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CONF-9103253--Summ

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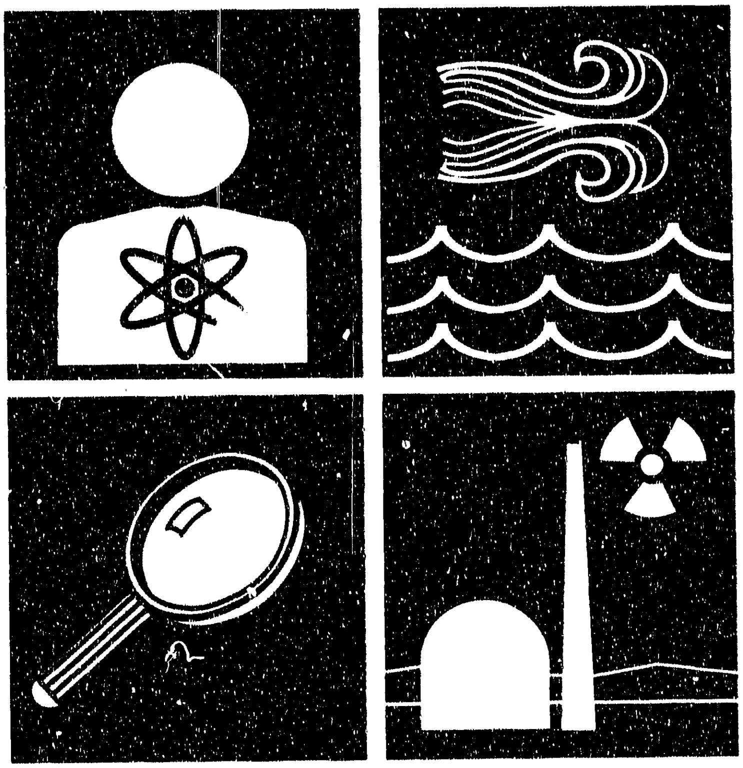
Summary of the March 25-26, 1991 Atmospheric Model Working Meeting

J. V. Ramsdell

July 1992



Letter report for the Technical Steering Panel
and the Centers for Disease Control
under Contract Number 18620

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SUMMARY OF THE MARCH 25-26, 1991 ATMOSPHERIC MODEL WORKING MEETING

Hanford Environmental Dose
Reconstruction Project

J. V. Ramsdell

July 1992

Letter report to the
Technical Steering Panel
and the Centers for Disease Control
Under Contract Number 18620

Battelle
Pacific Northwest Laboratories
Richland, Washington 99352

SUMMARY

Atmospheric transport and diffusion calculations for the initial phase of the Hanford Environmental Dose Reconstruction (HEDR) Project were made using the MESOILT2 computer code (Ramsdell and Burk 1991). This code implemented a Lagrangian trajectory, puff dispersion model using components from other models designed primarily for regulatory applications. Uncertainty in the dispersion calculations was estimated following model calculations. The results of the atmospheric dispersion calculations were summarized in frequency distributions by location for use in preliminary dose calculations.

Analysis of the results of the preliminary dose calculations showed that important information on spatial correlations was lost in summarization of the results of the atmospheric dispersion model calculations. Analysis of the results also showed that atmospheric model uncertainty should be based on model calculations rather than on estimates made independently from the model calculations. Correction of these weaknesses in the atmospheric dispersion model required a revision of the atmospheric model structure. A decision was made to update the level of science represented in the model as the model was restructured because many of the components of MESOILT2 do not represent the current state of the science in atmospheric dispersion modeling.

In early March 1991, a meeting was called to obtain guidance for revision of the atmospheric dispersion model. The participants (see Appendix A) met in Richland, Washington, on March 25 and 26, 1991. This report presents the results of that meeting. The results include a consistent set of equations that represent atmospheric processes important to the transport, diffusion, and deposition of material in the atmosphere and recommendations related to incorporation of uncertainty. Some aspects of wind field modeling and deposition were discussed but not resolved, and most details of implementation of the recommendations were left to those programming the code revisions.

The participants felt that it would be appropriate to reconvene the meeting to review the overall model organization and the implementation of the recommendations from the initial meeting when initial code development is complete.

CONTENTS

1.0 INTRODUCTION

In 1987, the U.S. Department of Energy (DOE) directed the Pacific Northwest Laboratory (PNL), which is operated by Battelle Memorial Institute, to conduct the Hanford Environmental Dose Reconstruction (HEDR) Project. The HEDR Project objective is to estimate radiation doses to individuals and population groups from exposure to historical, radioactive emissions from the Hanford Site. The project is being conducted under the direction of a Technical Steering Panel (TSP) selected by the Vice Presidents for Research at the major universities of Washington and Oregon. A December 1990 Memorandum of Understanding between the Secretaries of the DOE and the U.S. Department of Health and Human Services (DHHS) transferred responsibility for managing the DOE's dose reconstruction and exposure assessment studies, including the HEDR Project to the DHHS. However, the TSP continues in its technical direction role.

Phase I of the project, which ended in July 1990, was designed to determine whether enough information of sufficient quality was available to develop and demonstrate a dose estimating method. The product of Phase I was a set of more than 20 documents that describe the preliminary information found or reconstructed, preliminary dose-estimating models and computer codes, and preliminary estimates of doses and their uncertainties for representative individuals who may have lived near the Hanford Site during the early years of Hanford operations.

Analysis of the preliminary dose estimates (Simpson 1991a,b) revealed several weaknesses in the Phase I modeling approach. Two of the weaknesses related directly to the atmospheric dispersion model. The first weakness was that important information on spatial correlations was lost in summarizing the data in frequency distributions. The second weakness was in the method used to estimate uncertainties in the atmospheric dispersion model calculations. Uncertainty should be based on model calculations rather than on estimates made independently. These weaknesses have been corrected by revising the overall modeling approach to include Monte Carlo techniques for incorporating uncertainty in all components of the overall dose estimation process including the atmospheric dispersion model. This change in modeling approach required a major revision of the atmospheric dispersion model used in Phase I of the study.

In early March 1991, a meeting was called to obtain guidance for use in revision of the model. The meeting was held in Richland, Washington, on March 25 and 26, 1991. This report presents the results of that meeting. The results include 1) a consistent set of equations that represent atmospheric processes important to the transport, diffusion, and deposition of material in the atmosphere, and 2) recommendations related to incorporation of uncertainty. Some aspects of wind field modeling and deposition were discussed but not resolved, and most details of implementation of the recommendations were left to those programming the code revisions.

The meeting participants were told that the HEDR Project technical staff intends to estimate both the doses and the uncertainty in the doses using a Monte Carlo approach. They were also told that the purpose of the meeting was to provide guidance for restructuring and revising the MESOILT2 computer code (Ramsdell and Burk 1991) to make it consistent with the Monte Carlo approach. The participants were asked to re-examine the parameterizations used in the diffusion and deposition computations. The version of the model used in the Phase I calculations does not make much use of recent (last 20 years) developments in boundary layer meteorological theory or experiments.

Specific goals for the March 25-26, 1991, meeting were

1. select an appropriate set of relationships for estimating wind profiles, plume rise, diffusion coefficients, deposition velocities, washout coefficients, and mixing-layer thicknesses for use in the HEDR Project

2. determine methods for accounting for the effects of imprecision and uncertainties in the meteorological data and model parameterizations in the model diffusion and deposition calculations

3. consider distributions for the random variability to be used in the Monte Carlo simulations.

Participants were told that the following factors were to be considered as they worked toward their goals:

1. Computational factors are important. The Monte Carlo approach is computationally intensive. Based on model runs made for Phase I of the HEDR Project, the computational time for the atmospheric model is being discussed in terms of CPU days on Sun workstations. Storage for the model output is being discussed in terms of tens of gigabytes. Therefore, computational time is an important factor.

2. Attempt to come up with a set of relationships that describe the atmosphere in terms of continuous variables rather than discrete states. For example, attempt to build stability dependence into the model via the Monin-Obukhov length or Richardson Number. However, the use of stability classes might be needed to arrive at the Monin-Obukhov length or Richardson Number from available meteorological data. Similarly, it might be necessary to characterize surface roughness by gross classes because of limited data. Nevertheless, values of z_o that vary within the class range should be used rather than a typical value for the class.

3. Attempt to maintain temporal and spatial consistency among the parameters while introducing random variability into the model. It should be possible to maintain this consistency by introducing random variability in model variables that are independent and by propagating the variability to the dependent variables via the model parameterizations. For the purposes of the model, input values may be considered to be independent. These values include wind direction and speed, surface roughness, and perhaps stability class. Dependent variables might include u*, 1/L, plume rise, diffusion coefficients, deposition velocity, etc.

These factors were discussed early in the meeting and were generally open to modification. However, the limited computational resources and time were stressed.

The next chapter contains background information provided to the meeting participants. In addition, all participants were given a copy of the MESOILT2 documentation (Ramsdell and Burk 1991). They were also given a notebook containing copies of relevant papers in the open literature. Most of the papers in the notebooks are cited as references in this report.

Chapter 3 of this report covers the meeting deliberations. It lists the important alternatives considered and presents equations that describe the atmospheric processes. Recommendations of the participants are stated explicitly in Sections 3.1 through 3.5. They are implicit in Sections 3.6 through 3.8.

Chapter 4 covers issues that were not resolved at the workshop. These issues need further discussion as supporting information becomes available.

Chapter 5 contains information that supplements the workshop discussions. The sections on upper-level winds and mixing-layer depth describe data availability, and the section on sigma w for unstable atmospheric conditions presents an alternative set of equations.

The appendices contain information related to the meeting. Appendix A lists the participants, and Appendix B contains the agenda.

2.0 BACKGROUND

The following information was provided to participants in March 25-26, 1991, meeting on HEDR atmospheric modeling. TSP decisions since the meeting have expanded the model domain and extended the study period. These changes are not reflected in the material in this report.

2.1 TIME

The current period of primary interest is December 25, 1944, through December 31, 1947, because it is the period of the largest iodine-131 releases. In the future, this study period will be extended through at least 1955, and possibly through 1972. Model computations are made using a basic time-step of 15 min based on hourly meteorological data input. Puffs are released at 15-min intervals.

2.2 DOMAIN

The model domain is fixed in space and can be tied to a specific location on the earth's surface. Any position that can be identified by latitude and longitude, or other reference system, can be associated with a position in the model domain. The current domain includes most of eastern Washington and northeastern Oregon. It is likely to be extended to include all of eastern Washington and northeastern Oregon, as well as the western portion of northern Idaho. Figure 2.1 shows Washington, Oregon, and western Idaho. Mountains are indicated by the stippled region. Figure 2.2 shows the domain for Phase I of the study. Concentrations and surface contamination are computed at nodes of a Cartesian grid. Spacing between nodes is about 8 km. The wind field used for puff advection is defined on a Cartesian grid with 16-km spacing between nodes.

A separate set of calculations will be made for estimation of doses near the release point (<10-20 km). These calculations will be made using a straight-line plume model.

The vertical structure of the atmosphere in the model is limited to the boundary layer. The top of the boundary layer is defined by the mixing-layer

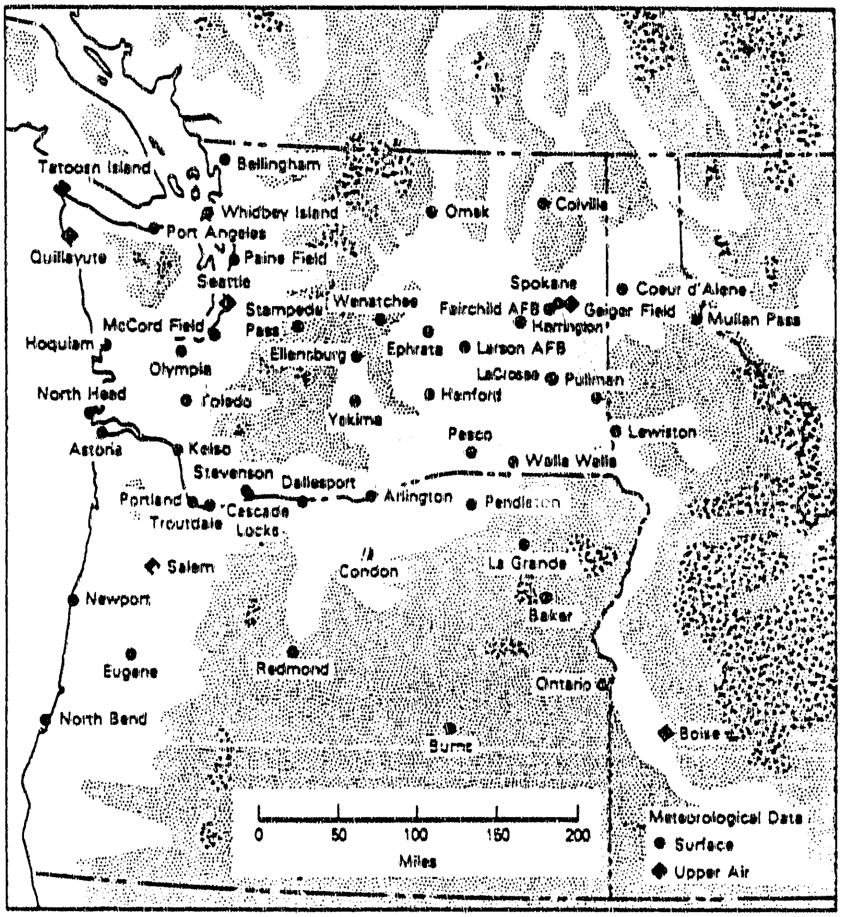

FIGURE 2.1. Meteorological Reporting Stations in Washington, Oregon, and Western Idaho, 1944-1947

depth. Advection of puffs released at ground level is based on winds at the 10-m level. Advection of puffs released at a level between 10 m and the top of the mixed layer is based on winds extrapolated to the release height, and advection of puffs released above the top of the mixing layer is based on winds extrapolated to the top of the mixing layer.

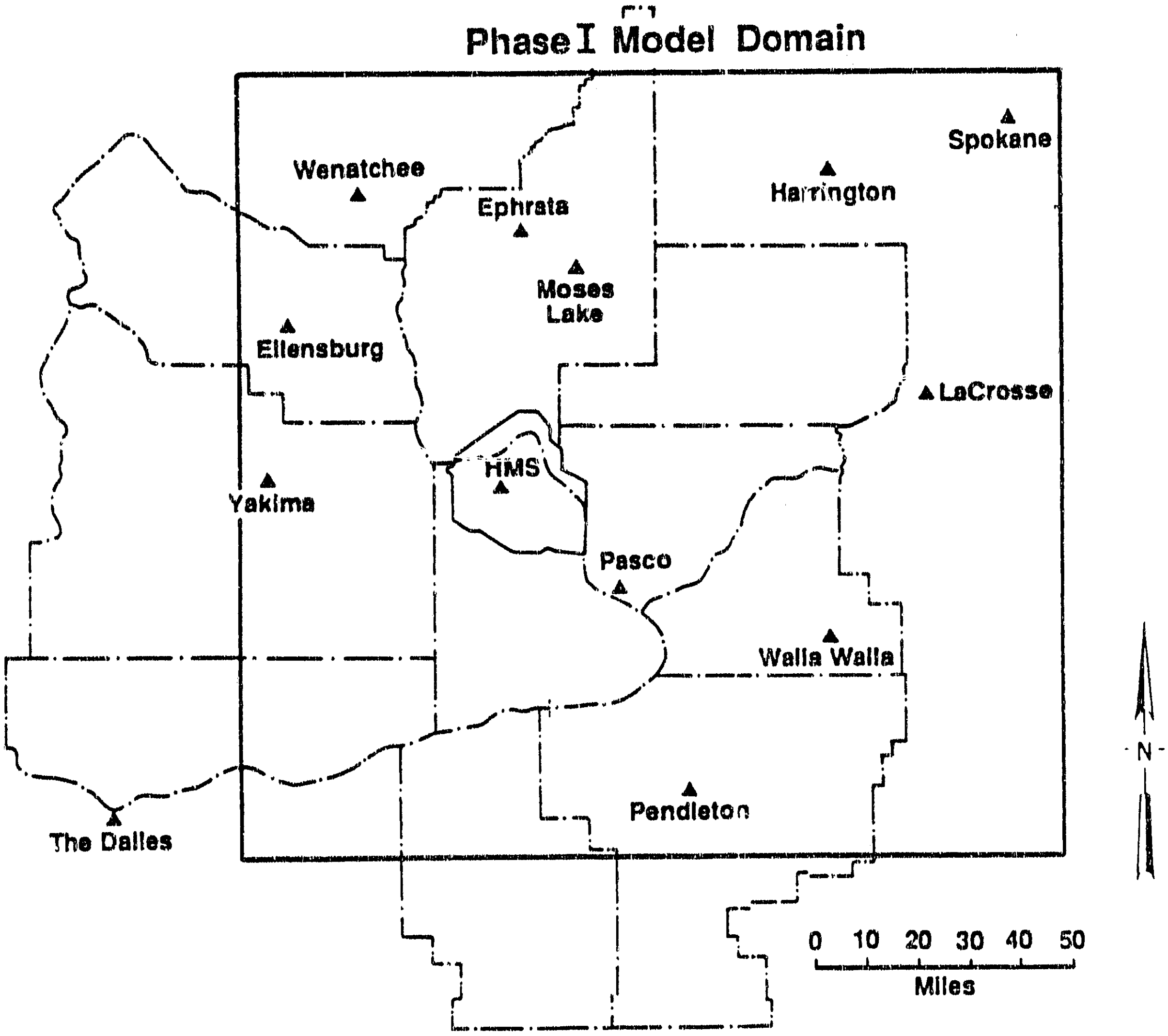

FIGURE 2.2. Meteorological Stations in the Vicinity of the HEDR Model Domain

2.3 METEOROLOGICAL DATA

Meteorological data from routine observations are available from 13 locations in and near the model domain for the primary period of interest. The records for eight of the locations are reasonably complete. Records for three additional locations are nearly complete, except that they are for limited hours. The records for the last two locations are for a limited period. Figures 2.1, 2.2, and 2.3 show the meteorological stations in the

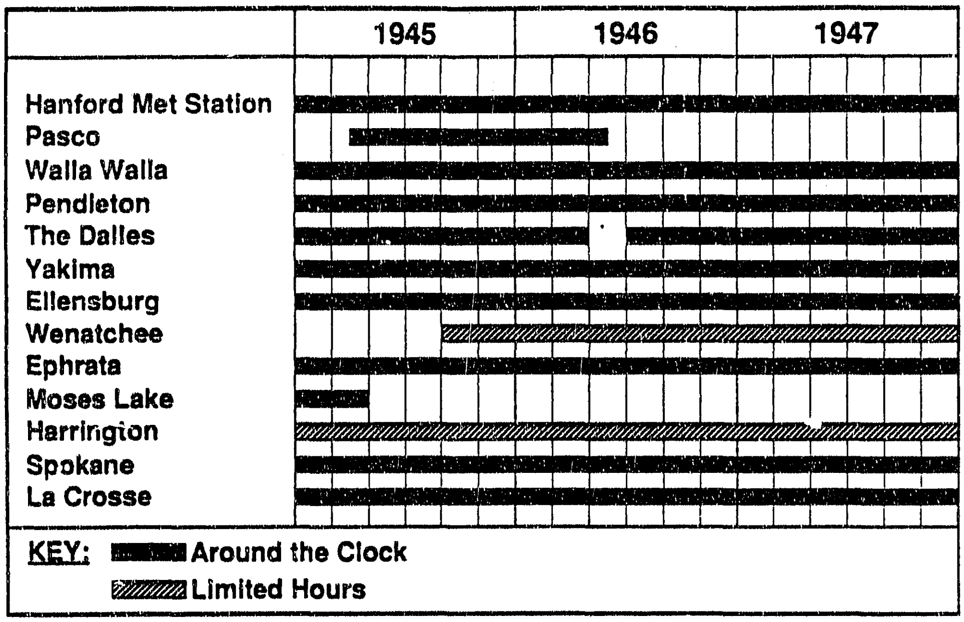

FIGURE 2.3. Meteorological Availability, 1944-1947

Northwest, show the model domain location, and indicate the extent of available meteorological records for the period of primary interest. HMS in Figure 2.2 is the Hanford Meteorology Station. The two fuel reprocessing plants that released most of the iodine-131 are located within 5 miles of the station. The solid line around the HMS shows the approximate boundary of the Hanford Site.

Wind direction, wind speed, and temperature are available for Hanford for the entire primary period of interest. Precipitation records begin in July 1946. Data for most of the other locations include wind, sky cover, weather (precipitation), and temperature. There are daily precipitation amounts for an additional 15 to 20 locations in and near the model domain.

The location and height of wind measurements is generally known. The observations were made with the standard anemometers and vanes of the period. All wind directions are recorded in compass points, and wind speeds are generally reported to the closest knot. Wind speeds at Hanford are reported in miles per hour.

The precipitation data included in the hourly observations generally are the qualitative intensities found under current weather (i.e., light snow, moderate rain, etc.). In a few cases there are hourly amounts in hundredths of an inch. The daily totals are in hundredths of an inch.

Most of the meteorological data for the period were available only on microfiche or paper copies of the original records. The wind data have been entered in our project data base manually. Any other data will have to be manually entered.

2.4 SURFACE ROUGHNESS

Many wind profile measurements (e.g., Horst and Elderkin 1970; Powell 1974) indicate that z_0 in the vicinity of the 200 Areas at Hanford is about 0.03 m. Surface roughness for the rest of the model domain will have to be estimated from topography, land use, and vegetation. Terrain elevations digitized at 30" latitude and longitude intervals (~1 km) are available. In addition, gross land use and vegetation data should be readily available.

2.5 MODEL PARAMETERS TO BE ESTIMATED

Equations, or at least guidance to where the equations can be found, should be selected for the following:

- extrapolation of winds within the boundary layer
- estimation of plume rise
- estimation of diffusion coefficients
- estimation of deposition velocities
- estimation of washout coefficients (secondary)
- estimation of the mixing-layer depth.

Consensus on some of these items should be reached very quickly. For example, the diabatic wind profiles (e.g., Panofsky and Dutton 1984, pp. 133-136) are reasonably well established, and Briggs' plume rise equations (e.g., Briggs 1975, 1984) seem to be almost universally accepted. Other items, for example, selection of washout coefficients, may not be settled.

2.6 INTERMEDIATE ATMOSPHERIC VARIABLES

Work will not be complete when the items listed above are settled. It will still be necessary to make sure that the calculations can be made with the available input data. It is likely that the relationships recommended by the group for wind profiles, estimating diffusion coefficients, etc., will involve intermediate variables such as u*, L, etc. Therefore, the group will spend some time discussing the process of getting from the input data to the final numbers.

3.0 MEETING DELIBERATIONS

The following sections contain the results of the meeting deliberations. Equations and references discussed in the meeting explicitly and implicitly have been included in the section. In some cases, background information has been added to assist members of the Technical Steering Panel in placing the meeting discussions in context of the Phase I model.

3.1 WIND PROFILES

Three methods of adjusting wind data for changes in height were considered during the meeting:

- interpolation between winds estimated at two or more levels using a wind field model
- power-law wind profiles in which the exponents are functions of stability
- diabatic wind profiles based on atmospheric boundary layer similarity theory.

3.1.1 Interpolation

Interpolation requires two wind fields, one near the surface and another at an upper level. Surface wind fields can be estimated from hourly weather data, but upper-level wind field data are available only twice a day. Currently there are four rawinsonde observation stations in the Pacific Northwest--Spokane, Boise, Salem, and Quillayute--that provide these data. The Quillayute station was established after the significant radionuclide releases to the atmosphere from operations at Hanford. Prior to establishment of the Quillayute station, rawinsonde measurements were made at Tatoosh Island and Seattle.

Assuming that the rawinsonde data are adequate, hourly winds at a representative upper level could be estimated by spatial and temporal interpolation from the twice-daily measurements. Then, wind speed and direction at the puff advection height could be estimated by interpolation between the surface and upper-level wind fields. This process estimates changes in wind direction as well as wind speed.

The general consensus was that winds at the 700-mb level (about 10,000 ft msl) would be more representative of the upper-level flow over the HEDR model domain than the 850-mb (about 5000 ft msl) winds because they would be less influenced by local topography. There was also consensus that the winds between 700 mb and a lower level, perhaps 1500 ft to 3000 ft msl, should be assumed to be independent of height. This assumption should lead to more realistic changes in wind direction and speed between the surface level wind field and the puff advection height.

3.1.2 Power-law Profile

Power-law wind profiles (e.g., Panofsky and Dutton 1984, pp. 130-131) have been in use for many years. In these profiles, the wind speed $u(z_2)$ at height z_2 is estimated from the wind speed $u(z_1)$ at height z_1 using the relationship

$$u(z_2) = u(z_1)\ (z_2/z_1)^{\alpha} \tag{3.1}$$

where the exponent α is function of atmospheric stability. The power-law profile does not address the change of wind direction with height.

Although the power-law profile is computationally simple and there is also a significant precedent for its use, the power-law profile doesn't include an explicit relationship with variables important in atmospheric boundary layer description. Specifically, it doesn't provide a relationship between wind speed, surface roughness, and stability that can be used to estimate the friction (atmospheric turbulence scaling) velocity u_*.

3.1.3 Diabatic Profile

Diabatic profiles are derived from atmospheric boundary layer similarity theory proposed by Monin and Obukhov (1954). The basic hypothesis of similarity theory is that in the atmospheric layer near the ground, a number of parameters, including wind profiles, should be universal functions of the friction velocity, a length scale, and the height above ground. A large body of experimental data supports Monin-Obukhov similarity theory.

In similarity theory, the length scale, L, is referred to as the Monin-Obukhov length and the ratio z/L is qualitatively related to atmospheric stability. When z/L is negative and large (e.g., <-2), the atmosphere is extremely unstable (convective). When z/L is near zero, the atmosphere is neutral, and when it is positive and large (e.g., >1), the atmosphere is extremely stable.

The diabatic wind profile is

$$u(z) = \frac{u_*}{k} [\ln(z/z_o) - f(z/L)] \qquad (3.2)$$

where u_* = function velocity

k = von Karman constant, which has a value of about 0.4

z = wind speed measurement height

z_o = a measure of local surface roughness (roughness length)

L = Monin-Obukhov length.

The term f(z/L) represents the effects of stability on the wind profile. In stable atmospheric conditions, f(z/L) has the form $-\alpha z/L$. Estimates of the value of α range from 4.7 to 5.2 (Panofsky and Dutton 1984, p. 136). In neutral conditions, f(z/L) is zero, and the diabatic profile simplifies to a logarithmic profile.

In unstable air, f(z/L) is more complicated. According to Panofsky and Dutton (1984), the most common form of f(z/L) for unstable conditions is based on work by Businger et al. (1971) and Paulson (1970). It is

$$f(z) = \ln\{[(1+x^2)/2] [(1+x)/2]^2\} - 2 \tan^{-1} x + \pi/2 \qquad (3.3)$$

where $x = (1 - 16 z/L)^{1/4}$.

Equation (3.2) provides a means of estimating the friction velocity from measured wind speeds when the surface roughness and Monin-Obukhov lengths can be estimated from other information. Typical roughness lengths have been determined for various types of topography, ground cover, and land use. For the HEDR model domain, they range from about 0.01 m to more than 1 m. Topography and land-use data are readily available with adequate resolution for use with the HEDR atmospheric transport model.

Golder (1972) provides a graphical relationship between the surface roughness length, the Pasquill stability class, and the Monin-Obukhov length. This relationship can be implemented numerically in the model. Estimation of intermediate variables is discussed in more detail later.

3.1.4 Recommendations

Following discussion of the alternatives, the consensus of the meeting participants was that the diabatic profile should be used to model the change in wind speed with height within the boundary layer. There was also a consensus to limit the use of the diabatic profile in stable atmospheric conditions. The wind speed at any height in the boundary layer should not be allowed to exceed the speed at the 850 or 700 mb pressure level. These levels correspond to about 5,000 and 10,000 ft above sea level, respectively.

The diabatic profile doesn't describe the change in wind direction with height. MESOILT2 and many similar dispersion models ignore this change. However, the participants felt that it may be important to model the change in wind direction. The method suggested for modeling the change in wind direction was to determine the upper-level wind direction (again 850 or 700 mb), assume that the wind direction at an as-yet-undetermined height (500 to 1000 m above the terrain) is the same as the upper-level direction, and linearly interpolate between the low-level and upper-level directions.

3.2 PLUME RISE

Plume rise was considered briefly. Although there is more than one method for estimating plume rise, the equations proposed by Briggs (1975, 1984) have gained a general acceptance unequaled by the other methods. Briggs' equations are implemented in the INPUFF model (Petersen and Lavdas 1986) and the MESOPUFF II model (Scire et al. 1984).

3.2.1 Unstable and Neutral Conditions

In unstable and neutral atmospheric conditions, the effective release height (stack height + plume rise) in INPUFF is given by

$$h_e = h_s' + 1.6\, F_b^{1/3}\, x_f^{2/3}\, U(h_s)^{-1} \qquad (3.4)$$

where h_e = effective stack height

h_s' = stack height, corrected for downwash if appropriate

F_b = buoyancy flux parameter

x_f = distance to final plume rise

$U(h_s)$ = wind speed at stack height.

The buoyancy flux parameter, F_b, is defined by

$$F_b = g[(T_p - T_a)/T_p]\ w_p\ r_s^2 \tag{3.5}$$

where g = gravitational acceleration

T_p = initial temperature in the plume

T_a = air temperature

w_p = vertical velocity of the plume at the stack exit

r_s = inside radius of the stack exit

and, the distance to final plume rise, x_f, is given by

$$x_f = \begin{cases} 3.5\ (14F_b^{5/8}) & F_b < 55\ m^4/s^3 \\ 3.5\ (34F_b^{2/5}) & F_b \geq 55\ m^4/s^3. \end{cases} \tag{3.6}$$

A minimum stack height wind speed of 1.37 m/s is assumed when the wind is near calm (<1.37 m/s).

Weil (1985) presents another equation, also attributed to Briggs, for estimating the final plume rise for windy, neutral conditions. It is

$$h_e = h_s' + 1.2\ F_n^{3/5}\ (1 + 1.2F_n)^{2/5}\ h_s' \tag{3.7}$$

where $F_n = F_b / [U(h_s)u_*^2 h_s']$.

3.2.2 Stable Conditions

In windy stable atmospheric conditions, the effective release height in INPUFF is

$$h_e = h_s' + 2.6\ F_b^{1/3}\ [SU(h_s)]^{-1/3} \quad (3.8)$$

where S is a stability parameter, $g\Gamma/T_a$, and Γ is the temperature lapse rate. If the wind speed is low during stable conditions, the effective release height is computed using

$$h_e = h_s' + 4\ F_b^{1/4}\ S^{-3/8}. \quad (3.9)$$

The effective release heights computed with Equations (3.8) and (3.9) are compared, and the lower value is used in the model.

3.2.3 Recommendations

The consensus of the meeting participants was to use equations for final plume rise for the model calculations [Equations (3.4-3.6), (3.8), and (3.9)]. It is not necessary to use equations for plume rise in the vicinity of the stack because it is several kilometers from the release points at Hanford to the nearest points at which air concentration and surface contamination are computed.

The participants also recommended that winds and temperatures measured at stack height be used in the plume rise calculation, when available. When the temperature at the release height is not available, a climatologically representative default value should be used. When the measured wind at the release height is not available, the wind will be estimated from the wind field using the same interpolation technique used to obtain winds for puff movement.

3.3 MIXING-LAYER DEPTH

The atmospheric mixing layer is the portion of the atmosphere near the earth's surface where turbulence is an effective mechanism in spreading material released to the atmosphere. The top of the mixing layer acts as a limit for the vertical diffusion of material released in the mixing layer. In models, mixing-layer depth refers to the height of the top of the mixing-layer above the ground.

The mixing-layer depth is generally a function of surface heat flux, surface roughness, and wind speed. It may be estimated from the temperature profile in rawinsonde observations or remote sensing instruments such as SODARs and LIDARs. Rawinsondes were just coming into use in the middle 1940s, and SODARs and LIDARs are recent developments.

3.3.1 Stable and Neutral Conditions

Estimates of the mixing-layer depth may be made from surface meteorological data. For stable conditions, Zilitinkevich (1972) derives the expression

$$H = k\ (u_* L/f)^{1/2} \tag{3.10}$$

where H = mixing-layer depth

k = von Karman constant (~0.4)

L = Monin-Obukhov length

f = Coriolis parameter.

Pasquill and Smith (1983) indicate that constant values in the range 0.2 to 0.7 have been suggested in place of the von Karman constant in Equation (3.10), and authors referenced by Weil (1985) suggest constant values in the range 0.4 to 0.7.

For neutral conditions, the mixing-layer depth may be estimated from

$$H = \beta u_*/f \tag{3.11}$$

where β is a constant. Zilitinkevich (1972) assumes that β is equal to k; Pasquill and Smith (1983) suggest β has a value in the range 0.2 to 0.3; and Panofsky and Dutton (1984) suggest its range is 0.15 to 0.25.

3.3.2 Unstable Conditions

Panofsky and Dutton (1984) contains a derivation of a simple integral equation for H in unstable conditions. However, solution of the equation requires information that is not available for Hanford for the HEDR study period. The remaining alternatives are to estimate H from observed data or from climatology.

The nearest location with rawinsonde data suitable for use in estimating mixing-layer depths is Spokane, where rawinsonde observations are made twice daily. Mixing-layer depths are also estimated hourly by the Hanford Meteorological Station forecast staff.

3.3.3 Recommendations

The consensus was that the mixing-layer depths be estimated from surface meteorological observations during neutral and stable atmospheric conditions. For unstable conditions, the participants recommended that the mixing-layer depth be estimated from Spokane rawinsonde observations if the weather is similar over the model domain. If the weather is dissimilar, they recommended that climatology be used to estimate the mixing-layer depth.

Estimating the mixing-layer depth based on local conditions may lead to unrealistic spatial variations in the mixing-layer depth between meteorological stations. The participants recommended that some method be used to smooth out unrealistic variability. The two methods discussed were 1) estimating the mixing-layer depth at each location and then smoothing the estimates, and 2) fitting a surface to the estimates. Selection of a method was left as an open issue.

3.4 DIFFUSION COEFFICIENTS

There are numerous methods for estimating diffusion coefficients described in the literature. They have been compared and evaluated (e.g., Gifford 1976, Hanna et al. 1977, Randerson 1979, Irwin 1983, Weil 1985, Gryning et al. 1987). The general consensus is that diffusion coefficients should be estimated directly from atmospheric turbulence statistics. Meeting participants group didn't indicate any desire to deviate from this consensus.

Turbulence statistics are not available for use in the HEDR study. As a result, turbulence statistics must be estimated from atmospheric conditions, e.g., wind speed and stability, and surface roughness. Estimation of turbulence statistics is discussed under intermediate variables in Section 3.6.

Methods of estimating diffusion coefficients that are based entirely on stability classes or turbulence typing schemes and distance (e.g., the Pasquill-Gifford curves) were not considered at the meeting.

A puff diffusion model is being used in the HEDR Project to simulate plume diffusion. There is a theoretical difference between puff and plume diffusion coefficients. Puff models, including MESOILT2, INPUFF, and MESOPUFF II, generally use plume diffusion coefficients. However, one peer reviewer of MESOILT2 questioned the appropriateness of this practice. The question was placed before the meeting participants. The consensus of the participants was that the use of plume diffusion coefficients was justified for two reasons. The first reason is that the model is using puffs as a computational device to represent plumes. If puff diffusion coefficients were used, the results of model calculations would not approach the results of a straight-line Gaussian plume model when constant wind direction, wind speed, and stability are used as model input. The second reason is that the duration of releases at Hanford is longer than the time for plumes to travel from the source to most receptors in the model domain. Therefore, use of plume diffusion coefficients will continue in the revised model.

3.4.1 Recommendations

The equation recommended for estimating horizontal diffusion coefficients near the source is

$$\sigma_y = \sigma_v \, t \, f_y(t) \tag{3.12}$$

where σ_y = the horizontal diffusion coefficient

σ_v = the standard deviation of the component of the wind perpendicular to the mean direction

t = the travel time

$f_y(t)$ = a nondimensional function related to the travel time and turbulence time scale.

This relationship is used in the INPUFF model; MESOPUFF II uses stability classes and distance traveled to estimate diffusion coefficients. Thus, the recommendation on diffusion coefficients is to follow the procedure in INPUFF.

In the INPUFF model, the function $f_y(t)$ is computed using a relationship suggested by Irwin (1983). It is

$$f_y(t) = [1 + 0.9(t/T_i)^{1/2}]^{-1} \quad (3.13)$$

where t is the travel time and T_i is the turbulence time scale, which is assigned a value of 1000.

In Equation (3.12) with $f_y(t)$ defined by Equation (3.13), the diffusion coefficient increases as a function of time to the first power near the source and as a function of time to the one-half power at long times. This behavior is consistent with Taylor's (1921) theoretical result. However, Gifford (1977, 1982) presents a strong case based on both theory and observed plumes that horizontal diffusion increases at least linearly with time for several days. On this basis, the participants recommend that after 30 minutes of travel time, horizontal diffusion coefficient be computed using

$$\sigma_y = c\sigma_v t \quad (3.14)$$

where c is a constant equal to the value of $f_y(t)$ at 1800 s.

The recommended equation for estimating vertical diffusion coefficients is similar to Equation (3.12) with σ_z replacing σ_y, σ_w replacing σ_v, and $f_z(t)$ replacing $f_y(t)$, respectively. It is

$$\sigma_z = \sigma_w \, t \, f_z(t). \quad (3.15)$$

When this equation is applied to releases within the mixing layer, growth of σ_z is limited by the mixing-layer depth. When it is applied to releases above the mixing layer, σ_w is set to 0.01 m/s, and σ_z is limited by the effective release height.

INPUFF has two forms for the nondimensional function $f_z(t)$. In unstable and neutral conditions

$$f_z(t) = 1 \quad (3.16)$$

and in stable conditions (and above the mixing layer)

$$f_z(t) = [1 + 0.9(t/T_i)^{1/2}]^{-1} \quad (3.17)$$

where $T_i = 50$. Estimation of σ_v and σ_w is discussed under estimation of intermediate variables (Section 3.6).

3.5 DEPOSITION

MESOILT2 uses simple methods for calculating dry and wet deposition. The original purpose for including deposition in the MESOI family of models was to identify areas where field teams should be sent to measure surface contamination. In that context, simple deposition models were adequate. More sophisticated methods of calculating deposition need to be evaluated for the model for use in the HEDR Project.

3.5.1 Dry Deposition

MESOILT2 uses a dry deposition model that is a puff model equivalent of the source depletion model used in plume models. The rate of deposition of material on surfaces is proportional to the concentration near the surface. The proportionality constant between the concentration in the air and the flux of material to the surface is called a deposition velocity. A constant value of 0.01 m/s was assumed for deposition of iodine-131 in MESOILT2. The amount of material deposited on the surfaces is subtracted from the total mass in the puff to conserve mass. However, this procedure artificially propagates the mass deficit resulting from deposition throughout the puff instantaneously.

Alternative methods for estimating dry deposition proposed by Overcamp (1976), Horst (1977, 1980, and 1983) have not been used in applied models. Current generation, applied models estimate deposition using an approach based on an analogy with electrical systems. The deposition process is assumed to be controlled by a network of resistances, and the deposition velocity is the inverse of the total resistance of the network. In the simplest case, resistances are associated with atmospheric conditions; physical and chemical characteristics of the material; and the physical, chemical, and biological properties of the surface. Seinfeld (1986) describes the resistance analogy.

In the resistance analogy, typically, the total resistance is made up of three components: aerodynamic resistance, surface layer resistance, and transfer resistance. Thus, for a gas, the deposition velocity is computed as

$$v_d = (r_a + r_s + r_t)^{-1} \quad (3.18)$$

where v_d = deposition velocity

r_a = aerodynamic resistance

r_s = surface resistance

r_t = transfer resistance.

Equation (3.18) is used in the MESOPUFF II model. The aerodynamic resistance is a function of wind, stability, and surface roughness. The surface resistance is a function of wind and surface roughness and may be expressed in terms of a Schmidt number. Finally, the transfer resistance is associated with the characteristics of the depositing material and surface type. Equation (3.18) can be extended to calculation of deposition velocities for particulate material with relatively minor modifications.

Computation of deposition velocities by the resistance analogy does not deal directly with the problem related to depletion of the puffs. However, by selecting the methods of computing resistances so the deposition velocity decrease significantly during stable conditions, the magnitude of the problem can be reduced.

3.5.2 Wet Deposition

MESOILT2 includes a simple washout model for calculating wet deposition. Washout coefficients are functions of precipitation rate and precipitation type. The values of the washout coefficients are based on limited experimental work.

3.5.3 Recommendation

The consensus of the participants was to use the resistance analogy to estimate deposition velocities. There were no recommendations related to computing resistances or wet deposition.

3.6 ESTIMATION OF INTERMEDIATE VARIABLES AND PARAMETERS

The methods recommended by the meeting participants involve several intermediate variables or parameters that are not directly measured. Therefore, values of these variables must be estimated from available data. The methods that the working group recommended for estimating the intermediate variables are summarized here.

3.6.1 Surface Roughness (z_o)

The surface roughness length is a characteristic length associated with surface roughness elements. It arises as a constant of integration in derivation of the wind profile equations and is used in several other boundary relationships.

Texts on atmospheric diffusion and air pollution (e.g., Panofsky and Dutton 1984) contain tables that give approximate relationships between z_o and land use, vegetation type, and topographic roughness. Data on land use, vegetation types and topographic roughness are readily available for the HEDR model domain. Thus, the relationships in these tables can be used to estimate surface roughness.

3.6.2 Stability Class

Numerous methods exist for describing atmospheric stability. Most of these methods require information that is not readily available in normal meteorological records. However, Pasquill (1961) and Turner (1964) describe procedures for estimating atmospheric stability classes from routine meteorological measurements. The stability classes defined by Pasquill and Turner do not provide the continuous measures of stability that are desired, but they may be used as intermediate variables in estimating a continuous stability measure, the Monin-Obukhov length.

The Pasquill and Turner stability classes are both determined from solar radiation and wind speed. Turner's classification scheme is more detailed than Pasquill's scheme. Golder (1972) compares stability class estimates from the two schemes.

3.6.3 Monin-Obukhov Length (L)

Golder (1972) also provides a means for converting stability class estimates to estimates of the Monin-Obukhov length. Golder's Figure 2 and 3 relate z_0, 1/L and the Pasquill and Turner stability classes. Given z_0 and a stability class, these figures can be used to estimate a range for 1/L.

3.6.4 Friction Velocity (u_*)

Given a wind speed, the wind speed measurement height, z_0, and 1/L, the diabatic wind profile equation can be used to estimate u_*.

3.6.5 Sigma v (σ_v) and Sigma w (σ_w)

Hanna, Briggs, and Hosker (1982) present simple expressions relating the standard deviations of the lateral and vertical components of turbulence to the friction velocity and other atmospheric boundary layer parameters. These expressions are

$$\sigma_v = \begin{cases} u_* \, (12 - 0.5H/L)^{1/3} & \text{Unstable} \quad (3.19) \\ u_* \, 1.3\exp(-2fz/u_*) & \text{Neutral} \quad (3.20) \\ u_* \, 1.3(1 - z/H) & \text{Stable} \quad (3.21) \end{cases}$$

$$\sigma_w = \begin{cases} u_* \, 1.3\exp(-2fz/u_*) & \text{Neutral} \quad (3.22) \\ u_* \, 1.3(1 - z/H). & \text{Stable} \quad (3.23) \end{cases}$$

They also provide four equations for use in estimating σ_w in unstable conditions. The four equations involve a scaling velocity related to the surface heat flux and the mixing-layer height. The equations are not listed here; two alternatives that were not discussed at the workshop are presented later.

3.7 INCORPORATION OF UNCERTAINTY

One of the primary reasons for extensive revision of the MESOILT2 (Ramsdell and Burk 1991) code is to facilitate the incorporation of uncertainty in model calculations. When the number of sources of uncertainty is large and the variables in the model are correlated, a good deal of caution must be taken in the way in which uncertainty is incorporated. Among the potential problems is compounding the effects of uncertainty in an unrealistic manner.

The premise set forth at the beginning of the meeting was that unrealistic compounding of the effects of uncertainty in an atmospheric model could be avoided by careful selection of a self-consistent set of equations for the model and restricting addition of random components to only those variables which may be realistically assumed to be independent. This premise was disputed. Equations (3.1) through (3.23), which were recommended by the participants, are consistent.

Given the recommended equations, the participants considered the variables discussed in Sections 3.7.1 through 3.7.6 to be appropriate places to enter uncertainty. The variables are uncorrelated or weakly correlated. Uncertainty entered via these variables will propagate properly throughout the remaining model variables.

3.7.1 Surface Roughness

Surface roughness lengths can be estimated directly from measured wind profiles or they can be estimated from general characteristics of the surface such as topography and land use. Extensive wind measurements at the Hanford Meteorology Station show that the roughness length near fuel processing plants in the 200 Areas is in the range of 0.03 to 0.12 m. Roughness lengths for the remainder of the domain must be estimated from topography and land use.

Topography and land use may be used to classify the model domain into several roughness length classes. Each class can be assigned a roughness length range using typical values found in the meteorological literature. Tables 6.1 and 6.2 in Panofsky and Dutton (1984) provide guidance in establishing the classes and ranges.

In the vicinity of Hanford, surface roughness should be relatively independent of atmospheric conditions. Therefore, it was the consensus of the participants that the set of surface roughnesses used to describe the model domain should not be changed as a function of time. However, the uncertainty in the surface roughness lengths should be incorporated by random variation of roughness lengths between replications. Use of a stratified sampling procedure (e.g., Latin hypercube sampling) to select the roughness lengths was recommended.

The distribution to be assumed for roughness lengths within the roughness length classes was discussed briefly. Both uniform and log-uniform distributions were mentioned. However, neither distribution has a strong theoretical basis.

3.7.2 Stability Class

Atmospheric stability is a fundamental concept in meteorology, but it cannot be obtained directly from the data available for the study period. As a result, it must be estimated from the limited data that are available. Several methods of estimating stability are in use. It is well established that the methods do not give consistent results on an hour-by-hour basis.

Methods of estimating stability classes proposed by Gifford (1961), Pasquill (1962), and Turner (1964) are based on data that are available in routine meteorological observations. These methods form the basis of the procedure that the National Climatic Data Center uses to estimate stability classes from climatological data (Hatch 1988).

Golder (1972) compares stability class estimates made at five locations using the Pasquill and Turner methods. The results of this comparison, shown in Golder's Figure 3, show reasonable agreement among the hourly stability class estimates and provide a basis for estimating the uncertainty in the class estimates.

3.7.3 Monin-Obukhov Length

Stability classes are discrete estimates of atmospheric stability. However, in boundary layer similarity theory, stability is represented by the Monin-Obukhov length, L, which is a continuous variable. Figure 5 in Golder's 1972 paper provides a basis for converting stability class to Monin-Obukhov length. The figure may be used to estimate a range of Monin-Obukhov lengths that are consistent with a given surface roughness length and stability class.

Specific values of L can be obtained from the range when needed. The figure indicates that it is appropriate to assume that 1/L is uniformly distributed within the range.

3.7.4 Wind Speed

Wind speed measurements are subject to many errors. The largest errors in historical measurements are likely to be in the result of poor instrument exposure. It is difficult to estimate the magnitude of these errors. Within the context of atmospheric transport and diffusion modeling, these errors may be assumed to be a minor source of uncertainty in model predictions relative to uncertainties in wind direction and stability. No attempt will be made to correct wind speed data for potential measurement errors. However, uncertainty in wind speeds related to imprecision of the recorded wind speeds will be accounted for.

Wind speeds used in the model will be selected from a uniform distribution centered on the recorded speed. The width of the distribution will be determined by the precision of the recorded speeds.

3.7.5 Wind Direction

Wind direction data prior to 1965 are recorded by compass points (N, NNE, ..., S, ..., NW, N). Each compass point represents a 22.5° sector. This imprecision in the recorded wind direction data will be a significant source of uncertainty in atmospheric transport calculations. This uncertainty will lead to significant uncertainty in the concentration and dose estimates at specific points resulting from isolated, short-term releases. The magnitude of the uncertainty should decrease as the number of releases and integration period increase.

Imprecision in wind direction can be addressed by assuming that wind directions are randomly distributed within the reported sector. However, imprecision is not the only source of uncertainty in wind directions. The recorded directions for stations other than Hanford are the result of brief observations made once each hour; they are not hourly averages. Thus, the direction may not be representative of the true hourly average. In addition, wind directions are expected to have greater uncertainty during low wind speeds than during high speeds.

Wind direction errors may also be caused by other factors including unrepresentative instrument exposures, instrumentation errors, and observer bias. To the extent that the errors are random and unsystematic, they are difficult or impossible to identify and correct in historic data. Frequently, however, the existence of errors associated with observer bias can be detected by examining wind direction summaries.

The meeting participants generally agreed (not unanimously) that the wind direction uncertainty should be treated by assuming that the wind direction is uniformly distributed within the reported 22.5° sector. An alternative, which was discussed at length, is to expand the sector width as the wind speed decreases. There was agreement that the uncertainty increases as the wind speed decreases, but there was no consensus on details of how much to expand the sector width, or how to relate the expansion to wind speed. Ultimately, the group agreed that it would be better to risk understating the wind direction uncertainty than to expand the sector width without a firm technical basis.

The discussion on wind direction uncertainty led the meeting participants to the general conclusion that we should base our treatment of uncertainty in the model input variables on what we know. We should not base it on what we feel.

3.7.6 Mixing-Layer Depth

The participants recommended that the mixing-layer depth be computed from the friction velocity and Monin-Obukhov length during stable and neutral atmospheric conditions. Therefore, variations in the estimated values of the friction velocity and Monin-Obukhov length will lead to variations in the mixing-layer depth during these conditions. In unstable conditions, the mixing-layer depth will be estimated from climatological data at the Hanford Meteorology Station. These data may be used to estimate a range of variability and distribution of mixing-layer depths as well as a mean value. Uncertainty in mixing-layer depths during unstable conditions can be modeled by selecting random values from an empirical distribution based on Hanford data.

3.8 MODEL VALIDATION

The subject of model validation was discussed briefly by the working group. The discussion centered on two topics. The first was the meaning of validation, and the other was data sets for use in validation.

The group consensus was that if model validation is construed as proof that a model will give accurate concentration or dose estimates under all conditions for all locations, then model validation is impossible. On the other hand, if model validation is construed as a demonstration that a model produces results that are generally consistent with observed data in one or more test cases, then validation is a realistic goal.

In this broader sense of validation, the group noted that there are several data sets that might be used to evaluate the transport and diffusion portions of the atmospheric model. These data sets include data on krypton-85 releases at Hanford and the Department of Energy's Savannah River Plant and data from dispersion experiments at the Idaho National Engineering Laboratory. The group also suggested that there might be other environmental monitoring data from Hanford that could be used for model evaluation.

4.0 OPEN ISSUES

The meeting agenda covered many topics related to revision of the atmospheric model. Several important topics were not on the agenda, notably, wind field modeling and treatment of the various forms in which iodine can exist in the environment. In addition, the meeting participants did not dwell at length on the details of implementation of their recommendations. These topics remain as issues to be discussed later.

4.1 WIND FIELD MODELING

Discussion of wind field modeling was omitted from the meeting agenda because the topic is being addressed in a separate HEDR task element and the work in the element was not at a suitable stage for review. Nevertheless, some time was spent discussing wind field models. The importance of the wind field model was stressed in the discussion.

4.2 IODINE PARTITIONING

Iodine exists in the atmosphere in many forms. Burger (1991) states that the iodine may be released in several forms as reactor fuel is dissolved, and that three of these forms last long enough to be considered atmospheric emissions. The three forms are elemental iodine (or ICl), organic iodides, and iodine attached to particulates.

The partitioning of the iodine is significant because the literature (e.g., Sehmel 1980) indicates that these forms have different deposition characteristics. For example, reported deposition velocities for elemental iodine are of the order of 1 cm/sec, deposition velocities for typical atmospheric particulates are generally ≤ 0.1 cm/sec, and deposition velocities for methyl iodide are generally $<10^{-2}$ cm/sec. The amount of iodine entering the milk pathway via deposition depends on the deposition velocity for and the amount of iodine in each form.

Burger (1991) discusses reactions of iodine in the atmosphere. It is clear from this discussion that the reactions are complex and that it is unlikely that they can be modeled in a rigorous fashion in the HEDR atmospheric model. However, it is also clear from the importance of the milk pathway in estimating doses from iodine that the atmospheric model should in some way account for the partitioning of iodine between forms.

Alternative methods for treating the iodine partitioning problem will be identified and evaluated. Following peer review of the evaluation, the results will be presented to the Technical Steering Panel for consideration.

4.3 MODEL IMPLEMENTATION

Details of implementation of the recommendations made at the meeting depend on many factors, some obvious and others that can only be discovered during implementation. Therefore, participants in the meeting did not specify details of implementation of the group's recommendations. However, they were willing to reconvene the meeting to review the overall organization of the revised atmospheric dispersion code and the details of implementation of the recommendations when the code is completed.

5.0 POSTSCRIPT

This section presents information on several topics that have come to light following the working group meeting.

5.1 UPPER-LEVEL WINDS

Rawinsonde observations in the northwest United States were limited to Medford, Oregon, prior to 1947. Thus, the data do not exist for this period to permit estimation of upper-level winds directly from observations. However, constant height and constant pressure charts are available for 1944 through 1947, except for a 2-month period in 1945. Upper-level winds may be extracted manually from these charts. Surface weather charts are also available for the entire period. Geostrophic winds can be estimated from surface pressures or isobars for the period when the upper-level charts are missing. Gridded surface pressures and 500 mb heights are available starting in 1946.

5.2 MIXING-LAYER DEPTH

Spokane rawinsonde soundings cannot be used to estimate mixing-layer depth during unstable atmospheric conditions for the early years of the HEDR study period because the data are not available. Therefore, we will use climatological estimates of mixing-layer depth for unstable conditions. These climatological estimates may be based on hourly mixing-layer depth estimates made at the Hanford Meteorology Station in recent years. Climatological estimates of mixing-layer depths will provide backup for missing data during neutral and stable conditions. These estimates may also be used to provide a check on computed mixing-layer depths.

5.3 SIGMA w (σ_w) FOR UNSTABLE CONDITIONS

Hanna, Briggs, and Hosker (1982) divide the atmosphere into four layers relative to H, the mixing-layer depth, for the purpose of computing σ_w for unstable conditions. This division provides more detail than is needed for HEDR because the releases are relatively close to the bottom of the mixing layers that are common in unstable atmospheric conditions.

Several methods of estimating σ_w have been suggested in the literature in addition to the method suggested by Hanna et al. Panofsky et al. (1977) suggest two possible relationships. The simpler of their relationships appears to fit experimental data better. It is

$$\sigma_w = 1.3\ u_* \ (1.0 - 3.0\ z/L)^{1/3} \tag{5.1}$$

where the symbols are as previously defined. A more recent relationship given by Gryning et al. (1987) is

$$\sigma_w = u_* \ \{1.5[z/(kL)]^{2/3}\ \exp(-2z/H) + (1.7 - z/H)\}^{1/2}. \tag{5.2}$$

One of these relationships may be selected for incorporation in the model.

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APPENDIX A

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APPENDIX B

AGENDA

APPENDIX B

AGENDA

AGENDA FOR
HEDR ATMOSPHERIC TRANSPORT MODEL MEETING

<u>March 25, 1991</u>

8:30	Convene -- Tower Inn Suite B
8:45	Introduction to HEDR
10:00	Break
10:15	Revisions to Agenda
10:30	Wind Profiles
11:15	Plume Rise
12:00	Lunch
1:00	Mixing-Layer Depth
2:00	Diffusion Coefficients
2:45	Break
3:00	Diffusion Coefficients Cont.
3:45	Deposition
4:55	Revisions to Tuesday Agenda
5:00	End of Session

<u>March 26, 1991</u>

8:00	Estimation of Intermediate Variables and Parameters
10:00	Incorporation of Uncertainty
12:00	Lunch
1:00	Model Validation
3:00	Summarize Results
5:00	End of Meeting

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