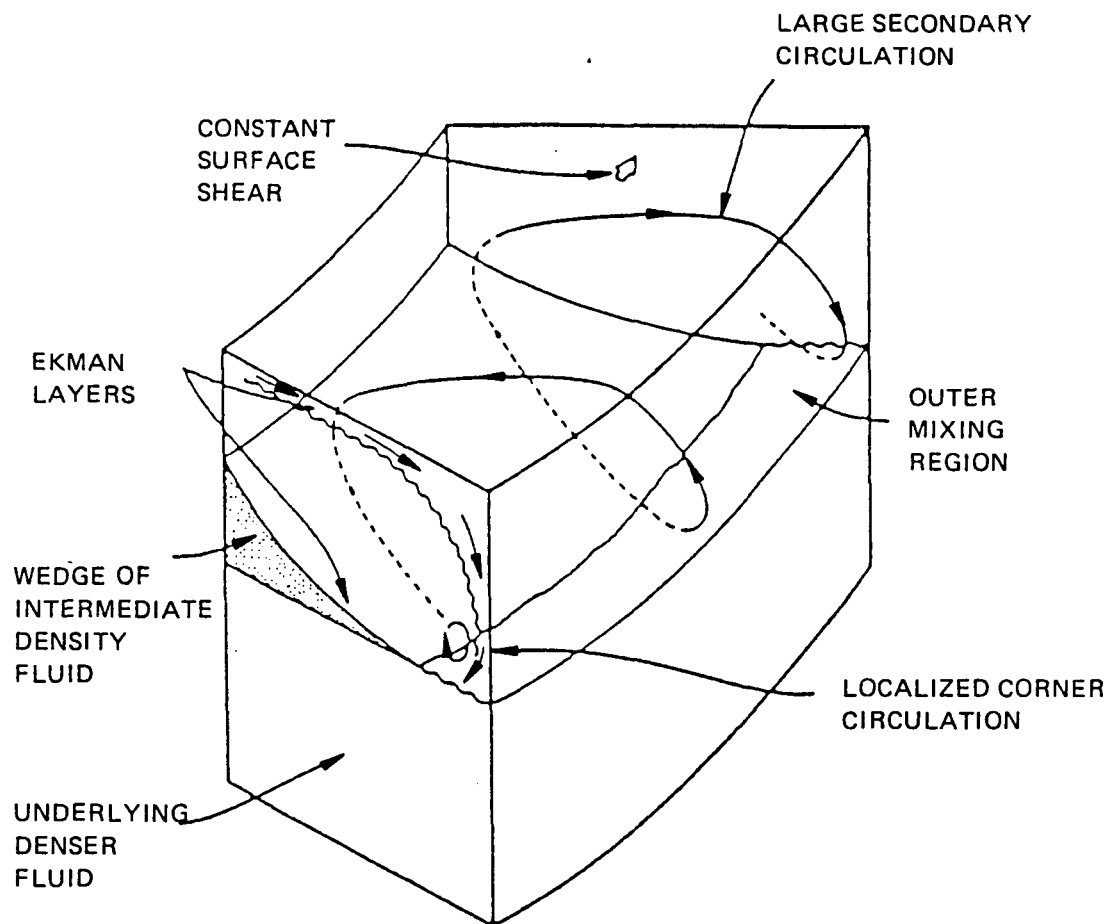


FIG. 3 — Conceptual flow model for moderate and high Richardson numbers ($Ri_* > 100$), showing outer interfacial mixing region, wedge of intermediate density fluid, secondary flow, and localized corner circulation.

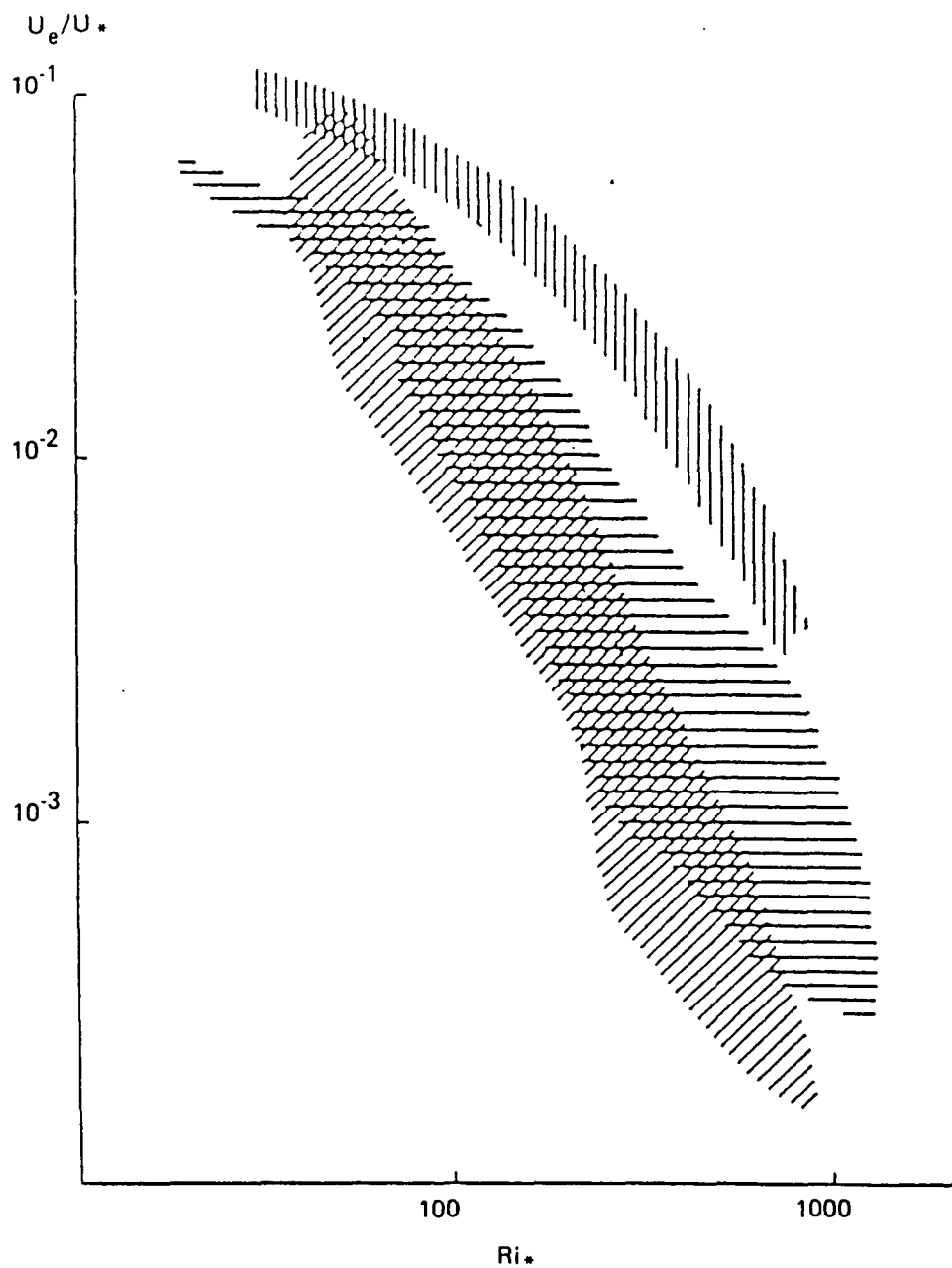


FIG. 4 — Measured entrainment rates of various investigators. The bands shown are envelopes of reported experimental data for various parametric variations, where the greatest variation was in the mean radius and values of H/W : ||||| is Kantha, Phillips, and Azad, $R_m = 65\text{cm}$, $H/W = 0.25$; ≡ is Deardorff and Willis, $R_m = 50\text{cm}$, $H/W = 0.38-1.5$; /// is Scranton and Lindberg, $R_m = 53\text{cm}$, $H/W = 0.25-0.37$. The data of Kato and Phillips fall in the band of data common to Deardorff and Willis and Scranton and Lindberg, and is not shown (for clarity).

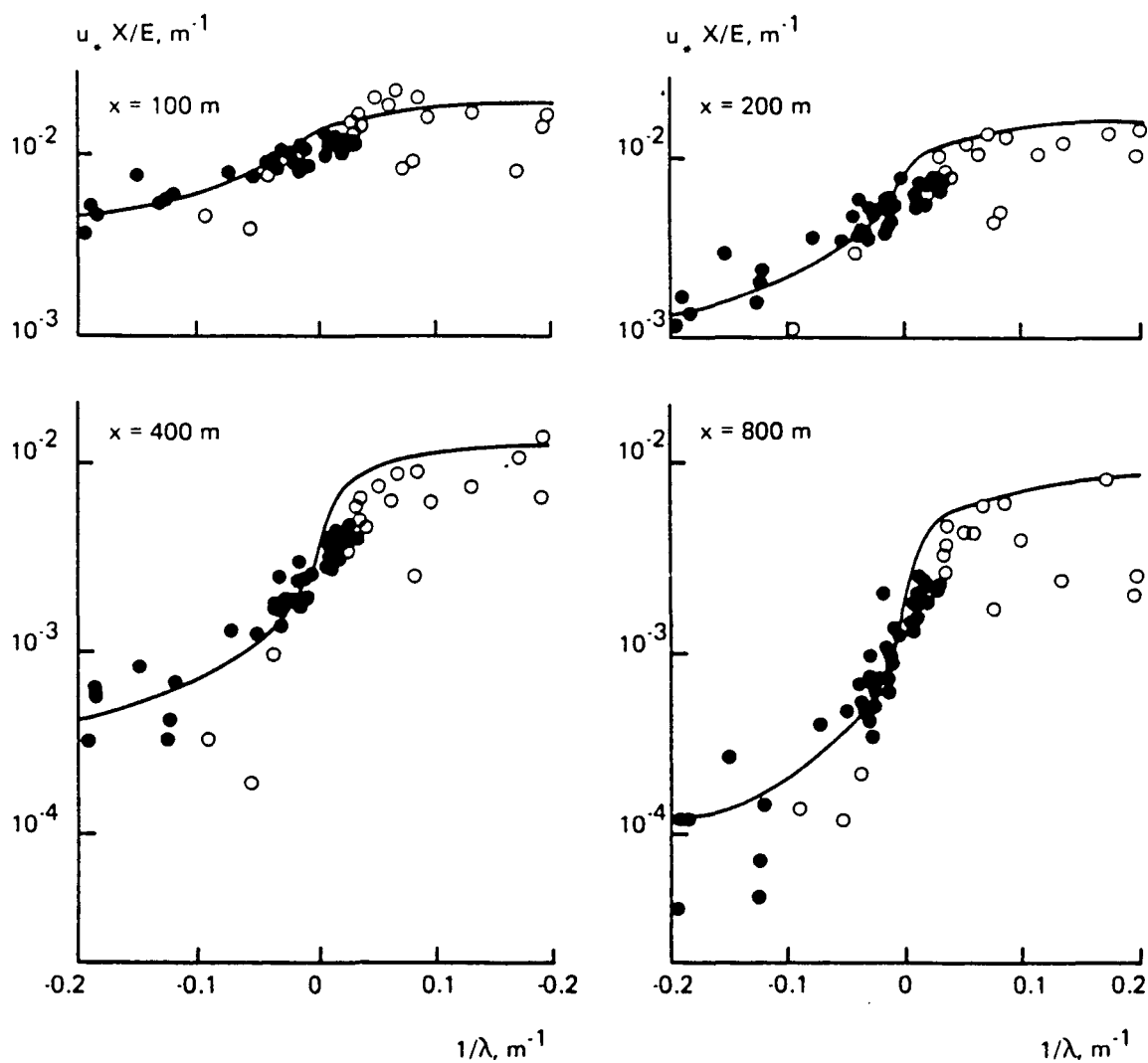


FIG. 5 — Measured (points) and predicted (curve) concentrations 100, 200, 400 and 800 m downwind of the source in the prairie grass experiments

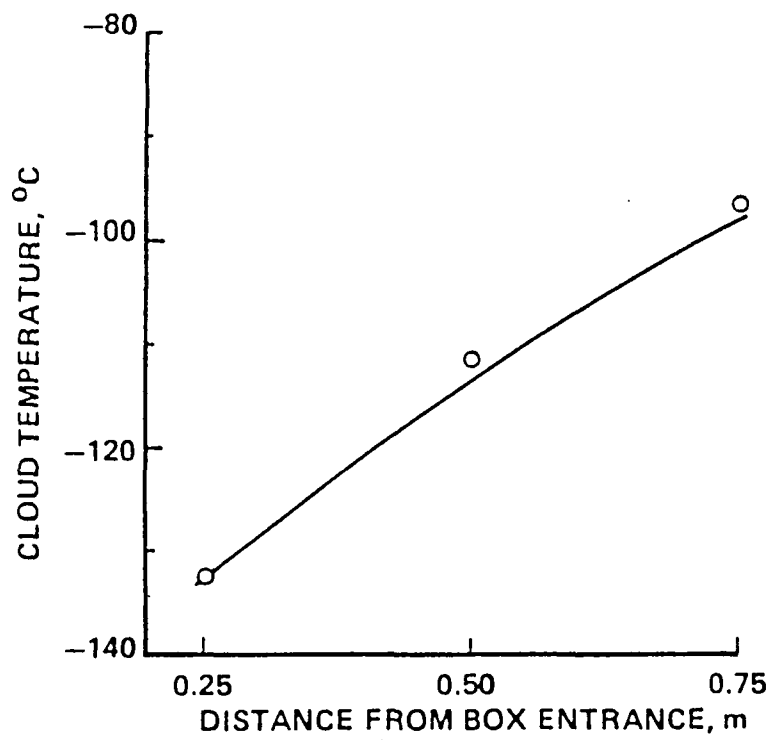


FIG. 6 — Temperature as a function of distance from box entrance, measured and calculated with HEGADAS;
Series 3 : Evaporation from copper plate, oil film on water surface.

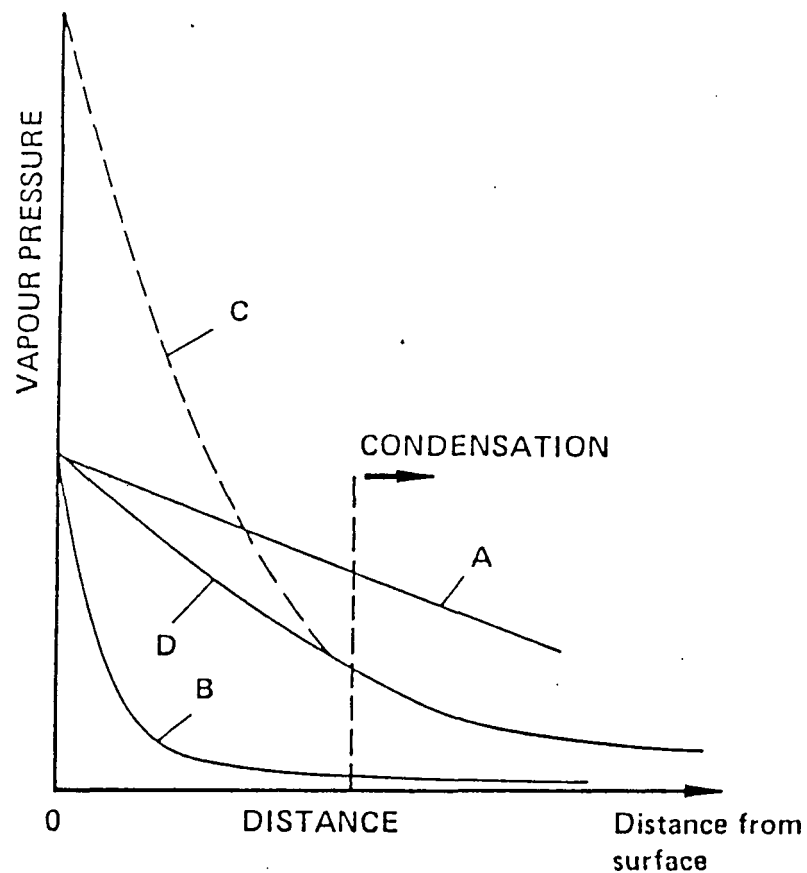


FIG. 7 — Vapour pressure profiles in the immediate vicinity of a vaporising surface (after Rosner, 1967)

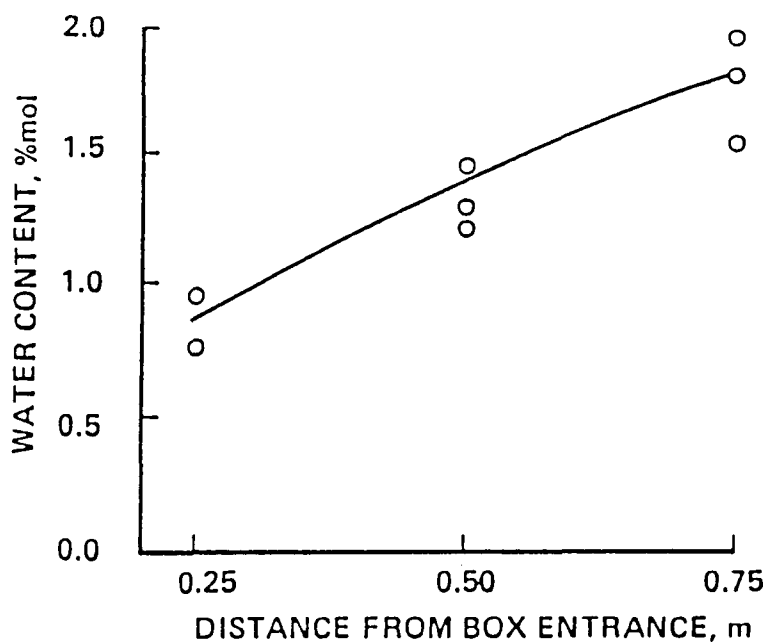


FIG. 8 — Water concentration as a function of distance; experimental data points; curve calculated with HEGADAS
Series 2: Evaporation from copper plate.

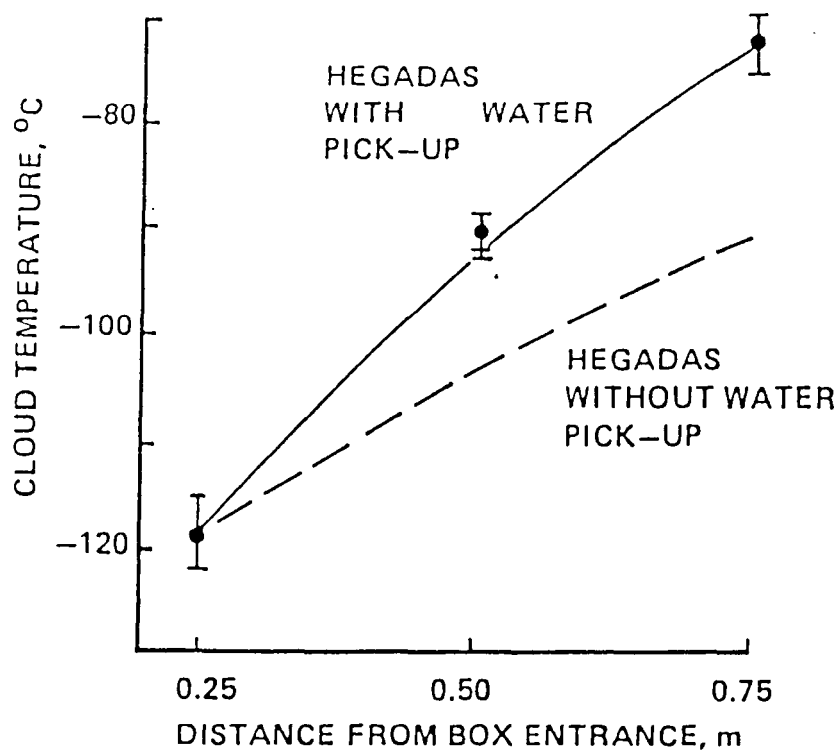


FIG. 9 — Temperature as a function of distance; the bars represent the experimental data, the curve results from a HEGADAS calculation.
Series 2: Evaporation from copper plate

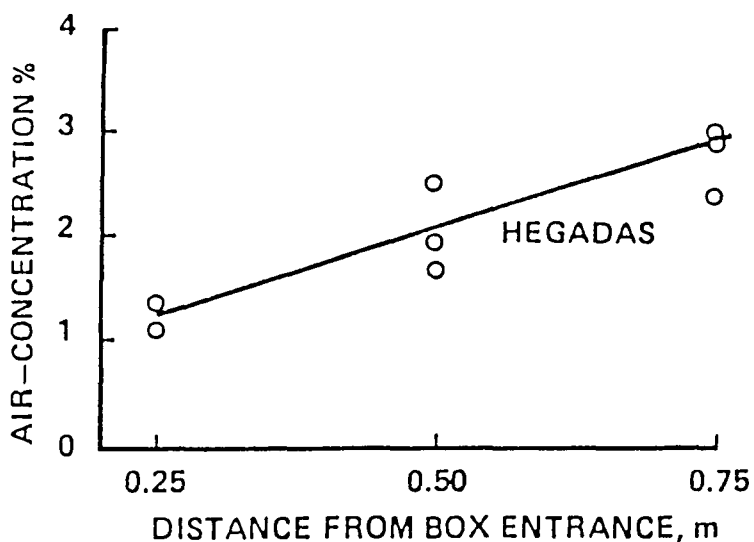


FIG. 10 — Air concentration (molar percentage of air in air/nitrogen mixture) as a function of distance; experimental data points and curves, calculated with HEGADAS
Series 2: Evaporation from copper plate.

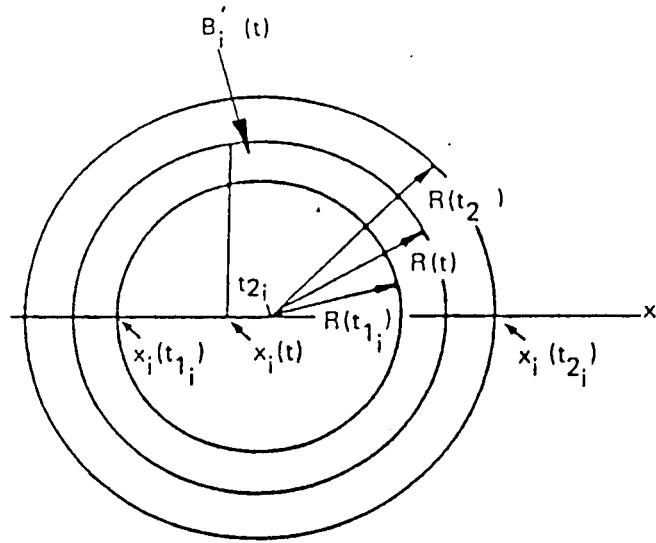


FIG. 11 — Parameters associated with observer "i"

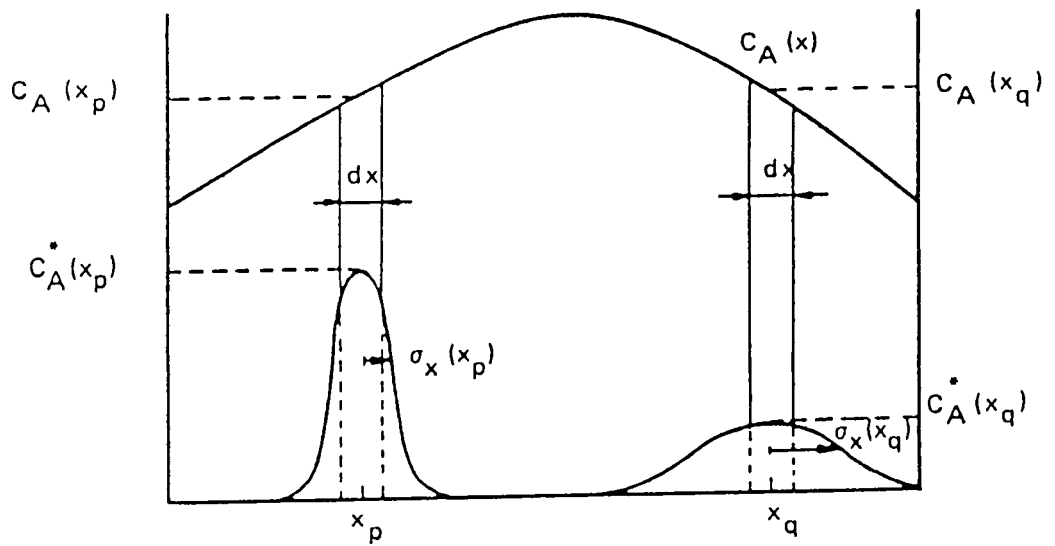


FIG. 12 — Correction of the concentration distribution $C_A(x)$ for dispersion in the x-direction

APPENDIX A

The thermodynamics of a mixture of evaporating liquefied gas,
moist air and entrained water. Calculation
of temperature and density in subroutine THERMO

A.1 Introduction

This appendix details the thermodynamic equations needed for calculating the temperature and density of a cloud of cold hydrocarbon gas, mixed in arbitrary proportions with ambient air with the possible inclusion of evaporating droplets of liquefied gas and of water picked up from the sea surface. The equations form the basis of subroutine THERMO. Figure A1 indicates the dependence of various quantities on others and so the necessary sequence of calculations.

A.2 Notation

y_{wg}	molar ratio: wet gas/total mixture
ω'_1	molar ratio: water initially in air/dry air
ω'_2	molar ratio: water initially in gas ("picked up")/gas
y	molar proportions: $y_g + y_a + y_w = 1$ $y_{w1} + y_{w2} + y_{w3} = y_{wv} + y_{wn} = y_w$
r_h	relative humidity in atmosphere (fraction; $0 < r_h < 1$)
P_v	water vapour pressure (mm Hg)
P	atmospheric pressure (in current HEGADAS version $P = P_{st}$)
P_{st}	standard atmospheric pressure = 760 mm Hg
M	molecular weight (kg/kmol)
c_p	specific heat (molar; J/mole/K)

h_{gv}, h_{wv}, h_{wf}	heat of vaporisation of gas, water; heat of fusion of water at 0°C (all molar)
T, T'	temperature in K and °C. $T = T' + 273.15$
T_{st}	standard temperature: 273.15°K
T'_s	surface temperature (°C)
T'_{bpg}	boiling temperature of gas (°C)
ρ	density
V	molar volume
V_o	molar volume at s.t.p., 0.0224 m ³
D	heat transferred from surface per mole of mixture
n	moles

Subscripts

g	gas (hydrocarbon)
gv, gl	gas in vapour phase, liquid gas
gl_0	gas as liquid aerosol at time $t = 0$
a	air (dry)
w	water
w_1, w_2	water initially in air, gas
w_3	water from surface
wv, w_1, w_i	water vapour, liquid water, ice
wn	non-vapour water (liquid or solid)
m	mixture (i.e. total cloud)

A.3 Thermodynamic equations

The molar proportions of the various components in the mixture can be calculated from their definitions and the definition of the vapour pressure of water:

$$\omega_1' = \frac{r_h P_v(T_a)/P}{1 - r_h P_v(T_a)/P} \quad \dots (A.1)$$

$$y_g = \frac{y_{wg}}{1 + \omega_2'} \quad y_a = \frac{1 - y_{wg} - y_{w3}}{1 + \omega_1'} \quad \dots (A.2)$$

$$y_{w2} = \frac{y_{wg} \omega_2'}{1 + \omega_2'} \quad y_{w1} = \frac{(1 - y_{wg} - y_{w3}) \omega_1'}{1 + \omega_1'}$$

$$y_{wv} = \min \left[\frac{(y_g + y_a) P_v(T_m)/P}{1 - P_v(T_m)/P}, y_w \right] \quad \dots (A.3)$$

$$y_{wn} = y_w - y_{wv} \quad \dots (A.4)$$

An empirical expression for the vapour pressure of water $P_v(T)$ is given below. Since the temperature of the mixture is initially unknown, the temperature at the previous time step should be used in (A.3). The estimate is improved by iteration.

The mixture temperature is calculated by evaluating the enthalpy of each component of the mixture before and after mixing and equating the initial and final total enthalpies. In all cases enthalpy will be taken to be zero at 0°C in the gaseous state. Specific heats will be assumed to be independent of temperature. (The specific heat of methane in fact varies by ±2% from its mean between -161°C and 20°C.)

$$\text{Enthalpy of air initially} = n_m y_a T_a' c_{pa} \quad \dots (A.5)$$

$$\text{finally} = n_m y_a T_m' c_{pa}$$

$$\begin{aligned}
 \text{Enthalpy of water initially} &= n_m c_{pwv} (y_{w1} T'_a + y_{w3} T'_s) \\
 &\dots (A.6) \\
 &+ n_m y_{w2} (T'_s c_{pw1} - h_{wv})
 \end{aligned}$$

Enthalpy of water finally

$$\begin{aligned}
 &= n_m y_{wv} T'_m c_{pwv} + n_m y_{wn} (T'_m c_{pw1} - h_{wv}) \quad \text{for } T'_m > 0 \\
 &= n_m y_{wv} T'_m c_{pwv} + n_m y_{wn} (T'_m c_{pwi} - h_{wv} - h_{wf}) \quad \text{for } T'_m < 0
 \end{aligned}$$

Here it is assumed that the non-vapour water is ice when the temperature is below 0°C. Supercooled water should not be found since the initial temperature of the cloud (for LNG) is low enough to ensure ice nucleation.

$$\text{Enthalpy of gas initially} = n_m y_g T'_g c_{pg} - n_m (y_{g1o}/y_{go}) y_g h_{gv} \quad \dots (A.7)$$

$$\text{finally} = n_m y_g T'_m c_{pg}$$

assuming that all the gas has evaporated in the final state.

The term between brackets in (A.7) denotes the molar ratio of initial liquid gas to initial dry gas.

$$\text{Heat transferred from sea surface} = n_m D \quad \dots (A.8)$$

Equating total enthalpy before and after mixing gives:

$$\begin{aligned}
T'_m = & [y_a T'_a c_{pa} + (y_{w1} T'_a + y_{w3} T'_s) c_{pwv} + y_{w2} T'_s c_{pw1} \\
& + (y_{wn} - y_{w2}) h_{wv} + \underline{y_{wn} h_{wf}} + y_g T'_g c_{pg} \\
& - (y_{g10}/y_{go}) y_g h_{gv} + D] ./ \\
& [y_a c_{pa} + y_{wv} c_{pwv} + \underline{y_{wn} c_{pwi}} + y_g c_{pg}] \quad \dots (A.9)
\end{aligned}$$

Equation (A.9) is only correct if T'_m is less than 0°C . Otherwise the underlined terms should be changed: the first to zero, and the second to $y_{wn} c_{pw1}$. In computation it will be necessary to try both forms, and if one is self-consistent then that is correct. If assuming $T'_m < 0$ gives a result > 0 and vice-versa, then the ice is partially melted and $T'_m = 0$.

If all the liquid gas has not evaporated in the final state then equation (A.9) is wrong. A proper treatment for the presence of unevaporated liquefied gas requires a knowledge of the vapour pressure as a function of temperature, since under the equilibrium conditions the temperature will fall below the boiling point of the liquid gas T'_{bpg} until the vapour pressure is equal to the partial pressure of the gas in the gas-air mixture. In the absence of vapour pressure data, the subroutine takes the simplistic assumption that the temperature does not fall below T'_{bpg} . When the temperature T'_m is equal to the boiling point of the liquid gas T'_{bpg} , equation (A.9) can be inverted to determine how much liquid gas has vaporised:

$$\begin{aligned}
(y_{g10}/y_{g0}) y_g - y_{g1} &= [y_a c_{pa} (T'_a - T'_{bpg}) \\
&+ (y_{w1} T'_a + y_{w3} T'_s - y_{wv} T'_{bpg}) c_{pww} \\
&+ y_{w2} T'_s c_{pw1} - y_{wn} T'_{bpg} c_{pwi} \quad \dots (A.10) \\
&+ y_g c_{pg} (T'_g - T'_{bpg}) + (y_{wn} - y_{w2}) h_{wv} \\
&+ y_{wn} h_{wf} + D] / h_{gv}
\end{aligned}$$

The ratio of the density of the mixture to that of (moist) air at the same temperature is:

$$\rho_o / \rho_{aw} = \frac{(y_g M_g + y_a M_a + y_w M_w) (1 + \omega_1')}{(y_{gv} + y_a + y_{wv}) (M_a + \omega_1' M_w)} \quad \dots (A.11)$$

assuming that the liquid is in a aerosol small enough to move with the gas and so contribute to the dynamics of the cloud, but has negligible volume.

The actual density of the mixture is then given by:

$$\rho_m / \rho_{aw} = \frac{\rho_o}{\rho_{aw}} / \frac{T_m}{T_a} \quad \dots (A.12)$$

and the molar volume by:

$$\frac{V_m}{V_o} = (y_{gv} + y_a + y_{wv}) \frac{T_m}{T_{st}} \frac{P_{st}}{P} \quad \dots (A.13)$$

A.4 Empirical function for water vapour pressure

For temperatures from 0°C to 50°C the vapour pressure of water $P_v(T)$ can be calculated, in bars, for T' in degrees C, from Lowe and Ficke(1974):

$$P_v = a_0 + T' (a_1 + T' (a_2 + T' (a_3 + T' (a_4 + T' (a_5 + a_6 T'))))))$$

where $a_0 = 6.1078$

$$a_1 = 4.4365 \times 10^{-1}$$

$$a_2 = 1.4289 \times 10^{-2}$$

$$a_3 = 2.6506 \times 10^{-4}$$

$$a_4 = 3.0312 \times 10^{-6}$$

$$a_5 = 2.0341 \times 10^{-8}$$

$$a_6 = 6.1368 \times 10^{-11}$$

Below 0°C, the following is adequate for the vapour pressure of ice:

$$P_v(T) = b_1 \exp(-b_2/T)$$

where $b_1 = 2.624 \times 10^{10} \text{ mmHg} = 3.498 \times 10^7 \text{ bars}$

$$b_2 = 6134 \text{ K.}$$

Table A1. Some useful physical constants for hydrocarbons, water and air

Physical constant	Methane	Ethane	Propane	n-Butane	Ethylene	Propylene	Nitrogen	Air	Water vapour
Molecular weight M_g (g/mole)	16.04	30.07	44.0	58.13	28.05	42.08	28.016	28.964	18.016
Boiling point T'_{bpg} ($^{\circ}\text{C}$)	-161.5	-88.6	-42.07	-0.5	-103.7	-47.5	-195.8	-	-
Latent heat of vaporisation at boiling point h_{gy} (J/mole)	8200	14 700	18 800	22 400	13 500	18 400	5578	-	45 000 at 0°C
specific heat (J/mole/K) (vapour)	34.4	48.0	68	96.6	39	60.4	29.3	29.1	Heat of fusion H_{wf} : 6010 (c_{pwy}) 33
(liquid)									(c_{pwl}) 75.5
(solid)									(c_{pwi}) 37.9 ⁺
Liquid density at b.p. (kg/m^3)	424	548	580	603	570	591	807	-	-
Thermal diffusivity/ (temperature) ² , ($\text{m}^2/\text{s K}^2$)	2.6×10^{-10}	0.95×10^{-10}	0.61×10^{-10}	0.41×10^{-10}	1.20×10^{-10}	-	2.7×10^{-10}	2.5×10^{-10}	-
Kinematic viscosity/ (temperature) ² , ($\text{m}^2/\text{s K}^2$)	1.92×10^{-10}	0.85×10^{-10}	0.50×10^{-10}	0.34×10^{-10}	1.00×10^{-10}	0.54×10^{-10}	2.0×10^{-10}	1.8×10^{-10}	-
Upper flammable limit (%)	15.0	12.8	9.4	8.4	30	11	-	-	-
Lower flammable limit (%)	5.0	2.9	2.1	1.8	2.7	2.0	-	-	-

⁺ A better value for the mean between 0°C and the boiling point of the gas T'_{bpg} is: $c_{pwi} = 37.0 + 0.066 T'_{bpg}$ with T'_{bpg} in degrees C.

APPENDIX BWind velocity and observer velocityB.1 The wind velocity profile

The best way of describing the wind velocity in the atmosphere surface layer is (Businger, 1973):

$$u_x(z) = \frac{u_*}{k} \left[\ln \frac{z + z_R}{z_R} - \Psi_1 \left(\frac{z}{\lambda} \right) \right] \quad \dots (B.1)$$

where

$$\Psi_1(z/\lambda) = -6.9 z/\lambda \quad \text{for } 1/\lambda > 0 \text{ (stable atmosphere)} \quad \dots (B.2)$$

and

$$\begin{aligned} \Psi_1(z/\lambda) = & 2 \ln \left[(1+a)/2 \right] + \ln \left[(1+a^2)/2 \right] - 2 \tan^{-1}(a) \\ & + \pi/2 \text{ for } 1/\lambda < 0 \quad \text{(unstable atmosphere)} \quad \dots (B.3) \end{aligned}$$

$$\text{with } a = (1 - 22 z/\lambda)^{1/4} \quad \dots (B.4)$$

However, to be consistent with the similarity profiles for the concentration, equation (2.2), we have to use a wind velocity profile of the form

$$u_x = u_o \left[\frac{z}{z_o} \right]^\alpha \quad \text{(equation (2.2)).}$$

The value of α is determined from the best fit with expression (B.1).

Expression (B.1) is used directly in calculating u_* for given $u_x(z=z_o)=u_o$;

the value of u_* is used in the differential equation for S_z (equation (3.4)) and in calculating the value of Ri_* (equation (3.6)).

B.2 Relation of observer velocity u_1 to wind velocity u_x

The observers are released from the point $x = -R_{\max}$, where $R_{\max}$

is the maximum radius of the secondary source $R(t)$. The average transport velocity of the vapour molecules for given S_z is expressed by relation (3.10):

$$u_{eff} = u_o \left[\frac{S_z}{z_o} \right]^\alpha \frac{1}{\Gamma[1/(1+\alpha)]} \quad \dots (B.5)$$

At location X the value of S_z and accordingly u_{eff} differ from observer to observer and consequently some observers may overtake others. This possibility calls for an observer velocity which is a function of x only. Therefore an element of arbitrariness has to be introduced into the observer velocity calculation.

In the two-dimensional case the growth of S_z with x is determined by differential equation (3.8), which can be solved for a neutrally buoyant situation to give:

$$\left[\frac{S_z}{z_o} \right]_{\rho_E = \rho_a} = \left[\frac{k}{z_o} \frac{u_*}{u_o} \frac{(1+\alpha)^2}{\Phi(0)} (x - x_o) \right]^{\frac{1}{1+\alpha}} \quad \dots (B.6)$$

If we take $x_o = -R_{max}$ and substitute equation (B.6) into equation (B.5), the observer velocity will be given by:

$$\frac{u_o}{\Gamma[1/(1+\alpha)]} \left[k \frac{u_*}{u_o} \frac{(1+\alpha)^2}{\Phi(0)} \frac{(x + R_{max})}{z_o} \right]^{\frac{\alpha}{1+\alpha}} \quad \dots (B.7)$$

This velocity is definitely too high in a stably stratified situation, since the growth of S_z with x is influenced considerably by vertical density gradients. Therefore, for the observer velocity we put:

$$u_i(x) = C_o \left[\frac{x + R_{max}}{z_o} \right]^{\frac{\alpha}{1+\alpha}} \quad \dots (B.8)$$

The constant C_o is determined by calculating with the pertinent values of u_o , u_* and ρ_E the value of S_z at the end of a steady-state source of length $L = \sqrt{\pi} R_m$, where R_m is the radius of the secondary source when the take-up rate $\pi R^2 Q^*$ is maximum; for the value of Q^* in this calculation the take-up flux at the same time is taken. The observer velocity at $x = \frac{\sqrt{\pi}}{2} R_m$ is then taken to be

$$u_i \left(x = \frac{\sqrt{\pi}}{2} R_m \right) = \frac{u_o}{\Gamma[1/(1+\alpha)]} \left[\frac{S_z \left(x = \frac{\sqrt{\pi}}{2} R_m \right)}{z_o} \right]^\alpha \quad \dots (B.9)$$

By substituting this expression into equation (B.8) we find:

$$C_o = \frac{u_o}{\Gamma[1/(1+\alpha)]} \left[\frac{S_z \left(x = \frac{\sqrt{\pi}}{2} R_m \right)}{z_o} \right]^\alpha \left[\frac{\frac{\sqrt{\pi}}{2} R_m + R_{max}}{z_o} \right]^{-\frac{\alpha}{1+\alpha}} \quad \dots (B.10)$$

$$u_i(x) = \frac{u_o}{\Gamma[1/(1+\alpha)]} \left[\frac{S_z \left(x = \frac{\sqrt{\pi}}{2} R_m \right)}{z_o} \right]^\alpha \left[\frac{x + R_{max}}{\frac{\sqrt{\pi}}{2} R_m + R_{max}} \right]^{\frac{\alpha}{1+\alpha}} \quad \dots (B.11)$$

APPENDIX CCloud shape correction for gravitational spreading in the wind direction

In low wind velocities HEGADAS simulations of time-dependent spills show considerable gravitational spreading of high density vapour clouds (e.g. propane) after the initial slumping of the vapour blanket.

Since the HEGADAS model allows for gravitational spreading in the crosswind direction only, the calculated crosswind dimensions are too large and the dimensions in wind direction too small as already indicated in Section 7.

As cloud shape becomes a parameter of increasing importance in more refined hazard assessment methods, we have designed a cloud shape correction routine for the time-dependent HEGADAS computer program. The basic consideration for this correction is that the gravitational spreading velocity should be the same in all directions. The HEGADAS model generates a cloud at a specified point of time consisting of elements with calculated height, length, width and concentration. These elements retain their length while travelling downwind and spreading in the crosswind direction. Leaving height and concentration unchanged, as well as the product of length and width of each element, the width is reduced and the length increased in such a way that the amount of spreading in the downwind direction of the cloud as a whole equals the spreading in the crosswind direction. A subroutine of the HEGADAS time-dependent computer program contains the mathematical formulation of this correction which is briefly outlined below; the notation is consistent with Section 6.

Let L_c be the calculated cloud length and W_c the cloud width at a specified point at time t . As initial cloud width we take the maximum diameter of the gas blanket above the source, $2R_{max}$. We correct cloud width and length now in such a way that the spreading S in downwind direction equals the spreading in crosswind direction. This means, if we define L'_c and w'_c as corrected length and width, that $L'_c = L_c + S$ and $W'_c = 2R_{max} + S$.

Conservation of cloud surface area then requires: $L'_c \times W'_c = L_c \times W_c$
or

$$(L_c^* + S^*) \times (1 + S^*) = L_c^* \times W_c^* \quad \dots (C.1)$$

with $L_c^* = L_c/2R_{max}$, $W_c^* = W_c/2R_{max}$ and $S^* = S/2R_{max}$.

Given L_c^* and W_c^* , equation (C.1) can be solved for S^* :-

$$S^* = -0.5 (1 + L_c^*) + 0.5 [(1 + L_c^*)^2 + 4 L_c^* (W_c^* - 1)]^{1/2} \quad \dots (C.2)$$

so that

$$L'_c/L_c = (L_c^* + S^*)/L_c^* \quad \dots (C.3)$$

and

$$W'_c/W_c = (1 + S^*)/W_c^* \quad \dots (C.4)$$

Assume now that the uncorrected cloud consists of k elements with length Δx_i and width $B_{eff,i}$ ($i=1,k$). The cloud shape correction is started at the element where the maximum concentration c_A is found. (If the maximum is found in more than one element, the one located furthest from the source is chosen.) This element remains fixed at its location but its length and width are corrected as follows, in analogy to (C.2) - (C.4):

$$\Delta x'_i/\Delta x_i = (L_c^* + S_i^*)/L_c^* \quad \dots (C.5)$$

$$B'_{eff,i}/B_{eff,i} = (1 + S_i^*)/B_{eff,i}^* \quad \dots (C.6)$$

with

$$S_i^* = -0.5 (1+L_c^*) + 0.5 [(1 + L_c^*)^2 + 4L_c^* (B_{eff,i}^* - 1)]^{1/2} \quad \dots (C.7)$$

where

$$L_c^* = L_c / 2R_{max} \quad \dots (C.8)$$

and

$$B_{eff,i}^* = B_{eff,i} / B_i \quad \dots (C.9)$$

In expression (C.9), B_i is the half-width of element i at the source.

Again, these correction formulae satisfy the essential condition of conservation of element surface area:

$$\Delta x'_i \times B'_{eff,i} = \Delta x_i \times B_{eff,i}$$

The shape correction of the elements upwind and downwind of the first one are performed in an identical way.

Correction (C.6) is applied to both the middle part and the Gaussian flanks of the crosswind concentration profile:

$$b'_i / b_i = S'_{yi} / S_{yi} = (1 + S_i^*) / B_{eff,i}^*$$

No correction is applied when $b_i = 0$.

After the correction gravitational slumping, dispersion in the wind direction is taken into account as described in Section 6.3.

APPENDIX DLaboratory experiments on heat and mass transfer
into a cold nitrogen gas flow

Laboratory experiments were performed to test the aspects of heat transfer, water vapour transfer and convective entrainment in the model. Results have been presented in the main text. The experimental setup is summarised here; more details have been given by Colenbrander and Puttock (1984).

Three series of experiments were performed. In series 1 a steady stream of liquid nitrogen (-196°C) was released into a 1m wide and 0.2m deep tray filled with water up to about 3cm below the brim. The nitrogen, floating on the water surface, evaporated and the cold, dense vapour entered a perspex box, the flow being homogeneously distributed over the width of the box (see Figure D1). The box contained a water layer 0.2m deep, over the surface of which the vapour was flowing. The nitrogen left the box through an opening over its entire width. The opening was provided with a flow restriction consisting of vertical bars with a triangular cross-section. The length and width of the box were equal (1m), and the height was 0.6m. On top a lid was placed to prevent air currents in the room from affecting the flow in the box. Holes in the lid allowed air to flow in and out freely.

In series 2 the water surface in the evaporation tray was covered with a copper plate from which the nitrogen was evaporated. Hot water was circulated through the tray below the plate to provide the heat of vaporisation.

In series 3 this copper plate was used again, but in addition the water surface in the box was covered with an oil film. This was done to prevent water vapour transfer from the water surface into the nitrogen vapour stream.

At locations A, B and C (0.25, 0.50 and 0.75m from the box entrance) temperatures and concentrations in the vapour stream were measured. A mass spectrometer was used to measure the concentrations of nitrogen, oxygen and water, from which were calculated air entrainment and water (vapour) pick-up into the nitrogen vapour stream.

The water temperature in the box was measured, as well as a vertical temperature profile in the vapour stream at location B, which indicated the vapour layer thickness. In all test runs the temperature was measured simultaneously at all locations. But the concentrations could only be measured at one fixed location during a run. Repeat runs were performed so that concentration measurements could be obtained at a number of locations.

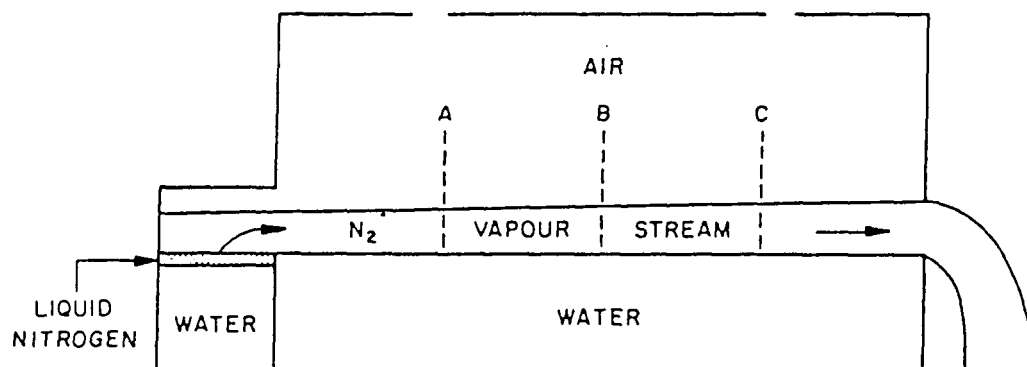


FIG. D1 SCHEMATIC REPRESENTATION OF THE EXPERIMENTAL SET-UP

APPENDIX ESummary of HEGADAS equations

For clarity the complete set of equations solved by HEGADAS is summarised in this appendix.

The HEGADAS formulation of dispersion involving vertical entrainment is given by:

$$\frac{d}{dx} \left[u_{eff} B_{eff} H_{eff} / V_m \right] = Q_e B_{eff} \quad (E.1)$$

with

$$Q_e = \left[k u_T (1+\alpha) / (V_o \Phi(Ri_T)) + Q_{wv} \right] \quad (E.2)$$

In this expression

$$u_T = [u_*^2 + (0.2 w_*)^2]^{1/2} \quad (E.3)$$

$$w_* = \left[\frac{g Q_H H_{eff}}{T_m \rho_m C_{pm}} \right]^{1/3} \quad (E.4)$$

$$Ri_T = g' \frac{H_{eff}}{u_T^2} \quad (E.5)$$

with $g' = g[\rho_m(c=c_A) - \rho_a(z = H_{eff})] / \rho_a(z = 0)$ (E.6)

The temperature T_m and density $\rho_m(c=c_A)$ of the gas/air mixture as well as the specific molar volume V_m are computed in the thermodynamic subroutine THERMO.

Expressions for u_{eff} , B_{eff} and H_{eff} read:

$$u_{eff} = u_o \left[\frac{S_z}{z_o} \right]^\alpha \frac{1}{\Gamma(\frac{1}{1+\alpha})} \quad (E.7)$$

$$B_{eff} = b + \frac{\sqrt{\pi}}{2} S_y \quad (E.8)$$

and

$$H_{eff} = \frac{\Gamma(\frac{1}{1+\alpha})}{1+\alpha} S_z \quad (E.9)$$

Hence Equation (E.1) may also be written as:

$$\frac{d}{dx} \left[\left(b + \frac{\sqrt{\pi}}{2} S_y \right) \left[\frac{S_z}{z_o} \right]^{1+\alpha} \sqrt{V_m} \right] = \frac{1+\alpha}{u_o z_o} \left(b + \frac{\sqrt{\pi}}{2} S_y \right) Q_e \quad (E.10)$$

Above the source S_y is taken to be zero and b as well as c (and V_m) are taken to be constant and hence Equation (E.10) reduces to

$$\frac{d}{dx} \left[\left[\frac{S_z}{z_o} \right]^{1+\alpha} \right] = \frac{1+\alpha}{u_o z_o} V_m Q_e \quad (E.11)$$

Since heat transfer from the earth's surface and water vapour pick-up are neglected above the source ($D = 0$ and $y_{w3} = 0$), Equation (E.11) is the only differential equation to be solved above the source. Q_e then reduces to:

$$Q_e = [ku_*(1+\alpha)/(V_o \Phi(Ri_*))] \quad (E.12)$$

If the atmosphere cannot take up directly by diffusion the gas flux emitted by the source, a 100% gas blanket is formed in the model formulation. The dimensions of the gas blanket are determined iteratively in such a way that the molar flow rate of gas transported by the wind equals the emission rate. This calculation is done along the lines set out by Colenbrander (1980, Section 2.3), who also discusses the case of no formation of a gas blanket. This occurs if the atmospheric take-up is greater than the emission rate. Then the ground-level gas concentration above the source is less than 100%, while the source dimensions are determined by the source specification. The constant value of c above the source is again determined iteratively so as to satisfy continuity of gas molar flow rate.

Downwind of the source, at distances where the middle part of the concentration profile b has not yet disappeared, the entrainment relation (E.11) is solved together with four additional differential equations.

The first of these four is an equation describing heat transfer:

$$\frac{d}{dx} [D u_{eff} B_{eff} H_{eff} / V_m] = Q_H B_{eff} \quad (E.13)$$

or

$$\frac{d}{dx} \left[D \left(b + \frac{\sqrt{\pi}}{2} S_y \right) \left[\frac{S_z}{z_o} \right]^{1+\alpha} / V_m \right] = \frac{1 + \alpha}{u_o z_o} \left(b + \frac{\sqrt{\pi}}{2} S_y \right) Q_H \quad (E.14)$$

The second equation describes the pick-up of water vapour:

$$\frac{d}{dx} [y_{w3} u_{eff} B_{eff} H_{eff} / V_m] = Q_{wv} B_{eff} \quad (E.15)$$

or

$$\frac{d}{dx} \left[y_{w3} \left(b + \frac{\sqrt{\pi}}{2} S_y \right) \left[\frac{S_z}{z_o} \right]^{1+\alpha} / V_m \right] = \frac{1 + \alpha}{u_o z_o} \left(b + \frac{\sqrt{\pi}}{2} S_y \right) Q_{wv} \quad (E.16)$$

The third additional equation deals with the lateral gravitational spreading of the plume:

$$\frac{dB_{eff}}{dt} = C_E \left[g H_{eff} \left(1 - \frac{\rho_a(z=0)}{\rho_m} \right) \right]^{\frac{1}{2}} \quad (E.17)$$

or

$$\frac{d}{dx} \left(b + \frac{\sqrt{\pi}}{2} S_y \right) = C \left[1 - \frac{\rho_a(z=0)}{\rho_m} \right]^{\frac{1}{2}} \left[\frac{S_z}{z_o} \right]^{\frac{1}{2}-\alpha} \quad (E.18)$$

where we use 1.15 for the spreading constant C_E and

$$C = C_E \frac{(gz_o)^{\frac{1}{2}}}{u_o} \left[\Gamma\left(\frac{1}{1+\alpha}\right) \right]^{\frac{3}{2}} (1+\alpha)^{-\frac{1}{2}} \quad (E.19)$$

Finally an equation is added to describe the crosswind atmospheric dispersion:

$$S_y \frac{dS_y}{dx} = \frac{4\beta}{\pi} \left(b + \frac{\sqrt{\pi}}{2} S_y \right)^2 \left[\frac{\delta \sqrt{\pi/2}}{b + \frac{\sqrt{\pi}}{2} S_y} \right]^{1/\beta} \quad (E.20)$$

where β and δ are constants in a relation, determining the crosswind spreading of a plume, emitted by a point source.

To close the set of equations, c is determined by dividing the molar flow rate of emitted gas by the total flow rate $u_{eff} B_{eff} H_{eff}/V_m$ in the plume. Given y_{wg} , c , D and y_{w3} , the plume temperature T_m , density $\rho(c)$ and specific molar volume V_m are calculated in the subroutine THERMO. Hence the 7 unknowns S_z , S_y , b , D , y_{w3} , c and V_m are determined by solving the set of 5 coupled ordinary differential Equations (E.10), (E.14), (E.16), (E.18) and (E.20), together with the integral molar mass and enthalpy balances (THERMO).

Downwind of the point $x = x_t$ where b becomes zero, gravitational spreading is neglected and hence (E.18) is dropped from the set of

equations. Since the crosswind concentration profile is completely Gaussian for $x > x_t$, Equation (E.20) can be solved, giving

$$S_y = 2 \delta(x + x_v)^\beta \quad (\text{E.21})$$

where x_v is determined from the expression

$$S_y(x_t) = 2 \delta(x_t + x_v)^\beta \quad (\text{E.22})$$

For $x > x_t$ Equations (E.10), (E.14) and (E.16) reduce to

$$\frac{d}{dx} \left[\left(\frac{S_z}{z_o} \right)^{1+\alpha} / V_m \right] = \frac{1 + \alpha}{u_o z_o} Q_e \quad (\text{E.23})$$

$$\frac{d}{dx} \left[D \left(\frac{S_z}{z_o} \right)^{1+\alpha} / V_m \right] = \frac{1 + \alpha}{u_o z_o} Q_H \quad (\text{E.24})$$

and

$$\frac{d}{dx} \left[y_{w3} \left(\frac{S_z}{z_o} \right)^{1+\alpha} / V_m \right] = \frac{1 + \alpha}{u_o z_o} Q_{wv} \quad (\text{E.25})$$

Stability Class (Pasquill)	δ 10 min	δ_I	β
A	0.527	0.264	0.865
B	0.371	0.186	0.866
C	0.209	0.105	0.897
D	0.128	0.064	0.905
E	0.098	0.049	0.902
F	0.065	0.033	0.902

Table III-2. Constants in experimentally determined crosswind dispersion coefficient for a point source $S_y = \delta x^\beta$.

$\delta_{10 \text{ min}}$ are the values for an averaging time for the concentration measurement of 10 min. If the averaging time is t sec. δ_t can be calculated, using the following formula:

$$\delta_t = \delta_{10 \text{ min}} \left(\frac{t}{600} \right)^{0.2}$$

The values for δ_I apply to instantaneous sources; these values are recommended for use in dispersion calculations for flammable gases.

Source: "Methoden voor het berekenen van de gevolgen van het vrijkomen van gevaarlijke stoffen". TNO, 2nd ed.

APPENDIX 4. THE JET RELEASE MODEL HFJET

Contents

A4.1: Introduction

A4.2: Model Formulation

A4.3: Range of Applicability

A4.4: Conclusions

References

§A4.1: Introduction.

A second model, HFJET, has been developed for the prediction of near release conditions following a high momentum, initially horizontal release to a coflowing atmosphere. HFJET is a simplified version of the basic HFPLUME in which the influence of gravity, crosswinds, atmospheric turbulence, and gradients within the atmosphere have all been neglected. Account is taken of the ground surface only as a geometrical constraint; ground drag and impact related pressure forces are neglected.

These simplifications are sweeping, and severely limit the range of downwind distances for which HFJET may be expected to predict experimental data. Nonetheless the substantial simplification of the underlying differential/algebraic system permits the development of a fast running, robust code, in which the principal features of HF/moist-air thermodynamics may be examined. The development of HFJET preceeded that of HFPLUME. The latter, more complex, model has benefited substantially from experience gained, and problems solved, in the development of the former.

§A3.2: Model Formulation.

The simplifications introduced in the model HFJET allow almost complete integration (Appendix 1, Wheatley 1987) of the differential/algebraic system for jet motion. The system comprises 1 differential and 6 algebraic equations for the solution or "state"

$$(T, y_{HF}, x_{\ell}^{HF}, x_{HF}; u, D; dm/dt).$$

The differential/algebraic system is, for two-phase equilibrium, as follows:

$$\begin{aligned} dm/dt &= A u; (u - u_{\infty}) / (u_{\square} - u_{\infty}) = x_{HF}; \\ (h + (1/2)u^2 - h_{\infty} - (1/2)u_{\infty}^2) / (h_{\square} + (1/2)u_{\square}^2 - h_{\infty} - (1/2)u_{\infty}^2) &= x_{HF} \\ 1 &= y_{HF} + y_{(HF)_2} + y_{(HF)_6} + y_{(HF)_8} + y_{H_2O}^{HF} + y_{H_2O} + y_{N_2O_2}, \\ \beta x_{N_2O_2} \rho_g(T, P_{\infty}; y_{HF}) &= \rho(1 - c/\rho) x_{N_2O_2}^{\infty}; \\ dm/dt|_{HF} &= x_{HF} dm/dt; d/ds(dm/dt) = Entr_{jet}. \end{aligned}$$

[Notation: A cross-sectional area, ρ mean jet density, c mass-concentration HF, u jet flow-speed, h mean jet enthalpy, β mixture void fraction, x_{HF} mass-fraction mixture that is HF $dm/dt|_{HF}$ the (steady) HF mass-flux, $dm/dt - dm/dt|_{HF}$ the mass-flux of entrained air $Entr_{jet}$ jet entrainment rate per unit jet length Of the affices " ∞ " refers to ambient conditions " $\square$ " to conditions at the release orifice or pipe break, "g" to the vapour phase; HF, $(HF)_2$, ... , N_2O_2 to the several chemical species present.]

Ground impact is represented by a simple geometrical change in the assumed jet cross-section. An airborne jet, for which the jet radius $D/2$ is less than the release height h, has a circular cross-section; otherwise the cross section is the major segment of a circle of diameter D and centre h. This results in the auxiliary equation

$$\begin{aligned} A &= \begin{cases} \pi/4 D^2 & , 2h/D > 1, \\ L [\cos^{-1}(-2h/D) + \sqrt{(1 - 4h^2/D^2)}] D^2, & 0 \leq 2h/D \leq 1. \end{cases} \end{aligned}$$

§A3.3: Range of Applicability.

The range of applicability of simplified HFJET model may be found by direct comparison with the full HFPLUME algorithm. Such an approach, while certainly valid, destroys any computational advantage in using the simpler model. What is required are approximate validity criteria based upon the jet description generated by HFJET. Consider first the neglected effect of gravity in deflecting the plume centre-line. Fluid within the jet convected at representative speed u experiences a downward acceleration $(1-\rho_\infty/\rho)g$, which over a (horizontal) displacement s results in a vertical deflection z such that

$$z/h \approx (1/2)(1-\rho_\infty/\rho)(gh/u^2)(s/h)^2 \ll 1.$$

In addition it is assumed that "jet" entrainment dominates all other mechanisms, and in particular heavy-gas entrainment. Comparison of the neglected with the present terms results immediately in the validity condition

$$u/u_\infty \ll 1 + \kappa / [\frac{1}{2}(Ri_\star)\eta(\rho/\rho_\infty)e_{jet}](u_\star/u_\infty),$$

$$Ri_\star = 2gh(\rho/\rho_\infty - 1)/u_\star^2.$$

Assuming that conditions are approximately neutral we may estimate the friction velocity $u_\star$ from the logarithmic profile

$$u_\infty = (u_\star/\kappa)\ln(1+h/z_r),$$

in which z_r is the surface roughness, κ von Karman's constant. It then follows from the horizontal momentum equation that the mass-concentration x_{HF} must satisfy for the validity of HFJET the extreme inequality,

$$x_{HF} >> \kappa^2 / [\frac{1}{2}(Ri_*) \eta(\rho/\rho_\infty) e_{jet}] / (u_\square / u_\infty - 1) / \ln(1+h/z_r),$$

in which $u_\square$ is the release velocity at the discharge orifice.

Consider the likely range of displacement and concentration for which the computer model HFJET is (approximately) valid. We take a representative release of evaporating liquid HF for which the velocity "immediately post flash" might be 50m/s, reducing rapidly toward unity, with a representative value 10m/s. The initial density ratio might be 10::1, with a representative value perhaps 2::1; the release height might be 1m; the wind-speed 5m/s; and the surface roughness 1cm. We obtain the specific forms, $s \ll 7m$; $x_{HF} >> 0.5\%$. Clearly therefore the jet model is valid only in the near source region to a distance perhaps 10m, or to a concentration of some 1%_{HF} by mass. In particular the "Goldfish" series of experimental releases (Blewitt 1988), for which data were first captured at 20m downwind of release, lie beyond the range of applicability of HFJET. Comparison with HFPLUME indicates that HFJET is (broadly) satisfactory for prediction at 20m, but **not** for 40m, 60m, 100m and 200m downwind of release. This is consistent with the observed behaviour of HF releases: video recordings clearly illustrate plume slumping within 20m downwind of release. the model has been run to some 200m downwind of release.

§A3.4: Conclusions.

Comparison of HFJET and HFPLUME with (admittedly limited) experimental data confirms the order of magnitude estimates developed above for the range of validity of the simplified model HFJET. The range of model applicability ($<10m, >1\%_{HF}$) is restrictive; nonetheless it is sufficient to allow description of a jet incident upon "spray curtains" (Blewitt 1988) placed some 6m from the

point of release. In particular mean temperature, HF concentration, phase composition, and flow speed at such spray barriers may all be estimated. It is possible to extend the range of model validity by incorporating heavy-gas entrainment and (perhaps) gravity slumping in a manner similar to that proposed by Raj and Morris (1987). We recommend the use of the more complex model HFPLUME, except for the near-field when computational cost or time is at a premium.

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APPENDIX 5. DESCRIPTION OF HF THERMODYNAMICS MODEL IN HEGADAS

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A5.1. Introduction	A5.2
A5.2. Theory; adopted nonlinear thermodynamic equations	A5.3
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A5.1. Introduction

This chapter describes the thermodynamic model for mixing of HF with humid air, which is implemented in HEGADAS: The thermodynamics for HF is complex because of formation of HF-polymers, depolymerisation of the gas to the monomer state HF (endothermic reaction), and exothermic reaction of HF with water vapour in the ambient air.

The thermodynamic model adopted in the HGSYSTEM programs has been described in detail in Chapter 2. This model is based on a revised version by Schotte (1988) of his original HF-model (see Schotte (1987)). Both models include as mixture components:

- a vapour mixture, consisting of water, air, HF-monomer (HF), HF-dimer $(\text{HF})_2$, HF-hexamer $(\text{HF})_6$, HF-octamer $(\text{HF})_8$, and $\text{HF} \cdot \text{H}_2\text{O}$ complex,
- an aqueous HF fog, i.e. a liquid fog consisting of water and HF monomer.

The revised model differs from the original model in the following:

- it adopts modified formulae for the partial vapour pressures of HF and water, which are also valid for high molar fractions of HF,
- it does not assume the initial HF prior to the mixing to be purely gaseous, but it also allows for liquid HF to be present.

Section A5.2 describes the HF model adopted in HEGADAS. See Chapter 2 for a validation of this model against experiments.

A5.2. Theory; adopted nonlinear thermodynamic equations

This section describes the consecutive steps in the HF thermodynamic model adopted in the HEGADAS program. See Schotte (1987,1988) for details not covered in this section.

In this section first notations are introduced for the molar fractions, molar flows, pressures, enthalpy terms etc. (before and after mixing), and the input data to the HF model are given. Subsequently the basic set of thermodynamic equations governing the HF model is derived. This set consists of two (in the absence of liquid fog) or three (with fog) equations for two or three basic unknowns. These unknowns are the fugacity of the HF-monomer, the mixture temperature, and (in case of fog) the molar fraction x of HF in the fog. Finally expressions are derived for the mixture volume and the mixture density.

NOTATION

y_{HF}	molar fraction of HF in a mixture of humid air and HF, with ALL HF based on HF-monomer
$y_{\text{HF}}^{\text{L}0}$	mass fraction of liquid in initial, pure HF (before mixing) = molar fraction of liquid in initial, pure HF with ALL HF based on HF-monomer)
y_{α}^0	molar fraction of species α in initial, pure HF vapour (before mixing); $\alpha = 11$ (HF monomer), 12 (dimer), 16 (hexamer) or 18 (octamer); $y_{11}^0 + y_{12}^0 + y_{16}^0 + y_{18}^0 = 1$
y_{α}	molar fraction of species α in vapour (after mixing); $\alpha = a$ (dry air), w (H_2O), c ($\text{HF} \cdot \text{H}_2\text{O}$), 11, 12, 16 or 18; the sum of these fractions must be 1: $y_a + y_w + y_c + y_{11} + y_{12} + y_{16} + y_{18} = 1$
x	molar fraction of HF (monomer) in aqueous fog (after mixing)

M_a	molar flow of dry air (before and after mixing), kmole/s
M_w	molar flow of water before mixing = molar flow of water vapour, $\text{HF}\cdot\text{H}_2\text{O}$ complex, and water in fog after mixing, kmole/s
M_{HF}	molar flow of HF with ALL HF based on HF-monomer, kmole/s
$M_{\text{HF}}^{\text{L}0}, M_{\text{HF}}^{\text{V}0}$	molar flow of initial liquid HF and HF vapour with ALL HF based on HF-monomer, kmole/s; $M_{\text{HF}}^{\text{L}0} = y_{\text{HF}}^{\text{L}0} M_{\text{HF}}$, $M_{\text{HF}}^{\text{V}0} = (1 - y_{\text{HF}}^{\text{L}0}) M_{\text{HF}}$
M_{tot}	total molar flow before mixing with ALL HF based on HF monomer, kmole/s; $M_{\text{tot}} = M_a + M_w + M_{\text{HF}}$
L	total molar flow of aqueous fog (after mixing), kmole/s
M_{vap}	total molar flow of vapour (after mixing), kmole/s; the number of moles after mixing must be equal to the number of moles prior to mixing, if ALL HF is based on HF-monomer: $(y_a + y_w + 2y_c + y_{11} + 2y_{12} + 6y_{16} + 8y_{18}) M_{\text{vap}} + L = M_{\text{tot}}$
f_1^0	fugacity of HF-monomer for initial, pure HF vapour (post-flash, before mixing; $f_1^0 = y_{11}^0$)
f_1	fugacity of HF-monomer (after mixing; $f_1 = y_{11}$)
$K_i(T)$	$K_i(T)=1$; $K_i(T)$ is equilibrium constant at temperature T for the dimer (i=2), hexamer (i=6), octamer (i=8) formation at temperature T, atm^{-i-1} ; see eq. 5 in Schotte (1988) for expressions $K_i(T)$
$K_c(T)$	equilibrium constant at temperature T for the formation of $\text{HF}\cdot\text{H}_2\text{O}$ complex at temperature T, atm^{-1} ; see eq. 5 in Schotte (1988) for expression $K_c(T)$
Φ_1	fugacity coefficient of HF in the gas phase; approximated by $\Phi_1=1$ in HEGADAS

P	total pressure, atm; approximated by $P=1$ in HEGADAS
P_w	partial vapour pressure of water (including $\text{HF}\cdot\text{H}_2\text{O}$), atm
P_{HF}	partial vapour pressure of HF (including $\text{HF}\cdot\text{H}_2\text{O}$), atm
$P_v(T)$	vapour pressure of water at temperature T , atm; see section A.4 of Appendix 3 to this Technical Report for the empirical function $P_v(T)$
r_H	relative humidity of the ambient air (fraction)
T_a	ambient temperature (Celsius)
T^0	temperature (Celsius) of initial, pure HF (post-flash)
T	final temperature (Celsius) of mixture
H_e	added heat from the surface (Joule / mole of mixture)
H^0	enthalpy departure (cal/mole of HF vapour) of the initial, pure HF vapour from the ideal monomeric gas (including added heat from surface)
H_{25}, H	enthalpy departure (cal/mole of HF vapour) of HF vapour from the ideal monomeric gas at 25°C and the final temperature T , respectively
ΔH_α	enthalpy of association of HF species α , cal/mole; $\alpha = 2$ (dimer, $\Delta H_2 = -12775$), 6 (hexamer, $\Delta H_6 = -41927$), 8 (octamer, $\Delta H_8 = -50121$) or c ($\text{HF}\cdot\text{H}_2\text{O}$, $\Delta H_c = -6266$)
$H_{\text{cond}}^{\text{HF}}$	heat of condensation of HF-monomer at 25°C, cal/mole; $H_{\text{cond}}^{\text{HF}} = 7231$
H_{cond}^w	heat of condensation of water at 25°C, cal/mole; $H_{\text{cond}}^w = 10519$

- H_{mix} heat of mixing of liquid HF and H_2O at $25^\circ C$, cal / mole of HF;
 $H_{mix} = H_{mix}(x) = 4500 \cdot (1-x^2)$
- C_p^α specific heat at constant pressure of species α , cal/mole/ $^\circ C$; $\alpha =$
 a [dry air, $C_p^a = 6.96$], w [water, $C_p^w = 8.05$], HFV [gaseous HF,
 $C_p^{HFV} = 6.96$], HFL [liquid HF, $C_p^{HFL} = C_p^{HFL}(T^0) = 12.01 + 0.0164T^0$]
- C_p^{fog} specific heat at constant pressure of liquid fog, cal/mole/ $^\circ C$;
 C_p^{fog} is given as a function $C_p^{fog}(x, T)$ of x, T by eq. (24) in
 Schotte (1988)

INPUT AND OUTPUT

In the program HEGADAS the HF thermodynamic routine THRMHF carries out the calculations for HF thermodynamics. This routine requires as input:

- the HEGADAS input parameters r_H (relative humidity), T_a (ambient temperature); these data need to be specified by the user
- the post-flash data T^0 (post-flash HF temperature) and y_{HF}^{L0} (post-flash liquid mass fraction of HF); these data are usually set in the flash calculations performed by one of the HGSYSTEM programs HFFLASH, HFJET or HFPLUME; they can also be directly input to HEGADAS by the user
- the HEGADAS solution variables y_{HF} (HF molar fraction) and H_g (added heat from surface); these data are functions of the downwind distance x ; they are set in the HEGADAS program during the solution in the downwind direction of the ordinary differential equations for the dispersion data

The calculations described below are carried out using the above input data. The routine THRMHF outputs calculated data required for further HEGADAS dispersion calculations, i.e. the mixture temperature T , the molar mixture volume V_m and the molar mixture density ρ_m .

DERIVATION AND SOLUTION TO EQUATIONS I,II,III FOR UNKNOWN f_1, T, x

1. SET ENTHALPY DEPARTURE OF THE INITIAL, PURE HF VAPOUR: H^0

- Set vapour-association (molar fractions $y_{11}^0, y_{12}^0, y_{16}^0, y_{18}^0$ of monomer, dimer, hexamer, octamer) of initial, pure HF by iterative solution for the fugacity $f_1^0 = y_{11}^0$ of the equation

$$y_{11}^0 + y_{12}^0 + y_{16}^0 + y_{18}^0 = 1 \quad (1)$$

whereby $y_{1i}^0 = y_{1i}(f_1^0, T^0)$, $i=1,2,6,8$ with

$$y_{1i}(f_1, T) = K_i(T) (f_1)^i / (\Phi_1 P) \quad (2)$$

- Set enthalpy departure H^0 of the initial, pure HF vapour from the ideal monomeric gas (including added heat H_e from surface),

$$H^0 = \frac{y_{12}^0 \Delta H_2 + y_{16}^0 \Delta H_6 + y_{18}^0 \Delta H_8}{y_{11}^0 + 2y_{12}^0 + 6y_{16}^0 + 8y_{18}^0} + \frac{H_e}{4.19 y_{HF}} \quad (3)$$

2. SET PARTIAL VAPOUR PRESSURES OF WATER AND HF: P_w, P_{HF}
[both including $HF \cdot H_2O$ complex]

- Set the partial vapour pressure P_w^{amb} of water in the ambient wet air (before mixing)

$$P_w^{amb} = r_H P_v(T_a) \quad (4)$$

- a In the absence of liquid fog ($L = 0$), set the partial vapour pressures as follows

$$P_w = (1 - y_{HF}) P_w^{amb}, \quad P_{HF} = y_{HF} P \quad (5)$$

b In the presence of liquid fog ($L > 0$), the partial vapour pressures are set as a function of x and T from the empirical expressions $p_w(x,T)$, $p_{HF}(x,T)$ given by Schotte (see eqs. (1) and (2) in Schotte (1988)). These expressions consist of different formulas for $x < 0.4738$ and $x > 0.4738$. In the HEGADAS formulation these expressions are smoothed (identical to the smoothing carried out in the program HFPLUME) to arrive at functions $p_w(x,T)$, $p_{HF}(x,T)$ which are everywhere continuous and differentiable; see Figure 1 for the values of these functions at the temperature $T = 26^\circ\text{C}$ Celcius. In the presence of fog, the amounts of HF and water in the vapour are smaller than in the absence of fog, and the partial vapour pressures must then be smaller than the pressures (5). Therefore the following values are adopted in HEGADAS for the partial pressures in the presence of fog,

$$P_w = \min(p_w(x,T), (1-y_{HF})P_w^{amb}), \quad P_{HF} = \min(p_{HF}(x,T), y_{HF} P) \quad (6)$$

3. SET MOLAR FLOWS BEFORE MIXING OF HF, WATER, AIR: M_{HF} , M_w , M_a

[the precise value of the total molar flow M_{tot} is irrelevant for the present discussion, and can be taken without loss of generality equal to unity]

$$\begin{aligned} M_{HF} &= y_{HF} M_{tot}, \quad M_w = (P_w^{amb}/P) (M_{tot} - M_{HF}), \\ M_a &= M_{tot} - M_{HF} - M_w \end{aligned} \quad (7)$$

4. SET MOLAR FRACTIONS OF SPECIES IN VAPOUR; SET TOTAL MOLAR FLOW OF VAPOUR [after mixing]

- Set molar fraction $y_{1i} = y_{1i}(f_1, T)$, $i=1,2,6,8$ (HF monomer, dimer, hexamer, octamer) from equation (2).
- Set molar fraction y_c of $\text{HF} \cdot \text{H}_2\text{O}$ complex. From

$$y_c = K_c(T) f_1 P_{wt} / (\Phi_1 P)$$

with the true partial pressure P_{wt} of water in the vapour given by $P_{wt} = P_w - y_c P$, it follows that

$$y_c(f_1, T) = (P_w/P) / [1 + \Phi_1 / (K_c(T)f_1)] \quad (8)$$

- Set molar fraction y_w of H_2O in vapour,

$$y_w = P_w/P - y_c \quad (9)$$

- Set molar fraction y_a of dry air in vapour,

$$y_a = 1 - P_{HF}/P - P_w/P + y_c \quad (10)$$

- Set total molar flow of vapour M_{vap} ,

$$M_{vap} = M_a/y_a \quad (11)$$

5. SET ENTHALPY DEPARTURE OF HF VAPOUR: H

[departure from the ideal monomeric gas, at the final temperature T]

$$H = \frac{y_{12}\Delta H_2 + y_{16}\Delta H_6 + y_{18}\Delta H_8 + y_c\Delta H_c}{y_{11} + 2y_{12} + 6y_{16} + 8y_{18} + y_c} \quad (12)$$

6. SET TERMS IN EQUATION I.

In equation I, the molar fraction of HF (including $HF \cdot H_2O$ complex) in the vapour equals the ratio P_{HF}/P of the partial vapour pressure of HF (including $HF \cdot H_2O$ complex) and the total pressure,

$$y_{11} + y_{12} + y_{16} + y_{18} + y_c = P_{HF}/P \quad (I)$$

Substituting equations (5) or (6), (2) and (8) into (I), it is seen that Equation I is an equation in terms of the unknowns f_1 and T in the

absence of fog, and an equation in terms of the unknowns f_1 , T , and x in the case of fog.

7. SET TERMS IN EQUATION II.

In the absence of fog ($L=0$), Equation IIa expresses the enthalpy balance in terms of the unknowns f_1 and T . In the presence of fog, the molar flow L of fog is first determined from the enthalpy balance. Then equation II is derived in terms of x , f_1 , T by imposing conservation of water.

The total change in enthalpy during mixing equals zero. Here the mixing process is assumed to consist of the following three phases:

- I. separate preheating of HF (at temperature T^0) and humid air (at temperature T_a) to 25°C , and at 25°C evaporation of liquid HF
- II. At 25°C , condensation of HF and H_2O to form aqueous HF (liquid fog)
- III. heating of vapour and fog from 25°C to final temperature T

Thus enthalpy balance yields

$$\Delta H_a + \Delta H_w + \Delta H_{\text{HF}}^{\text{I}} + \Delta H_{\text{HF}}^{\text{II}} + \Delta H_{\text{HF}}^{\text{III}} = 0 \quad (13)$$

in which the changes in enthalpy of air ΔH_a , water ΔH_w (excluding fog; including water in $\text{HF}\cdot\text{H}_2\text{O}$), and hydrogen-fluoride $\Delta H_{\text{HF}}^{\text{I}}$ (during phase I), $\Delta H_{\text{HF}}^{\text{II}}$ (during phase II; including water in fog), $\Delta H_{\text{HF}}^{\text{III}}$ (during phase III; including water in fog and HF in $\text{HF}\cdot\text{H}_2\text{O}$) are given by

$$\begin{aligned} \Delta H_a &= C_p^a M_a (T - T_a) \\ \Delta H_w &= C_p^w \{ M_w (25 - T_a) + [M_w - (1-x)L](T - 25) \} \\ \Delta H_{\text{HF}}^{\text{I}} &= M_{\text{HF}}^{\text{LO}} \{ C_p^{\text{HFL}} (25 - T^0) + H_{\text{cond}}^{\text{HF}} + H^{25} \} + \\ &\quad M_{\text{HF}}^{\text{VO}} \{ -H^0 + C_p^{\text{HFV}} (25 - T^0) + H^{25} \} \\ \Delta H_{\text{HF}}^{\text{II}} &= -(1-x)L H_{\text{cond}}^w - xL (H_{\text{cond}}^{\text{HF}} + H_{\text{mix}} + H^{25}) \\ \Delta H_{\text{HF}}^{\text{III}} &= (M_{\text{HF}} - xL) \{ C_p^{\text{HFV}} (T - 25) + H - H^{25} \} + C_p^{\text{fog}}(x, T) L (T - 25) \end{aligned} \quad (14)$$

By insertion of (14) into the overall enthalpy balance (13) it is easily seen that the term H^{25} falls out. In the absence of fog ($L=0$) equation (13) is applied as Equation II in terms of the unknown f_1 and T ,

$$\Delta H_a + \Delta H_w + \Delta H_{HF}^I + \Delta H_{HF}^{II} + \Delta H_{HF}^{III} = 0 \quad (L=0) \quad (IIa)$$

In the presence of fog, equation (13) is first used to determine the molar flow L . Subsequently conservation of water is imposed to obtain equation II in terms of the unknown f_1 , T , x . This equation expresses that the total molar flow of water after mixing (including $HF \cdot H_2O$ complex) equals the molar flow M_w of water before mixing,

$$(y_w + y_c)M_{vap} + (1-x)L = M_w \quad (L>0) \quad (IIb)$$

8. SET TERMS IN EQUATION III [in presence of fog only]

Equation III in terms of the unknowns f_1 , T , x expresses the conservation of HF, i.e. the total molar flow of HF based on HF-monomer after mixing equals the molar flow M_{HF} of HF before mixing,

$$(y_{11} + 2y_{12} + 6y_{16} + 8y_{18} + y_c)M_{vap} + xL = M_{HF} \quad (L>0) \quad (III)$$

9. ITERATIVE SOLUTION TO EQUATIONS I, II, III FOR BASIC UNKNOWNNS: f_1 , T , x

If a liquid fog is present ($L>0$), the equations (I), (IIb) and (III) are solved iteratively for the fugacity f_1 , the final temperature T and the molar fraction x of HF in the fog. If a liquid fog is not present ($L=0$), the equations (I) and (IIa) are solved iteratively for f_1 and T .

EVALUATION OF MOLAR MIXTURE VOLUME AND MIXTURE DENSITY

1. The molar mixture volume V_m , $m^3/kmole$ of mixture, is the ratio of the total volume flow (m^3/s ; volume of liquid fog can be neglected) and the total molar flow ($kmole/s$; vapour and fog). Thus it is seen that

$$V_m = \frac{[R (T+273.15)/P] M_{vap}}{M_{vap} + L} \quad (15)$$

with $R = 0.082 \text{ atm } m^3/K/kmole$ being the gas constant. Note that the term between brackets in the numerator of (15) signifies the molar volume of ideal gas ($m^3/kmole$)

2. The mixture density is the ratio of the total mass flow (kg/s ; vapour and fog) and total volume flow (m^3/s). Thus it is seen that

$$\rho_m = \frac{(m_a y_a + m_w (y_w + y_c) + m_{HF} (y_{11} + 2y_{12} + 6y_{16} + 8y_{18})) M_{vap} + (m_w (1-x) + m_{HF} x) L}{[R (T+273.15)/P] M_{vap}} \quad (16)$$

with $m_a = 28.95$, $m_{HF} = 20.01$, $m_w = 18.02$ the molecular weights of dry air, HF-monomer and water ($kg/kmole$). The ratio ρ_m / ρ_{amb} of the mixture density ρ_m and the density of the ambient humid air ρ_{amb} is output by the HEGADAS HF-thermodynamics routine. It is set from (16) and

$$\rho_{amb} = P m_{amb} / [R (T_a + 273.15)] \quad (17)$$

with the molecular weight of the humid air ($kg/kmole$) given by

$$m_{amb} = m_a [1 - p_w^{amb}/P] + m_w [p_w^{amb}/P] \quad (18)$$

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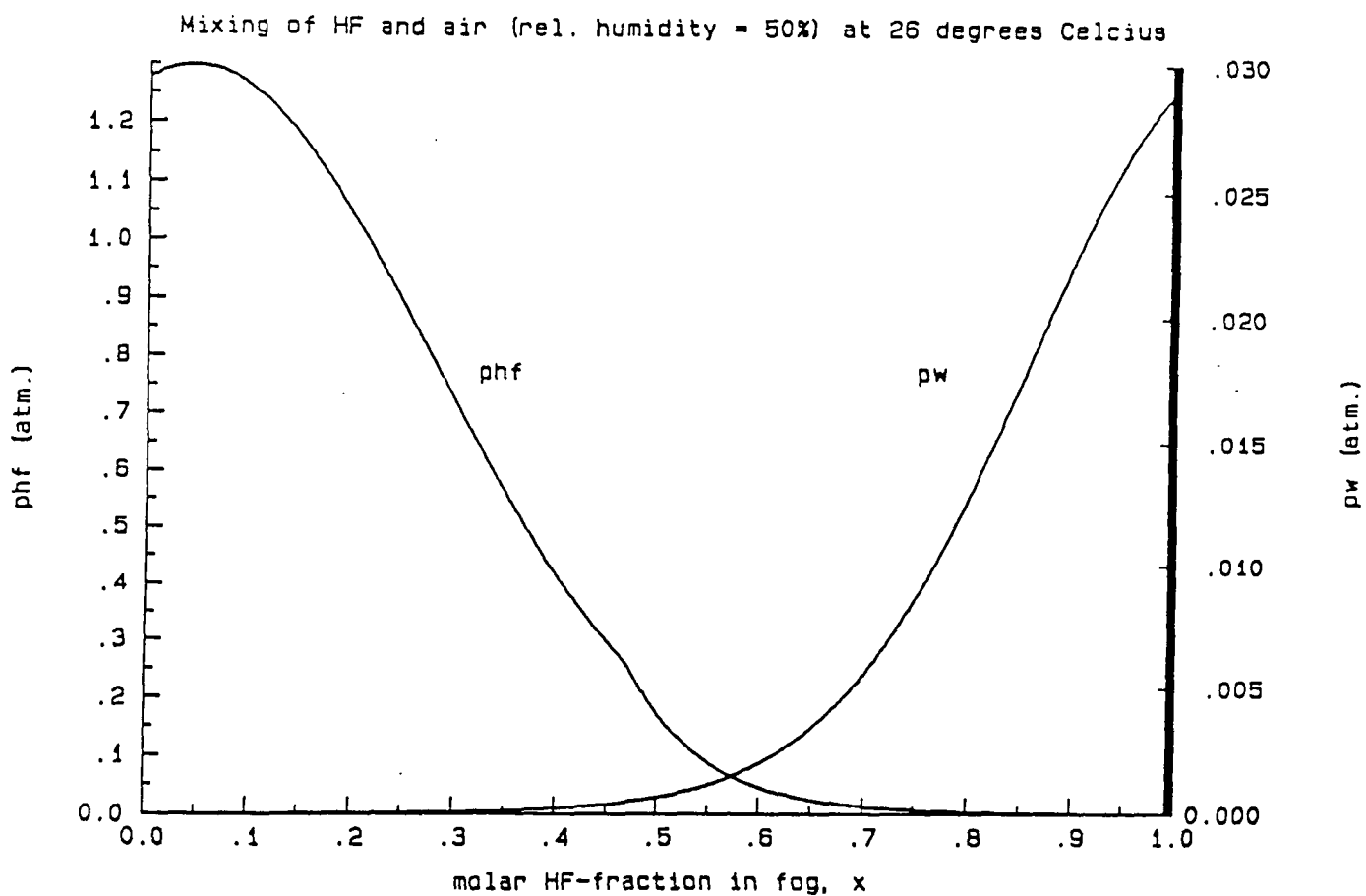


Fig. 1. Partial vapour pressures $p_{HF}(x,T)$, $p_w(T)$ of HF and water (after mixing of HF and humid air); p_{HF} , p_w are plotted against the molar fraction x in the aqueous HF-fog at the temperature $T = 26^\circ\text{C}$; $p_{HF}(x,T)$, $p_w(T)$ are derived by smoothing the expressions (1),(2) in Schotte (1987)

Glossary:

English Alphabet

A, A	scalar, vector cross-sectional area;
$A(s)$	cross-section area/surface at axis-displacement $s > 0$;
$A_{\square}$	plume area at release and before external flashing;
A_{∞}	surface of the control-volume $\tau(s)$ "at infinity", that is at great distance off-axis;
b_j	j^{th} Gaussian half-width;
Buoy	buoyancy force acting upon the plume;
$\text{Buoy}_{\text{Amb}}^{A(s)}$	buoyancy force per unit plume-axis length acting at the cross-section $A(s)$..;
c	local/"top-hat" mass-concentration HF; specific heat symbol; sound-speed;
c_{*}	plume centre-line mass-concentration (Gaussian model);
$c_{\square}$	HF mass-concentration at release;
$c_{\text{flash}}^{\text{post}}$	HF concentration immediately following flash;
c_g	vapour phase mass-concentration HF;
c_{HF}^g	mass-concentration HF monomer in the vapour phase;
$c_{(\text{HF})_2}^g$	mass-concentration HF dimer in the vapour phase;
$c_{(\text{HF})_6}^g$	mass-concentration HF hexamer in the vapour phase;
$c_{(\text{HF})_8}^g$	mass-concentration HF octamer in the vapour phase;
$c_{g, \text{H}_2\text{O}}^{\text{HF}}$	mass-concentration HF as part of the complex $\text{HF}=\text{H}_2\text{O}$;
c_p	specific heat at constant pressure;
$c_{p, \text{HF}}^{\text{H}_2\text{O}}$	isobaric specific heat dilute hydrofluoric acid;
C_D	gravity spreading coefficient; coefficient of discharge;

C_D^l	coefficient of (liquid) discharge;
C_D^g	coefficient of (gas/vapour) discharge;
dA	directed area element;
D	plume (effective) diameter;
D_y	transition width (horizontal) (asymptotic airborne plume);
D_z	transition width (vertical) (asymptotic airborne plume);
D_*	plume effective width (Gaussian) model;
$D_\square$	release orifice (effective) diameter;
dE/dt	flux of excess total-energy;
dm/dt	total entrained and released mass-flux;
$dm/dt _{HF}$	released mass-flux hydrogen fluoride;
dP_x/dt	"top-hat" horizontal excess-momentum flux;
dP_z/dt	"top-hat" vertical-momentum flux;
$Drag_{Amb}^{F(s)}$	scalar (horizontal) drag-force attributed to ground-surface shear over footprint area $F(s)$ at displacement $s>0$ (touchdown and slumped plumes);
Drag	vector drag force acting on the plume;
$Drag_{Amb}^{A(s)}$	vector drag acting on an airborne plume due to cross-wind vortices;
e	eccentricity (aspect ratio) of an ellipse;
e_{slump}^{grav}	entrainment coefficient associated with gravity slumping motion (touchdown and slumped plume);
e_{amb}^{turb}	entrainment coefficient for passive entrainment (airborne plume);
e_{jet}	"jet" entrainment coefficient;
e_{amb}^{turb}	entrainment coefficient associated with passive entrainment (airborne plume);
e_{wind}^{cross}	cross-wind entrainment coefficient;
e_{uwind}^{cross}	cross-wind entrainment coefficient associated with neutral releases;

ρ_{wind}^{cross}	cross-wind entrainment coefficient associated with density effects;
E_{er}	total-energy change due to ambient gradients;
$E_{er}^{A(s)}_{Amb}$	total-energy change attributed to gradients in the atmosphere at cross-section A(s);
$Entr$	entrainment per unit plume-axis length;
$Entr^{amb}_{turb}$	entrainment per unit plume-axis length attributed to passive dispersion (airborne plume);
$Entr^{grav}_{slump}$	entrainment per unit plume-axis length attributed to transverse gravity slumping (touchdown and slumped plumes);
$Entr_{jet}$	entrainment per unit plume-axis length attributed to shear between plume and atmosphere;
$Entr^{heavy}_{gas}$	entrainment per unit plume-axis length attributed to atmospheric turbulence as modified by density effects;
$Entr^{cross}_{wind}$	entrainment per unit plume-axis length attributed to cross-wind generated vortices (airborne plume);
$F(s)$	plume "footprint" area ("touchdown" and "slumped" plumes);
$g, \mathbf{g}$	scalar, vector acceleration due to gravity; (as affix) pertaining to the vapour/gas phase;
h	local/"top-hat" specific enthalpy; rectangular (slumped) plume height; depth of a cylindrical dense gas source; height above level ground;
h_{∞}	atmosphere specific enthalpy at height z; ambient enthalpy at the plume centroid height;
$h_{\square}$	plume enthalpy at release;
$h_{\infty}^{\square}$	atmosphere enthalpy at release height;
h_g	vapour phase specific enthalpy;
h_{HF}^g	specific enthalpy of HF monomer in the vapour phase;
$h_{(HF)_2}^g$	specific enthalpy of HF dimer in the vapour phase;

$h_{(\text{HF})_6}^g$	specific enthalpy of HF hexamer in the vapour phase;
$h_{(\text{HF})_8}^g$	specific enthalpy of HF octamer in the vapour phase;
$h_{g, \text{H}_2\text{O}}^{\text{HF}}$	specific enthalpy of the reacted complex $\text{HF}=\text{H}_2\text{O}$;
$h_{\text{H}_2\text{O}}^g$	specific enthalpy of free water-vapour in the vapour-phase;
$h_{\text{N}_2\text{O}_2}^g$	specific enthalpy of dry-air in the vapour-phase;
$h_{lg, \text{rtp}}^{\text{HF}}$	latent heat of evaporation HF liquid to HF-monomer at standard pressure and reference temperature (rtp);
$h_{lg, \text{rtp}}^{\text{H}_2\text{O}}$	latent heat of evaporation liquid water to water-vapour at standard pressure and reference temperature (rtp);
$\text{Impact}_{\text{Amb}}^{F(s)}$	impact pressure force at footprint area $F(s)$;
$ J $	Jacobian determinant for the "canonical" coordinate system;
k	gravity spreading coefficient;
K	reaction rate coefficient; ambient atmosphere diffusivity;
K_y	horizontal eddy-diffusivity in the undisturbed atmosphere;
K_z	vertical eddy-diffusivity in the undisturbed atmosphere;
$K_{(\text{HF})_2}^{\text{HF}}$	reaction rate coefficient for the reversible reaction between HF monomer and dimer;
$K_{(\text{HF})_6}^{\text{HF}}$	reaction rate coefficient for the reversible reaction between HF monomer and hexamer;
$K_{(\text{HF})_8}^{\text{HF}}$	reaction rate coefficient for the reversible reaction between HF monomer and octamer;
$K_{\text{H}_2\text{O}}^{\text{HF}}$	reaction rate coefficient for the reversible reaction between HF monomer and free water-vapour;
1	(as affix) pertaining to the liquid-phase;

ℓ	typical axial length scale (flow establishment); length of the intersection of cross-section A(s) and footprint area F(s); (as affix) pertaining to the liquid-phase;
ℓ_y	transverse (horizontal) eddy length-scale (undisturbed atmosphere);
ℓ_z	vertical turbulent eddy length-scale (undisturbed atmosphere);
L	Monin/Obukhov length;
$L_{\text{surface}}^{\text{free}}$	perimeter of a plume cross-section in contact with the ambient atmosphere;
m	mass;
N_2O_2	dry-air (oxygen/nitrogen mixture);
p	local/"top-hat" absolute pressure; (as affix) pertaining to constant pressure;
P/G	Pasquill/Gifford stability class;
p_∞, P_∞	ambient (absolute) pressure at height z;
P_{rtp}	reference (standard, absolute) pressure;
$p_{\text{sat}}^{\text{HF}}$	saturation partial pressure HF vapour above dilute hydrofluoric acid;
$p_{\text{sat}}^{\text{H}_2\text{O}}$	saturation partial pressure H_2O (free or bound) above hydrofluoric acid;
P	momentum within the plume cross-section;
r	radial distance from plume centre-line;
$\mathbf{r}(x, y, z)$	position vector of the plume centroid;
$\mathbf{r}_0(x_0, y_0, z_0)$	position vector of the release orifice;
R	universal gas constant;
Rate	reaction rate constant at standard pressure P_{rtp} ;
Ri_*	Plume (bulk) Richardson number;
rpt	reference temperature (25°C) and standard pressure (101kPa);
s	centroid displacement from release;
S	specific entropy;

Shear	shear force acting on the plume
$\text{Shear}_{\text{Amb}}^{A(s)}$	shear force acting on the plume at cross-section A(s) as the result of gradients within the ambient wind;
t	time;
T	absolute local/"top-hat" temperature Atmosphere Lagrangian time-scale;
T_g	absolute temperature at the roughness height (undisturbed atmosphere);
$T_{\text{ls}}^{\text{H2O}}$	normal freezing point of pure liquid water (absolute temperature, standard pressure);
T_y	horizontal Lagrangian time-scale undisturbed atmosphere;
T_z	vertical Lagrangian time-scale undisturbed atmosphere;
T_*	scale of turbulent temperature fluctuations (atmosphere);
T_∞	ambient temperature at given height; ambient temperature at plume centroid height;
$u(u_x, u_y, u_z)$	local/"top-hat" velocity;
u_*	atmosphere friction velocity; plume centre-line velocity (Gaussian model)
$u_\square$	plume/jet velocity at release;
$u_\infty^\square$	wind-speed at the release height;
$u_* T_*$	surface to air heat-flux (undisturbed atmosphere);
$\langle u'_y u'_y \rangle$	mean square velocity fluctuation in the transverse (horizontal) direction (undisturbed atmosphere);
$\langle u'_z u'_z \rangle$	mean square velocity fluctuation in the vertical direction (undisturbed atmosphere);
x	horizontal displacement of the plume centroid;
$x_{\text{HF}}^{\text{HF}}$	mass-fraction HF in the HF/moist-air mixture;
$x_{\text{HF}}^{\text{HF}}$	mass-fraction HF monomer in the vapour-phase;
$x_{(\text{HF})_2}$	mass-fraction HF dimer

	in vapour phase;
$x_{(\text{HF})_6}$	mass-fraction HF hexamer in vapour phase;
$x_{(\text{HF})_8}$	mass-fraction HF octamer in vapour phase;
$x_{\text{H}_2\text{O}}$	mass-fraction water-vapour in vapour phase;
$x_{\text{H}_2\text{O}}^{\text{HF}}$	mass-fraction $\text{HF}=\text{H}_2\text{O}$ complex in the vapour phase;
$x_{\text{N}_2\text{O}_2}$	mass-fraction dry-air in vapour phase;
x_1^{HF}	mass-fraction HF in liquid phase;
$x_{\square}$	horizontal displacement of release;
x	x-coordinate (HF partial-pressure) in the phase stability diagram;
x_g	x-coordinate assumed vapour-phase equilibrium state on the phase stability diagram;
X	vector of principal variables of a differential/algebraic system;
y	transverse (horizontal) displacement of the plume centroid;
$y_{\square}$	transverse (horizontal) displacement at release;
y_{HF}	molar fraction HF monomer in vapour phase;
y_{HF_2}	molar fraction HF dimer in vapour phase;
y_{HF_6}	molar fraction HF hexamer in vapour phase;
y_{HF_8}	molar fraction HF octamer in vapour phase;
$y_{\text{H}_2\text{O}}$	molar fraction free water-vapour in vapour phase;
$y_{\text{H}_2\text{O}}^{\text{HF}}$	mole-fraction $\text{HF}=\text{H}_2\text{O}$ complex in vapour phase;
$y_{\text{N}_2\text{O}_2}$	mole-fraction dry-air in vapour phase;

y_1^{HF}	mole-fraction (as monomer) liquid-phase that is HF;
Y	y-coordinate (H_2O partial-pressure) in the phase stability diagram;
Y_g	y-coordinate assumed vapour-phase equilibrium state on the phase stability diagram;
z	vertical displacement of the plume centroid; vertical distance above level ground ($z=0$);
z_c	height above ground of the centre of circular segment used in the description of plume "touchdown";
z_r	surface roughness;
$z_\square$	vertical displacement of release;

Greek Alphabet

β	mixture void-fraction;
γ	vapour-phase adiabatic constant (ratio of specific heats at constant pressure and volume)
γ^2, ε^2	turbulent Schmidt number;
Δ	difference between values;
Δh	specific enthalpy of reaction;
$\Delta h_{(\text{HF})_2}^{\text{HF}}$	enthalpy of reaction between HF monomer AND HF dimer;
$\Delta h_{(\text{HF})_6}^{\text{HF}}$	enthalpy of reaction between HF monomer AND HF hexamer;
$\Delta h_{(\text{HF})_8}^{\text{HF}}$	enthalpy of reaction between HF monomer AND HF octamer;
$\Delta h_{\text{H}_2\text{O}}^{\text{HF}}$	enthalpy of reaction between HF monomer and water-vapour;
$\Delta h_{\text{mix}}^{\text{rtp}}$	enthalpy (heat) of mixing pure HF liquid and pure liquid-water at standard pressure and 25°C (rtp);
ΔS	specific entropy of reaction;
$\Delta S_{(\text{HF})_2}^{\text{HF}}$	entropy of reaction between HF monomer AND HF dimer;
$\Delta S_{(\text{HF})_6}^{\text{HF}}$	entropy of reaction between

	HF monomer AND HF hexamer;
$\Delta S_{(HF)_8}^{HF}$	entropy of reaction between HF monomer AND HF octamer;
$\Delta S_{H_2O}^{HF}$	entropy of reaction between HF monomer and water-vapour;
ϵ	dissipation rate of turbulent kinetic energy in the ambient atmosphere;
ϵ_y	dissipation rate of turbulent kinetic energy attributed to horizontal eddies (undisturbed atmosphere);
ϵ_z	dissipation rate of turbulent kinetic energy attributed to vertical (turbulent) eddies (undisturbed atmosphere);
ζ	dimensionless length $(z+z_r)/L$;
θ	polar angle perpendicular to the local plume-axis;
κ	von Karman's constant;
μ	molecular weight;
μ_{HF}	molecular weight HF monomer;
$\mu_{(HF)_2}$	molecular weight HF dimer;
$\mu_{(HF)_6}$	molecular weight HF hexamer;
$\mu_{(HF)_8}$	molecular weight HF octamer;
μ_{H_2O}	molecular weight of water;
$\mu_{H_2O}^{HF}$	molecular weight $HF=H_2O$, that is of the association of HF-monomer and of water-vapour;
ρ	local/"top-hat" plume/mixture density;
ρ_*	plume centre-line density (Gaussian model);
ρ_∞	ambient density at height z; ambient density at the plume centroid height;
$\rho_\square$	plume density at release;
ρ_g	vapour phase density;
ρ_{HF}^g	partial density of

	HF monomer in the vapour phase;
$\rho_{(\text{HF})_2}^g$	partial-density of HF dimer in the vapour phase;
$\rho_{(\text{HF})_6}^g$	partial-density of HF hexamer in the vapour phase;
$\rho_{(\text{HF})_8}^g$	partial-density of HF octamer in the vapour phase;
$\rho_{g, \text{H}_2\text{O}}^{\text{HF}}$	partial-density of the reacted complex $\text{HF}=\text{H}_2\text{O}$;
$\rho_{\text{H}_2\text{O}}^g$	partial-density of free water-vapour in the vapour-phase;
$\rho_{\text{N}_2\text{O}_2}^g$	partial-density of dry-air in the vapour-phase;
ρ_l	liquid-phase density;
ρ_l^{HF}	liquid HF density;
$\rho_l^{\text{H}_2\text{O}}$	liquid water density;
σ_y	transverse (horizontal) plume standard deviation (Gaussian far-field);
σ_z	vertical plume standard deviation (Gaussian far-field);
$\sigma_{y,c}$	plume far-field standard deviation in the horizontal sense attributed to plume meander;
$\sigma_{z,c}$	plume far-field standard deviation in the vertical sense attributed to plume meander;
Σ	Reynolds stress tensor;
Σ_{xz}	xz-component of the Reynolds stress tensor within the plume boundary;
Σ_{xz}^∞	xz-component of the Reynolds stress in the undisturbed atmosphere at given height (general or plume centroid);
τ	Control volume for plume analysis;
ϕ	plume-axis inclination to the horizontal;
$\phi_\square$	inclination of plume immediately upon release;

Additional Symbols

$\times$	vector/"cross" product of vectors;
$\cdot$	scalar/"dot" product of vectors;
∇	Gradient/"del" operator;
$\nabla \cdot$	Divergence/"div" operator;
$\iint, \iiint$	surface, volume integral;
$\square$	appertaining to the release-orifice;
∞	appertaining to the undisturbed atmosphere;
$*$	appertaining to the plume-axis; relating to ambient conditions at the ground;
$ \cdot $	magnitude of a vector, determinant of a matrix, absolute value of a number;
$\rightleftharpoons$	reversible chemical reaction;
$=$	equality; chemical combination;
$'$	fluctuating component of a turbulence variable;
$\langle, \rangle$	turbulent (ensemble) average;
$(\cdot, \cdot, \cdot)$	vector formed from Cartesian components;
$\{ \cdot, \dots, \cdot \}$	set notation;