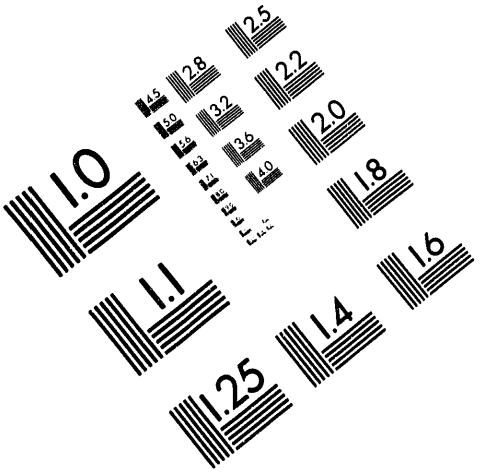

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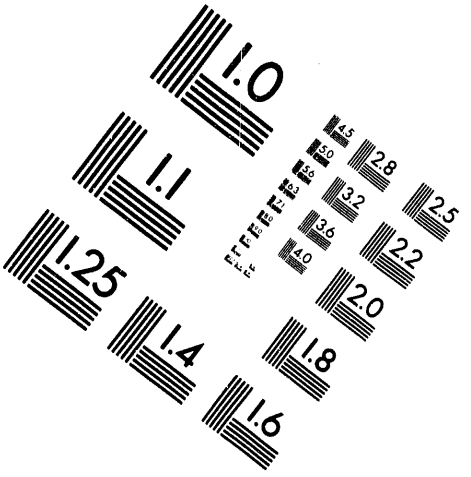

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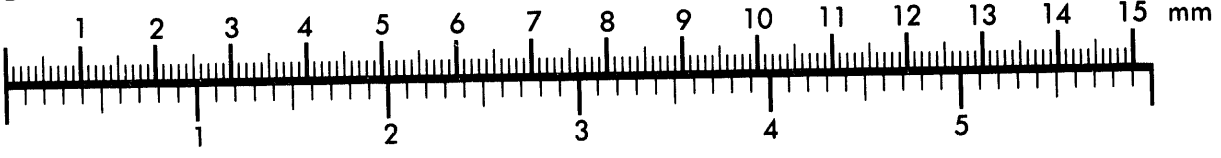

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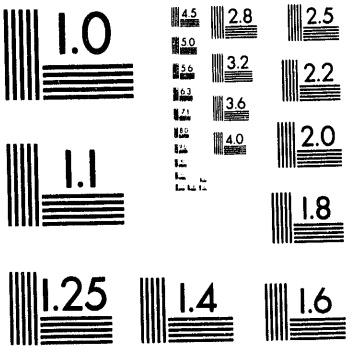

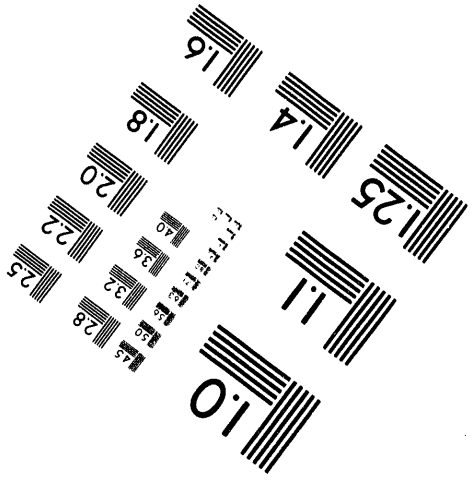

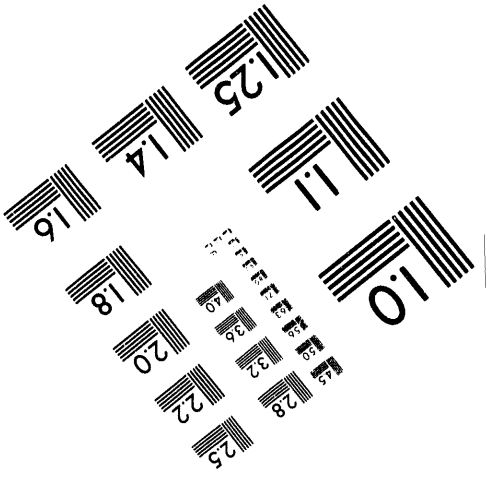

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FEM3C—An Improved Three-Dimensional Heavy-Gas Dispersion Model: User's Manual

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March 1994

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MASTER

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FEM3C—An Improved Three-Dimensional Heavy-Gas Dispersion Model: User's Manual

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ABSTRACT

FEM3C is another upgraded version of FEM3 (a three-dimensional Finite Element Model), which was developed primarily for simulating the atmospheric dispersion of heavier-than-air gas (or heavy gas) releases, based on solving the fully three-dimensional, time-dependent conservation equations of mass, momentum, energy, and species of an inert gas or a pollutant in the form of vapor/droplets. A generalized anelastic approximation, together with the ideal gas law for the density of the gas/air mixture, is invoked to preclude sound waves and allow large density variations in both space and time. The numerical algorithm utilizes a modified Galerkin finite element method to discretize spatially the time-dependent conservation equations of mass, momentum, energy, and species. A consistent pressure Poisson equation is formed and solved separately from the time-dependent equations, which are sequentially solved and integrated in time via a modified forward Euler method. The model can handle instantaneous source, finite-duration, and continuous releases. Also, it is capable of treating terrain and obstructions. Besides a K-theory model using similarity functions, an advanced turbulence model based on solving the $k-\varepsilon$ transport equations is available as well. Imbedded in the code are also options for solving the Boussinesq equations. In this report, an overview of the model is given, user's guides for using the model are provided, and three example problems are presented to illustrate the usage of the model.

1. INTRODUCTION

FEM3C is another upgraded version of FEM3 (a three-dimensional Finite Element Model) which was originally developed for simulating the atmospheric dispersion of liquefied natural gas (LNG) and other heavier-than-air gas (or heavy gas) releases. The FEM3 model (Chan, 1983) employs a modified Galerkin finite element method (GFEM) to solve the time-dependent conservation equations of mass, momentum, energy, and species of an inert gas, together with the ideal gas law for the density of gas/air mixture. Heat transfer between the ground surface and the vapor cloud is included via a bulk coefficient submodel and turbulence is parameterized via a K-theory submodel using similarity functions established in the atmospheric boundary layer. The model can simulate both continuous and finite duration releases with the resulting vapor cloud dispersion over either a flat or variable terrain. Over the years, FEM3 has been validated to a large extent using data obtained from both laboratory-scale and field-scale heavy-gas dispersion experiments (see, for example, Ermak *et al.*, 1982; Chan *et al.*, 1984, Ermak and Chan, 1985; Havens *et al.*, 1987).

Since 1984, the U.S. Army Chemical Research, Development and Engineering Center (CRDEC) has funded Lawrence Livermore National Laboratory (LLNL) to adapt and further develop FEM3 for CRDEC's applications. As a result, the capabilities of FEM3 have been significantly enhanced. In 1988, a newer version, called FEM3A (Chan, 1988), was released to CRDEC. The major improvements include the following: (1) capability for simulating

instantaneous releases involving multiple, overlapping sources, (2) the ability to treat obstructions such as buildings, dikes, and tanks, (3) improvement to the K-theory turbulence submodel, (4) addition of a phase-change submodel for treating vapor-liquid transition of the dispersed material, (5) implementation of an incomplete Cholesky conjugate gradient (ICCG) solver as a cost-effective alternative for solving the pressure field of large-scale problems, and (6) a more user-friendly code with simplified input. Some application and evaluation studies of FEM3A can be found in Ermak and Chan (1986), Rodean (1987a), and Chan *et al.* (1987a, 1987b).

Because the generalized anelastic equations solved in FEM3/FEM3A were originally derived as an extension of the classical Boussinesq equations to stretch the density change to a larger value (up to 0.6 for LNG-the material considered at the time), ensuring mass conservation was not thought to be an issue-as it is not considered an issue in the Boussinesq equations. In the past, the model has indeed been observed to conserve mass reasonably well, when density changes were in the LNG range. However, certain recent applications (Rodean, 1987b) revealed the lack of conservation of species mass and global mass was quite significant and sometimes deleterious, when much larger density changes (e.g., chlorine, hydrogen cyanide, and other chemical compounds) were involved. Thus the second upgrade of the FEM3 model was focused on extending FEM3A to solve also problems possessing large density changes in both space and time. The development entails solving a slightly modified set of governing equations, with only a slight increase in computational cost. Such a model, called FEM3B, was delivered to CRDEC in 1990.

Until 1990, turbulent mixing in FEM3 has been parameterized via a K-theory approach, in conjunction with the similarity functions established for atmospheric boundary-layer flow. Additionally, a number of ad hoc relations were devised to account for the presence of a dense-gas cloud, based largely on the experimental large-scale spills of dense gas performed by LLNL. The major shortcoming of an algebraic K-theory approach is the assumption that turbulence is in local equilibrium, i.e., transport or history of upstream effects on the turbulence are not accounted for except as reflected in the evolution of the mean variables. The assumption of local equilibrium is not valid for nonsteady or complex situations such as the source region or near obstacles. Thus, in order to further extend the range of applicability of FEM3, the FEM3B model has been further upgraded recently to include a more advanced turbulence submodel based on solving the $k-\varepsilon$ transport equations to better model the nonlocal conditions of turbulence. A theoretical and numerical description of the latest model, called FEM3C, is contained in Chan (1994).

The purpose of this manual is to provide non-programming users of FEM3C with the information necessary to use the model effectively. An overview of the model is briefly described in Section 2. User's guides for the preprocessor (PREFEM3C) and the main code (FEM3C) are presented in Sections 3 and 4, respectively. Finally, three example problems are included in section 5 to illustrate the usage of the model.

2. PROGRAM OVERVIEW

In this section, an overview of the FEM3C model is presented. Included are the major assumptions, main features, and program limitations. The overall program organization is also described.

2.1 Assumptions, Features and Limitations

FEM3C is a three-dimensional finite element model that has been developed primarily to simulate the atmospheric dispersion of heavier-than-air gas and liquid releases, using main frame computers such as the CRAYs. The model is based on solving the fully three-dimensional conservation equations of mass, momentum, energy, and species, together with a generalized anelastic approximation (i.e., $\nabla \cdot (\rho \underline{u}) = 0$ is the total mass conservation equation) to preclude sound waves and allow large density variations in both space and time. Thus, the model is restricted to simulations involving a basically incompressible fluid (more precisely, the mixture of air/pollutant). The ideal gas law is assumed to be valid for air and the species in vapor phase. Other assumptions pertaining to the submodels can be found in Chan (1994).

In the numerical aspects, the present model utilizes a modified Galerkin finite element method to spatially discretize the time-dependent conservation equations of mass, momentum, energy, and species, in conjunction with a modified forward Euler method to integrate the resulting ordinary differential equations (ODEs) in time. The particular elements used are quadrilaterals (in two dimensions, 2D) and hexahedrons (in three dimensions, 3D), with piece-wise constant approximation for the pressure unknown and bilinear (2D) or trilinear (3D) approximation for the remaining unknowns. These elements have been selected (over higher-order elements) for their ease of implementation, cost-effectiveness, and sufficient flexibility in treating arbitrary geometries. The numerical aspects of this model can be found in Gresho, *et al.* (1984).

The major features of FEM3C include the following:

(1) It solves both two-dimensional and three-dimensional problems.

(2) It models both isothermal and non-isothermal heavier-than-air gas/liquid releases. The code can be used to simulate the dispersion of a trace (neutrally buoyant) gas as well; however, the present version always solves the complete set of equations (as opposed to solving only the advection-diffusion equation for the trace gas) and thus is not as efficient as it could be for a trace gas.

(3) The model can handle multiple sources of instantaneous, continuous, and finite-duration releases.

(4) It models obstructions as well as variable terrain.

(5) Turbulence is parameterized via the K-theory approach. Two options are available: one using the similarity theory of the atmospheric boundary layer and the other via solving the $k-\varepsilon$ transport equations.

(6) A simple, local thermodynamic equilibrium submodel with temperature-dependent material properties is available to treat dispersion scenarios involving phase-change (between vapor and droplets) of the dispersed material.

(7) Direct and iterative methods are available for efficiently solving the pressure field.

Despite its versatility and a relatively wide range of applicability, FEM3C, like many other numerical models, has its limitations. For instance, many desirable features commonly encountered in the heavy gas/liquid releases such as the treatment of jet release, explosive sources, chemical reactions among the dispersed materials, are not yet available in the present model. Additionally, the following limitations should be recognized by the prospective user in order to avoid misuse:

(1) The K-theory turbulence submodel based on similarity functions is basically a local equilibrium model established in steady atmospheric boundary layers over flat terrain and thus should only be used for problems possessing either flat or gentle terrain. For situations involving complex geometry and obstructions, the $k-\varepsilon$ transport equation approach is indeed more appropriate. However, due to its inherent assumptions, such a submodel is by no means universal for all situations.

(2) The phase-change submodel in the present code is based on local thermodynamic equilibrium. Other physical processes such as rainout, drop-size dependence, and chemical reactions, are not included. Our limited experience with the present submodel suggests that it tends to overestimate the rate of droplet evaporation in the near field and underestimate the heavy-gas effects in the far field (Chan *et al.*, 1987b). Further assessment and improvements are highly desirable for simulating the dispersal of such vapor clouds.

(3) In order to maximize vectorization of the code, structured (or logical) grids (which may have variable grid spacings and irregular domains but must have constant number of mesh points in each direction) are assumed in the numerical algorithm. While such grids are probably very cost-effective for most applications including the treatment of obstructions with not-too-complex geometry, the computational penalties for complex situations may be significant due to less flexibility in element arrangement and more stringent stability limits. In such cases, unstructured grids (which are often used by finite element method) are perhaps more cost-effective.

2.2 Program Organization

FEM3C has been developed to serve as both a useful analysis code and an easily modifiable research tool. Composed of many task-oriented subroutines, the program package can be divided into four parts: a preprocessor (PREFEM3C), a main code (FEM3C), and two interactive postprocessors (PLOTRDM and EZPLOT). The function of PREFEM3C is to generate, from a small number of input lines, the bulk of input data (in the form of disk files) necessary to run the main code. Using the files generated by the preprocessor and an additional file containing run time parameters, FEM3C then performs the time-integration of the resulting discretized conservation equations. During the run, the main code generates various output files, in ASCII and binary forms, for diagnosis and post-processing by the graphics programs. PLOTRDM is a code for plotting velocity projections and contours of the field variables on selected planes, and for displaying the computed variables along any selected grid line. EZPLOT is used for plotting the time histories of field variables at preselected locations.

PREFEM3C and FEM3C are coded in standard FORTRAN and run under UNICOS on the CRAY-2 machines. The postprocessors, however, depend quite heavily on the graphics package available at LLNL and thus are not readily exportable. The contents of POLYPLOT, a binary input file to PLOTRDM, nevertheless, are described in Appendix A for possible adaptation by the user's post-processing code. The codes described herein are dynamically dimensioned and have been designed to solve efficiently problems of up to approximately 30,000 nodal points (requiring approximately 10 million word memory) on a CRAY-2 computer.

3. PREFEM3C USER'S GUIDE

3.1 Introduction

The function of the preprocessor (PREFEM3C) is to generate, from a small number of input lines, the bulk of the input data necessary to run the main code, FEM3C. These data include the physical properties and parameters of the simulation, mesh information, boundary conditions, initial conditions, finite element integrals (matrices), and the decomposed pressure matrix. These data are written into various disk files for use in FEM3C.

PREFEM3C is primarily composed of a number of modules that perform various functions. Each module is activated by a designated command and, if necessary, supplemented by subcommands and input data. The present preprocessor is restricted to logical grids only and the code is dynamically dimensioned. The size of problem that can be treated depends mainly on the available memory and cost considerations. The present codes have been constructed to efficiently solve problems of up to approximately 30,000 mesh points on a CRAY-2 computer, requiring about 10 million words of memory.

The input and output files of PREFEM3C are described next and instructions for preparing the PREPIN file are given in the last subsection.

3.2 Input and Output Files

Input to PREFEM3C is mainly contained in a file called PREPIN, which is sometimes supplemented by a file defining the nodal locations. After PREFEM3C has been executed, ten disk files are generated. Figure 3.1 is a sketch showing all the input/output files and Table 3.1 is a brief description of these files. Of the input files, PREPIN is always required, but COORDS and TERRAIN are optional as noted (and to be discussed in more details in Subsection 3.3). For the output files, PREPOT contains mainly the input parameters and the generated data and is used for verification purposes, FEM3INDF is a file which can be easily edited to become FEM3IN, an input file containing run-time parameters for the main code. The remaining output files provide the bulk of input data necessary to run the main code and will be further discussed in Subsection 4.2.

3.3 Preparation of Input File PREPIN

The first step in a numerical simulation via the finite element method usually involves the design of a mesh appropriate for the problem under consideration. Such a mesh should be sketched (not necessarily to scale or in great detail) to facilitate the preparation of input data. Figure 3.2 shows a three-dimensional structured grid together with the coordinate system (note the orientation of the Cartesian coordinate system and the correspondence between (x, y, z) and (I, J, K)) and node numbering (nodal points are always numbered first along the I-direction, then along the J-direction, and finally along the K-direction). A similar mesh for a two-dimensional problem is shown in Fig. 3.3. In both figures, the I-direction is assumed to be in the direction having the least number of mesh points so as to minimize the storage required by the direct equation solver, FISSLE (Taylor *et al.*, 1981). The depicted orientation of the coordinate system and node numbering are assumed in the code (for efficiency and the convenience of handling both two-and three-dimensional problems in the same code) and should be followed.

The design of an appropriate mesh usually involves the following considerations: characteristics of the problem, extent of the computational domain, computing costs, etc. For cost-effectiveness, the use of graded meshes consisting of fine zones in regions with large gradients of the field variables and coarse zones elsewhere is recommended. Regions requiring fine zones include those near the source, the ground surface, and obstructions. In order to minimize spatial truncation errors, the grid spacings between adjacent elements (or zones) should not vary too rapidly, say within ±20%. Also, since FEM3C is an explicit code, extremely small elements should not be used in order to avoid the stringent time-step size (which can lead to excessive computing costs) otherwise required to satisfy the stability limits (as opposed to accuracy requirement) of the discretized system of equations.

The input data to PREFEM3C are organized in a file called PREPIN, which is composed of various commands and, if required, certain subcommands and data. The following is a summary of the available commands and their functions, listed in the order usually appearing in the file:

PBSETUP — Set up problem identification and relevant parameters.

MATPROB — Select dispersed material from a look-up table of twelve preselected materials.

TDMPROP — Specify temperature-dependent material properties not included in the look-up table.

MESHGEN — Generate mesh point and element connectivities.

BCONGEN — Generate boundary conditions.

MTRXGEN — Generate various finite element matrices.

ICONGEN — Generate initial conditions of the field variables.

THISGEN — Generate arrays associated with time-history data at selected nodal points.

CALLFIS — Generate and decompose the pressure matrix.

ENDFILE — End-of-input deck.

It is permitted and sometimes desirable to include only an appropriate subset of the above commands in a preliminary set-up run. For example, since the finite element matrices and the decomposed pressure matrix are generally the most expensive to generate, one might want to defer generating these matrices until a satisfactory mesh has been obtained. This approach may prove to be useful in dealing with large-scale problems, especially to inexperienced users. Command THISGEN and its associated cards can always be omitted in the input deck if no time-history data of the computed variables are desired.

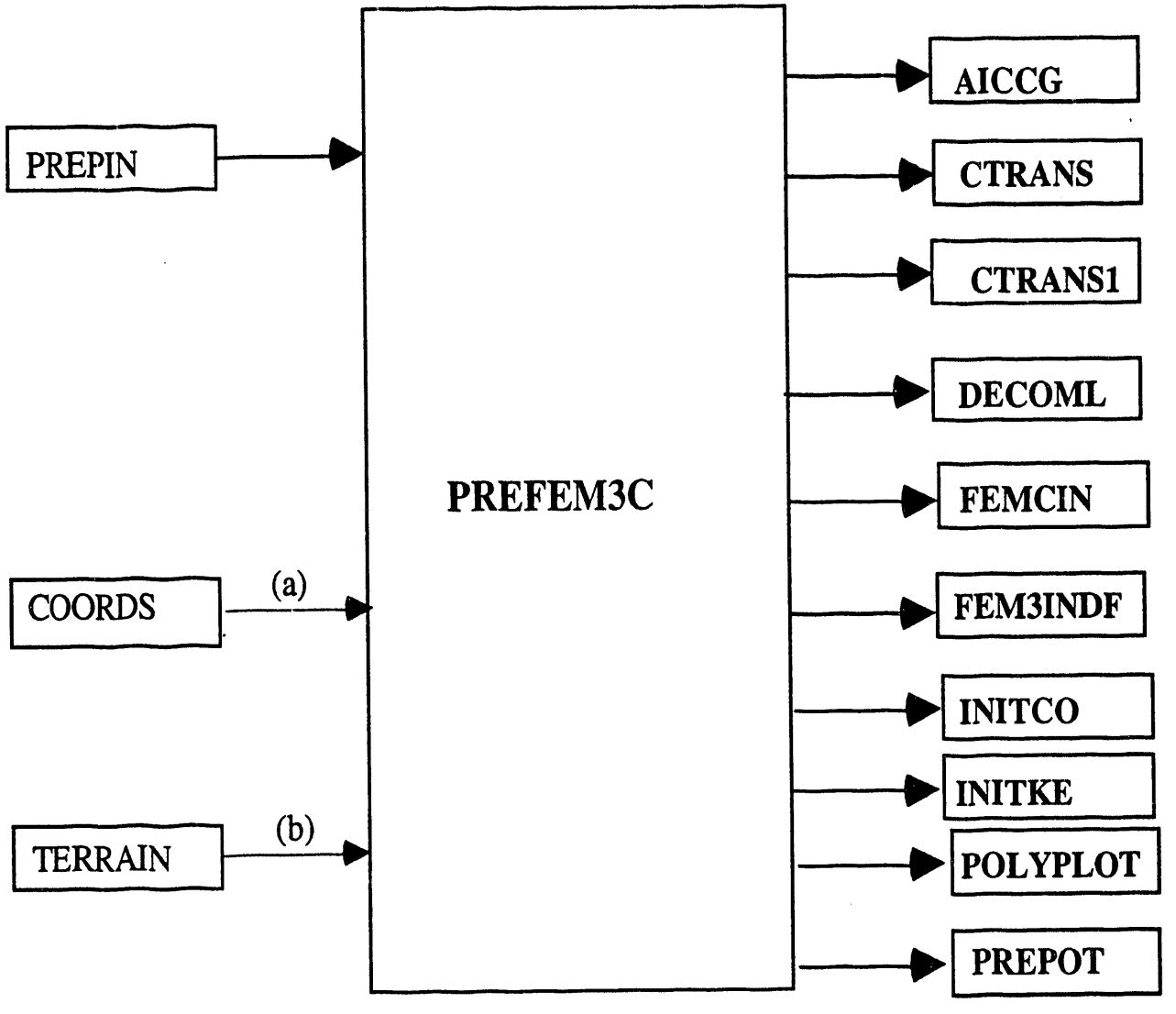

Fig. 3.1. Input and output files associated with PREFEM3C.
(a) File is required if subcommand COORD appears in PREPIN file.
(b) File is required if subcommand TERRA appears in PREPIN file.

Table 3.1. PREFEM3C input and output files.

Unit No.	File name	Description	File type	File access
5	PREPIN	First program input file	ASCII	Sequential
6	PREPOT	Program output file	ASCII	Sequential
7	INITCO	Initial conditions of velocity, temperature, and species concentration	ASCII	Sequential
8	DECOML	Decomposed pressure matrix	Binary	Random
9	CTRANS	Divergence Matrix	Binary	Sequential
9	CTRANS1	Half of the entries of the divergence matrix obtained with one-point quadrature	Binary	Sequential
10	POLYPLOT	Output file containing data for graphics	Binary	Random
10	COORDS	File containing all nodal coordinates (required only with COORD option)	ASCII	Sequential
10	TERRAIN	File containing the coordinates of nodal points on the ground surface (required only with TERRA option)	ASCII	Sequential
11	FEMCIN	Generated input data to FEM3C	Binary	Sequential
12	AICCG	File containing matrices associated with the iterative equation solvers	Binary	Sequential
14	FEM3INDF	Sample FEM3IN file	ASCII	Sequential
19	INITKE	Initial conditions of the k-ε fields	ASCII	Sequential

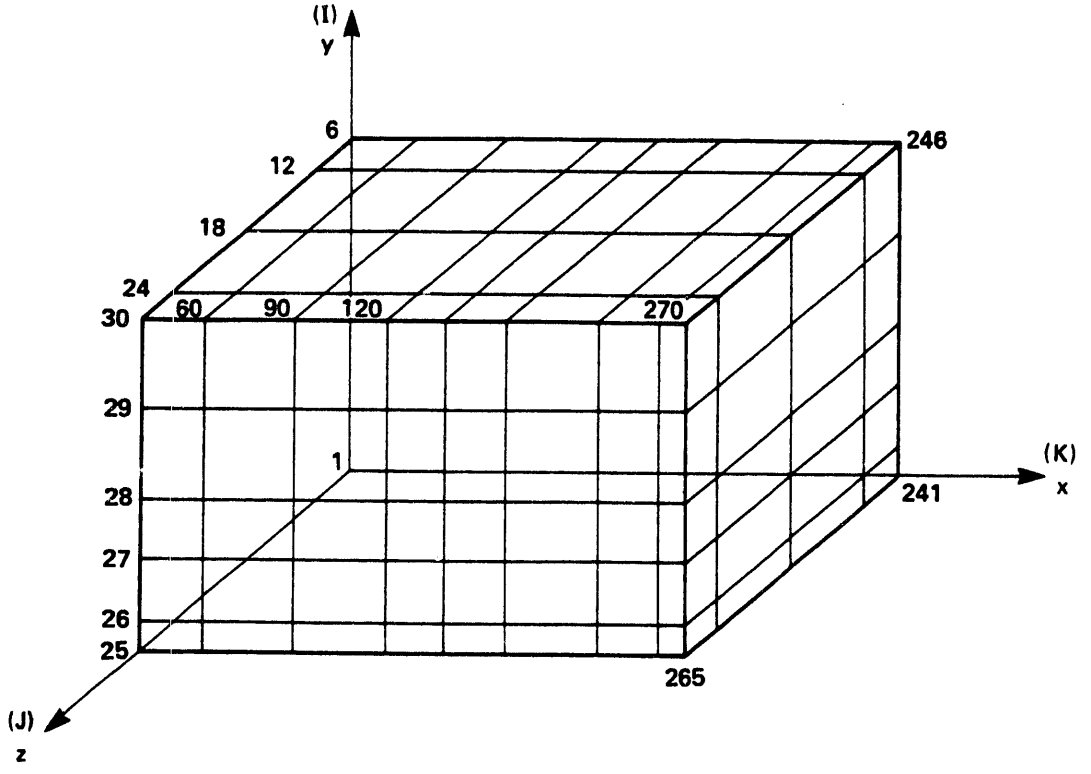

Fig. 3.2. Sketch of a three-dimensional graded mesh and its nodal numbers.

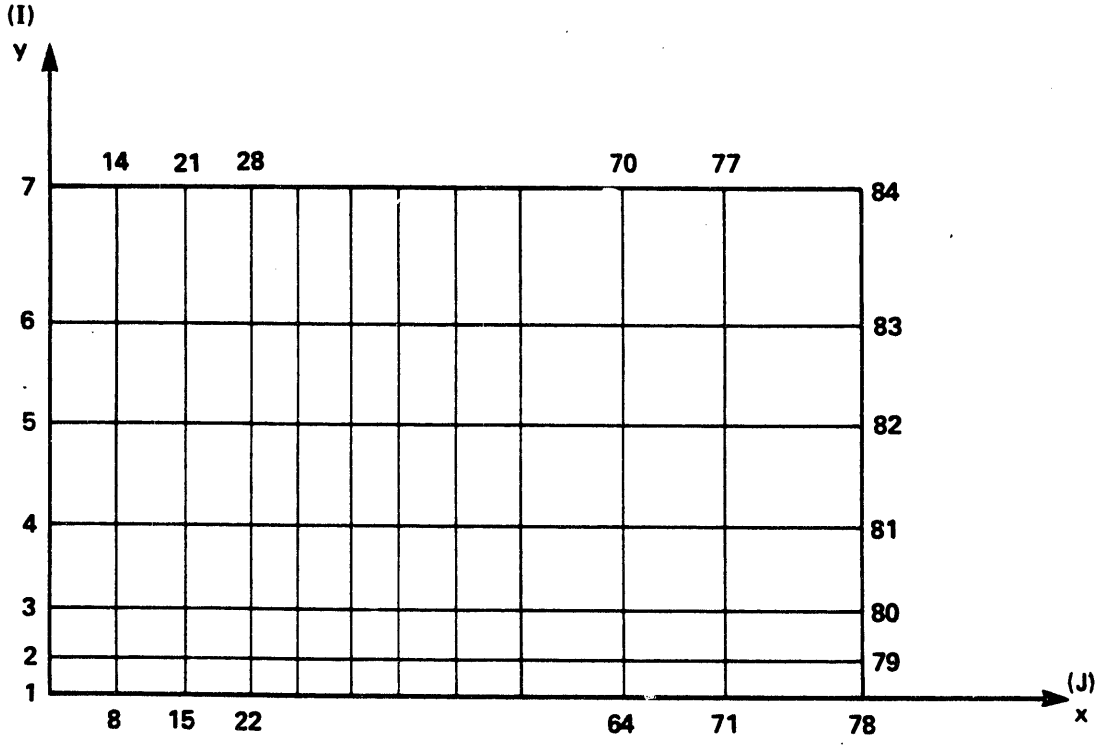

Fig. 3.3. Sketch of a two-dimensional graded mesh and its nodal numbers.

The following describes in detail the formats of the input cards (hereinafter cards and lines will be used interchangeably. In actuality, they are records in an input file) in each of the above groups. The types and formats (A, I, F) of the variables in the code follow usual FORTRAN conventions. All commands are composed of 7 letters (A7) and subcommands are designated by 5 letters (A5), all of which are to be input in lower-case letters exactly as specified. Unless specified otherwise, all integers are of I5 format, while floating-point numbers are of F10.0 format. The description of input given herein is for three-dimensional problems; the input file for a two-dimensional problem is similar except that the items within the brackets ([ ]) must be deleted and the format specifications modified accordingly. For example, the following node number generation card

IMN IMX JMN JMX [KMN KMX] RTO(1) RTO(2) [RTO(3)] NPMAP INDX

implies that the card is

IMN IMX JMN JMX KMN KMX RTO (1) RTO(2) RTO(3) NPMAP INDX

with format (6I5, 3F10.0, 2I5) for a three-dimensional problem, and it is

IMN IMX JMN JMX RTO(1) RTO(2) NPMAP INDX

with format (4I5, 2F10.0, 2I5) for a two-dimensional problem.

In the following, each command, together with any required subcommand(s) and data, is described in more detail.

3.3.1 Problem Heading and Parameter Cards

The function of problem heading and parameter cards is to set up problem identification, parameters, and problem size. There are four cards in this group which must appear in the following order.

Card 1: Problem setup command (A7).

Columns	Variable	Entry
1–7	ICMND	pbsetup

Card 2: Problem identification (10A8).

Columns	Variable	Entry
1–80	HEAD(10)	Problem identification to be used in labeling output.

Card 3: Problem size and parameters (7I5, 5X, F10.0, I5, F10.0).

Columns	Variable	Entry	Note
1–5	NDIM	Number of space dimensions. = 2, two-dimensional problem, = 3, three-dimensional problem.	
6–10	IMAX	Number of elements in the I-direction.	(1)
11–15	JMAX	Number of elements in the J-direction.	(1)
16–20	KMAX	Number of elements in the K-direction. For two-dimensional problems, KMAX is always set equal to 1 in the code.	(1)
21–25	NICS	Number of vectors required to store the initial conditions. = 5, simulations not involving phase-change, = 7, simulations involving phase-change (default).	
26–30	LQR	Quadrature rule to be used in evaluating certain finite element integrals and matrices. = 1, for 2-D rectangular elements and 3-D brick elements, = 2, for mesh with mildly distorted elements (default), = 3, for 3-D mesh involving variable terrain.	(2)
31–35	N1024	Number of blocks (1 block = 1024 decimal words) of working space for FISSLE, a direct solver for linear system of algebraic equations.	(3)
41–50	TLPS	Lapse rate of the temperature field.	(4)
51–55	IBOFLG	Flag indicating the set of governing equations to be solved. = 0, generalized anelastic equations, = 1, Boussinesq equations.	 (5)
56–65	BETA	Coefficient of volumetric expansion.	(6)

Notes:

(1) See Figs. 3.2 and 3.3 for definition of I-, J-, and K-directions. The product of IMAX, JMAX, and KMAX is the total number of elements, NUMEL.

(2) LQR indicates the desired level of approximations to be employed in obtaining the element volume and divergence matrix.

LQR=1 both the element volume and the divergence matrix are evaluated with one-point Gauss rule.

LQR=2 the element volume is evaluated with two-point Gauss rule and the divergence matrix is obtained by multiplying the derivatives of shape functions at element centroid with the corresponding element volume.

LQR=3 both the element volume and divergence matrix are obtained with two-point Gauss rule, which is exact for distorted elements.

Unless hexahedrons (distorted three-dimensional elements) are present, the use of LQR=1 is adequate (see Table 3.2). For a mesh with highly distorted elements, a value of 3 is recommended because both element level and global mass balances are maintained. On the other hand, a value of 2 (which is the default value) is adequate for meshes involving only mildly distorted elements.

(3) N1024 is the (temporary) working space, in blocks of 1024 words, to be allocated to the skyline solver FISSLE (Taylor *et al.*, 1981) for constructing and decomposing the pressure matrix. If no value is given, it is set equal to the maximum working space required by FISSLE (which is the sum of column heights + NUMEL + 3, rounded up to multiples of 1024, plus NUMEL words) and the pressure is solved in-memory in the main code, FEM3C. If computer memory size allows, solving the pressure in-memory is recommended, because the I/*O* costs associated with solving the pressure are then minimal. For problems that cannot fit in-memory, a nonzero value as large as the memory size permits is recommended to minimize the I/*O* costs of updating the pressure solution.

(4) It is the value of γ defined in the following equation

$$T = T_0 - \gamma y \ .$$

Corresponding to the above temperature profile, there exist a hydrostatic pressure field and a motionless state. For reasons of numerical accuracy and convenience of applying outflow boundary conditions, the above base state has been eliminated from the momentum equations in the FEM3C model. However, it is to be noted that the temperature field being calculated in the code is still the departure temperature from a reference value to be specified in card 4.

(5) The Boussinesq formulation is an add-on feature and included herein mainly for the purpose of validating the $k-\varepsilon$ turbulence submodel for isothermal flow test cases. Its non-isothermal counterpart, however, remains to be tested.

(6) This input is required only when the Boussinesq formation is desired and the flow is non-isothermal. Its default value is 0.003.

Table 3.2. Number of Gauss points required in each coordinate direction to evaluate various element matrices exactly.

Elements matrices	Rectangle and parallelogram	General quadrilateral	Brick and parallelepiped	General hexahedron
M^e (Lumped Mass)	1	2	1	2
K^e (Diffusion)	2	>3[a]	2	>3[a]
N^e (Advection)	2	2	2	3
C^e (Divergence)	1	1	1	2
Ω^e (Element Volume)	1	1	1	2

[a]It is not generally possible to evaluate K^e exactly using Gauss quadrature.

Card 4: Physical properties (8F10.0).

Columns	Variable	Entry	Note
1–10	TREF	Reference temperature.	(1)
11–20	TL	Temperature of the dispersed material.	(2)
21–30	RML	Molecular weight of the (gas) species.	(3)
31–40	CPL	Specific heat of the dispersed material.	(3)
41–50	PREF	Ground level pressure of the ambient air.	(4)
51–60	RMA	Molecular weight of the ambient air.	(4)
61–70	CPA	Specific heat of the ambient air.	(4)
71–80	GRAV	Constant of gravitational acceleration.	

Notes:

(1) Reference temperature is the background temperature based on which the departure temperature is calculated in the code. It is to be given in absolute temperature (K) if SI units are used.

(2) TL is the temperature of the (gas) species in an all-vapor simulation; it is the liquid temperature if the simulation involves phase-change.

(3) These variables represent the physical properties of the species in vapor. In the code, default values for NG vapor (consisting of 95% methane, 4% ethane, and 1% propane) are assumed. Their values are RML = 16.88 and CPL = 2180 J/kg-K, respectively.

(4) These are properties of the ambient air and their default values are: PREF=101,325 Newtons/m^2, RMA = 28.96, and CPA= 1005 J/kg-K, respectively.

3.3.2 Material Property Specification Cards

For dispersion simulations involving phase-change, additional material properties (usually temperature-dependent) must also be specified. These include the following (see Appendix B for details about the equations and units):

Antoine equation for saturation vapor pressure,

$$\log P_v = A - B/(T + C) \ . \tag{3.1}$$

Watson relation for heat of vaporization,

$$\lambda_v = \lambda_{vb}\left(\frac{T_c - T}{T_c - T_b}\right)^n \ . \tag{3.2}$$

Specific heat for the vapor material,

$$C_{pv} = a_v + b_v T + c_v T^2 + d_v T^3 \ . \tag{3.3}$$

Specific heat for material in liquid phase,

$$C_{p\ell} = a_\ell + b_\ell T + c_\ell T^2 + d_\ell T^3 \ . \tag{3.4}$$

There are two ways to specify the values of the coefficients in the above equations: either use the appropriate values from a look-up table in the code for twelve preselected materials or use user-supplied values.

In the first case, two cards are required, namely,

Card 1: Material selection command (A7).

Columns	Variable	Entry
1–7	ICMND	matprob

Card 2: Name of selected material (A5).

Columns	Variable	Entry
1–5	ICMND	MNAME

Notes:

MNAME is one of the following five-character (including leading blanks, if any) right-justified symbols for the preselected materials. For clarity, the alphabets in the symbols are capitalized but should be typed *in lower case* for input purposes. The appropriate coefficients are tabulated in Appendix B.

Symbol	Formula	Name
H2S	H_2S	hydrogen sulfide
C3H6	C_3H_6	propylene
C3H8	C_3H_8	propane
CL2	Cl_2	chlorine
NH3	NH_3	ammonia
C2H3C	C_2H_3Cl	vinyl chloride
SO2	SO_2	sulfur dioxide
COCL2	$COCl_2$	phosgene

C2H4O	C_2H_4O	ethylene oxide
HF	HF	hydrogen fluoride
N2O4	N_2O_4	nitrogen tetroxide
HCN	HCN	hydrogen cyanide

If the dispersed material is not one of the above or it is necessary to change any of the coefficients, the following three cards are required:

Card 1: Material property definition (A7).

Columns	Variable	Entry
1–7	ICMND	tdmprop

Card 2: Coefficients for Antoine equation and Watson relation (7F10.0).

Columns	Variable	Entry	Note
1–10	PA	A	(1)
11–20	PB	B	(1)
21–30	PC	C	(1)
31–40	HV1	λ_{vb}	(2)
41–50	T1	T_b	(2)
51–60	TC	T_c	(2)
61–70	EXN	n	(2)

Notes

(1) These are the desired values of the coefficients in Eq. (3.1).

(2) These are the desired values of the coefficients in Eq. (3.2).

Card 3: Coefficients for specific heats (8F10.0).

Columns	Variable	Entry	Note
1–10	AV	a_v	(1)
11–20	BV	b_v	(1)
21–30	CV	c_v	(1)
31–40	DV	d_v	(1)
41–50	AL	a_ℓ	(2)
51–60	BL	b_ℓ	(2)
61–70	CL	c_ℓ	(2)
71–80	DL	d_ℓ	(2)

Notes:

(1) These are the coefficients in Eq. (3.3) for the specific heat of the vapor material.

(2) These are the coefficients in Eq. (3.4) for the specific heat of the material in liquid phase.

3.3.3 Mesh Generation Cards

Mesh information, including nodal locations and their connectivities, are generated with command "meshgen" and its associated input cards. Four options are presently available for defining the nodal locations. For simple geometries, one option may suffice; for more complicated geometries, it may be advantageous to use a combination of the available options. Since logical grids are assumed, element connectivities are generated automatically (no input is required) with both the nodal points and elements numbered first along the I-direction, then along the J-direction, and finally along the K-direction. For instance, the node numbers associated with the first element in Fig. 3.2 are (1, 7, 37, 31, 2, 8, 38, 32) and the node numbers of the first element in Fig. 3.3 would (1, 8, 9, 2). The following describes the necessary cards and available options for generating the nodal points and their coordinates.

First Card: Mesh generation command (A7).

Columns	Variable	Entry
1–7	ICMND	meshgen

Option A—COORD. This subcommand will read all nodal coordinates from a file named COORDS, with format (10X, 3F12.6). The COORDS file contains in each line the node number (which is not read) and its coordinates x, y, z (x, y for a 2-D problem), which are arranged in sequential order according to the global node number. This file is always available from a run in

which option TERRA has been exercised. It can also be easily constructed by extracting the coordinate information in the PREPOT file.

Card a: Option A subcommand (A5).

Columns	Variable	Entry
1–5	ICMND	coord

Notes:

The above is the only card required for using this option. If no other option is being used, a card with subcommand "endms" should follow to terminate the "meshgen" command.

Option B-DIGIX. With this option, nodal locations are generated as the intersecting points of a series of preselected planes perpendicular to the coordinate axes. They are generated in blocks, and as many blocks as needed may be generated under this subcommand. To generate nodal locations within a block, at least four cards (excluding the subcommand card at the beginning and a blank card at the end of the option) are required. A blank card is used to terminate this subcommand. This option is useful in generating graded mesh consisting of brick-type elements within a box-like computational domain.

Card a: Option B subcommand (A5).

Columns	Variable	Entry
1–5	ICMND	digix

Notes:

This card is to be followed immediately by cards *b* through *e* to define the coordinates for the block of nodal points being generated. For an additional block of nodal points, cards similar to *b* through *e* must be repeated and placed before the blank card.

Card b: Node number generation card (6I5).

Columns	Variable	Entry
1– 5	IX1	Beginning index in the x-direction.
6–10	IX2	Ending index in the x-direction.
11–15	IY1	Beginning index in the y-direction.
16–20	IY2	Ending index in the y-direction.
21–25	[IZ1]	Beginning index in the z-direction.
26–30	[IZ2]	Ending index in the z-direction.

Notes:

This card defines a block of nodal points for which the nodal numbers and their coordinates will be generated.

Card(2) c: x-coordinates definition card(s) (8F10.0).
The location of planes perpendicular to the x-axis are defined by this group of card(s). There are (IX2-IX1 + 1) entries with 8 entries in each line.

Card(s) d: y-coordinates definition card(s) (8F10.0).
These cards are similar to those described above, except the planes are perpendicular to the y-axis and the number of entries is (IY2-IY1 + 1).

Card(s) e: z-coordinates definition card(s) (8F10.0)

These (IZ2 - IZ1 + 1) entries of z-coordinates for planes perpendicular to the z-axis are required only for three-dimensional problems.

Card f: Blank card to terminate Option B.

Option C-MAPPX. Option C employs the concept of isoparametric mapping to generate the nodal coordinates. First, nodal locations in the transformed co-ordinate system $(\xi-\eta-\zeta)$ are generated, either uniformly or continuously graded, in a way similar to what is done with the DIGIX option. These coordinates are then transformed to the physical space by isoparametric mapping, currently done by means of the trilinear mapping functions (in two dimensions, three mapping options are available). Again, mesh points can be generated in blocks and four (three in two dimensions) cards are required for defining a block of mesh points. Finally, a blank card is used to terminate this subcommand. Figures 3.4 and 3.5 display respectively the relationship between the physical space and the transformed space for 2-D and 3-D problems. This option supplements the previous one and is useful in generating mesh points involving sloping terrain and/or irregular regions of a computational domain. The usage of this option is illustrated by the second example problem in Section 5.

Card a: Option C subcommand (A5).

Columns	Variable	Entry
1 – 5	ICMND	mappx

Card b: Mapped region and parameters (6I5, 3F10.0, 2I5).

Columns	Variable	Entry	
1–5	IMN	Beginning index in the I-direction.	(1)
6–10	IMX	Ending index in the I-direction.	(1)
11–15	JMN	Beginning index in the J-direction.	(1)
16–20	JMX	Ending index in the J-direction.	(1)
21–25	[KMN]	Beginning index in the K-direction.	(1)
26–30	[KMX]	Ending index in the K-direction.	(1)

31–40	RI	Grading factor in the I-direction.	(2)
41–50	RJ	Grading factor in the J-direction.	(2)
51–60	[RK]	Grading factor in the K-direction.	(2)
61–65	NPMAP	Desired mapping function. = 4, 2-D bilinear function (Default), 8, 2-D quadratic Serendipity function, 12, 2-D cubic Serendipity function. = 8, 3-D trilinear function (Default).	(3)
66–70	INDX	Grading control parameter. = 0, grading to be controlled by the grading factors in columns 31 through 60, ≠ 0, control locations in the $(\xi-\eta-\zeta)$ system to be specified in cards $f-h$.	(4)

Notes:

(1) These indices define a group of nodes for which the nodal numbers and their locations are to be generated.

(2) These are the grading factors in the transformed space and their values can be less than or greater than 1. However, in order to minimize spatial truncation errors, values close to unity, preferably in the range of 0.9 and 1.1, are recommended. The default values are 1.0. The method of geometric grading is employed, i.e.,

$$\Delta X_2 = r\Delta X_1$$

$$\Delta X_3 = r\Delta X_2 = r^2\Delta X_1$$

$$\vdots$$

$$\Delta X_n = r^{n-1}\Delta X_1$$

where ΔX_1 is the size of the first element, r is the grading factor, and n is the number of elements in the direction being considered.

Thus for a length of L divided into n elements, one has

$$L = \Delta X_1 + \Delta X_2 + \ \ldots \ + \Delta X_n = \frac{(1-r^n)}{(1-r)}\Delta X_1.$$

(3) The mapping options, together with the corresponding control nodes, are displayed in Figs. 3.4 and 3.5. See, for example, Zienkiewicz (1971) for the definition of the mapping functions.

(4) This flexibility is provided for cases where the grading cannot be done conveniently with the above scheme. In this case, cards f through h are required to define the desired plane locations in the transformed space.

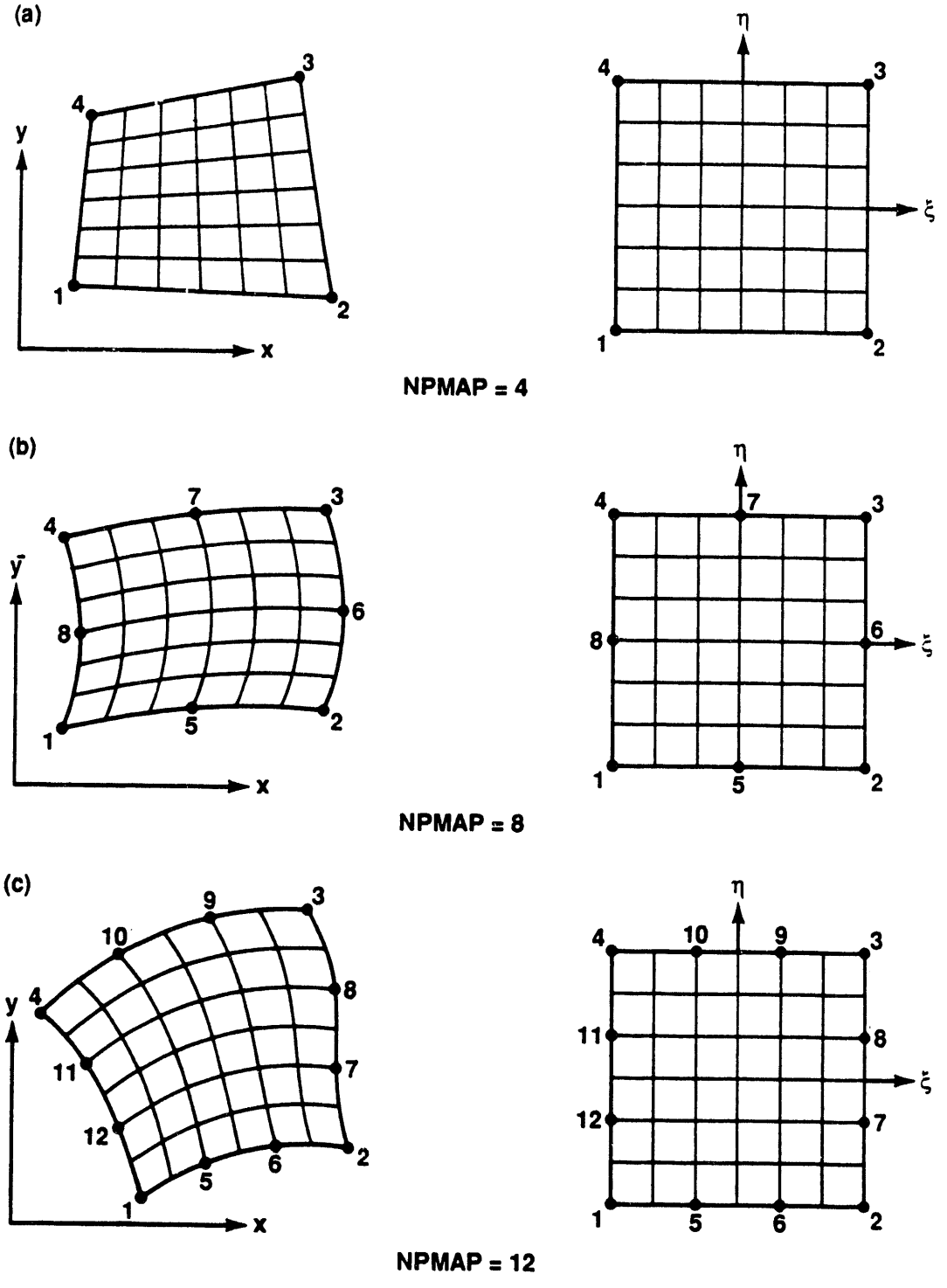

Fig. 3.4. Two-dimensional "mapping" using the Serendipity function: (a) linear, (b) quadratic, and (c) cubic. In each case, a grid consisting of 7×7 grid points has been generated. For definition of the Serendipity functions, see, for example, Zienkiewicz (1971).

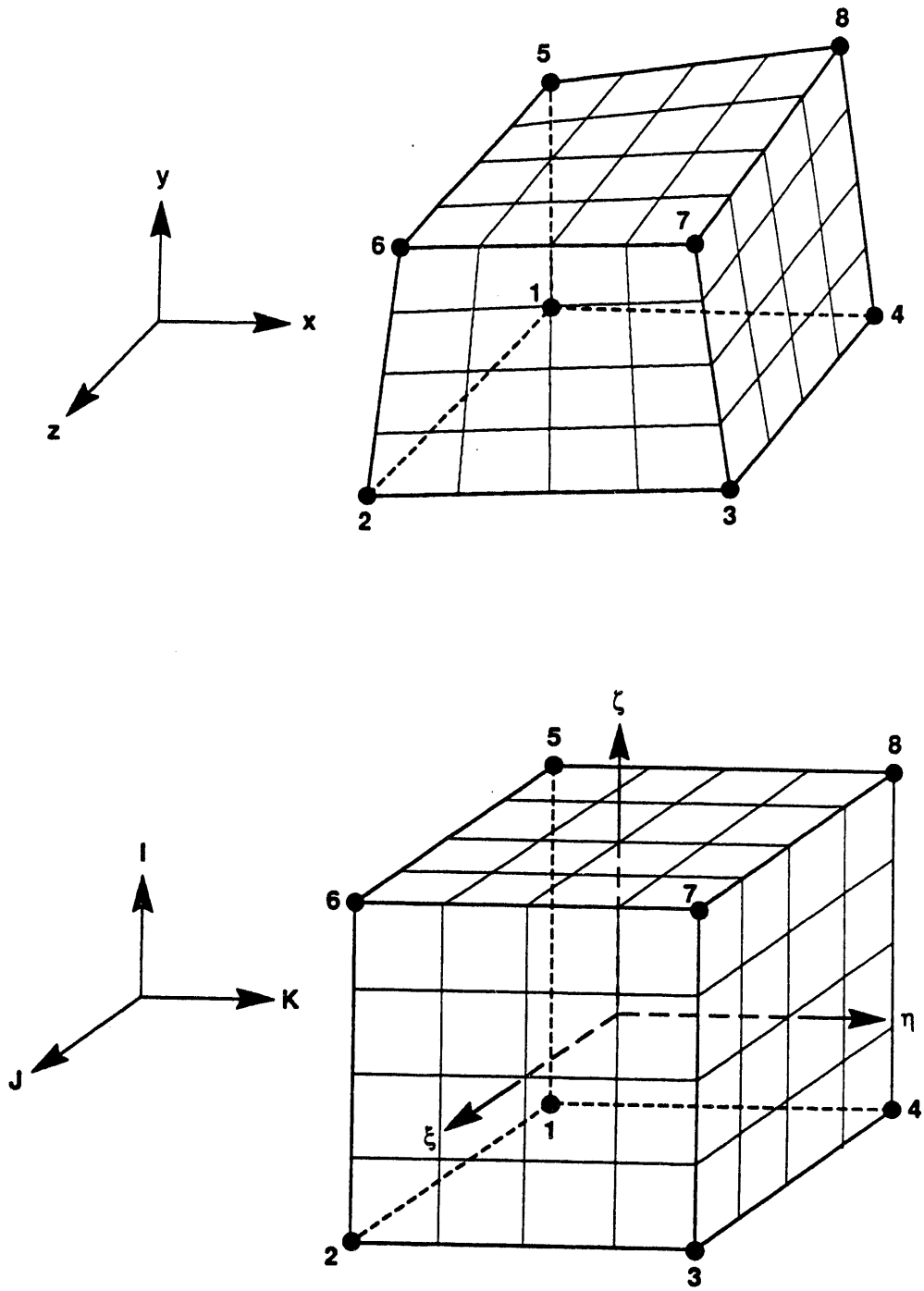

Fig. 3.5. Three-dimensional "mapping" using trilinear functions. In the figure, a grid consisting of $5 \times 5 \times 5$ grid points has been generated.

Card c: x-coordinates definition card (8F10.0).

Columns	Variable	Entry
1–10	CX (1,1)	x-coordinate of corner node No. 1.
11–20	CX (1,2)	x-coordinate of corner node No. 2.
21–30	CX (1,3)	x-coordinate of corner node No. 3.
31–40	CX (1,4)	x-coordinate of corner node No. 4.
41–50	[CX (1,5)]	x-coordinate of corner node No. 5.
51–60	[CX (1,6)]	x-coordinate of corner node No. 6.
61-70	[CX (1,7)]	x-coordinate of corner node No. 7.
71–80	[CX (1,8)]	x-coordinate of corner node No. 8.

Notes:

The relative positions of the corner nodes are shown in Fig. 3.4 and 3.5. The above entries are the x-coordinates of the eight corner nodes of a brick or a general hexahedron. If bilinear mapping is employed for two-dimensional problems, only the first four entries are required. If NPMAP=12, two cards are required for the twelve entries.

Card d: y-coordinates definition card (8F10.0).

Columns	Variable	Entry
1–10	CX (2,1)	y-coordinate of corner node No. 1.
11–20	CX (2,2)	y-coordinate of corner node No. 2.
21–30	CX (2,3)	y-coordinate of corner node No. 3.
31–40	CX (2,4)	y-coordinate of corner node No. 4.
41–50	[CX (2,5)]	y-coordinate of corner node No. 5.
51–60	[CX (2,6)]	y-coordinate of corner node No. 6.
61-70	[CX (2,7)]	y-coordinate of corner node No. 7.
71–80	[CX (2,8)]	y-coordinate of corner node No. 8.

Card e: z-coordinates definition card (8F10.0).

Columns	Variable	Entry
1–10	CX (3,1)	z-coordinate of corner node No. 1.
11–20	CX (3,2)	z-coordinate of corner node No. 2.
21–30	CX (3,3)	z-coordinate of corner node No. 3.
31–40	CX (3,4)	z-coordinate of corner node No. 4.
41–50	[CX (3,5)]	z-coordinate of corner node No. 5.
51–60	[CX (3,6)]	z-coordinate of corner node No. 6.
61-70	[CX (3,7)]	z-coordinate of corner node No. 7.
71–80	[CX (3,8)]	z-coordinate of corner node No. 8.

Notes:

These are the z-coordinates of the eight corner nodes. This card is required only for three-dimensional problems.

If INDX $\neq 0$, the following additional cards are required to specify the desired nodal locations in the local coordinates (ξ, η, ζ), similarly to the DIGIX option.

Card(s) f: ξ location definition card(s) (8F10.0).
These are the desired local coordinates in the ζ-direction.
There should be (JMX – JMN + 1) entries, ranging from -1.0 to 1.0.

Card(s) g: η location definition card(s) (8F10.0).
These are the desired local coordinates in the η-direction.
There should be (KMX – KMN + 1) entries, ranging from -1.0 to 1.0, for 3-D problems. In the case of a 2-D problem, the number of entries is (IMX – IMN + 1).

Card(s) h: ζ location definition card(s) (8F10.0)
These are the desired local coordinates in the ζ-direction, ranging from -1.0 to 1.0, and are required for 3-D problems only. The total number of entries is (IMX – IMN + 1).

Card i: Blank card to terminate option C.

Option D—TERRA. This option is provided to generate mesh involving arbitrary terrain. A file called TERRAIN and two input cards are required to use this option. File TERRAIN contains the (x, y, z) coordinates of all nodal points on the ground surface (I = 1), which is discretized a priori and the (x, y, z) coordinates are stored in the format (34x, 3E13.6), one line per nodal point, and arranged first along the J-direction and then along the K-direction. Executing this option will generate the vertical coordinates via an iteractive process (the horizontal coordinates are kept unchanged) for the remaining nodes above the ground surface. A COORDS file containing all nodal locations is also generated for future use (see Option A).

Card a: Option D subcommand (A5).

Columns	Variable	Entry
1– 5	ICMND	terra

Card b: Vertical coordinates generation card (I5, 7F10.0).

Columns	Variable	Entry	Note
1– 5	NY	Number of nodes in the vertical direction.	(1)
6–15	YMAX	Vertical coordinate of the top surface.	(2)
16–25	FST	Height of the first layer of elements.	(3)
26–35	XSCALE	Scaling factor for x-coordinates.	(4)
36–45	YSCALE	Scaling factor for y-coordinates.	(4)
46–55	[ZSCALE]	Scaling factor for z-coordinates.	(4)
56–65	TOL	Convergence tolerance in the iteractive process used to determine the vertical coordinates.	(5)
66–75	YTOP	The final coordinate of the top surface.	(6)

Notes:

(1) Since the I-direction is currently assumed to be aligned with y-coordinate, NY = IMAX + 1.

(2) YMAX defines the preliminary location of the top surface used in generating the missing vertical coordinates. The final location of the top surface, however, may differ [see note (6)].

(3) This parameter specifies the distance between nodes on the ground surface and those immediately above them, thereby ensuring that model predictions and available measurements at the same height (say, 1 m), can be compared directly without the need for vertical interpolation.

(4) These are scaling factors applied to the data read from disk file TERRAIN. The default values are 1.0.

(5) The default value for TOL is 0.001 * YMAX.

(6) If YTOP > YMAX, the top surface will be moved to YTOP (other surfaces remain unaltered) after all vertical coordinates have been generated; otherwise, it remains at the height of YMAX. This is sometimes done so as to minimize the possible adverse effects of the approximate boundary conditions employed on the top surface, while retaining a fine mesh resolution near the ground.

Last card: Mesh generation termination subcommand (A5).

Columns	Variable	Entry
1 – 5	ICMND	endms

Notes:

The above card is always required to terminate the function of the "meshgen" command.

3.3.4 Boundary Conditions Data Cards

The boundary conditions treated in the present model can be generally categorized as forced (also called essential) and natural. The former is associated with specifying the unknown variables including velocity components, temperature, mass fraction of species, turbulence kinetic energy, the dissipation rate of turbulence kinetic energy, and pressure; the latter is associated with specifying normal/tangential stresses, heat flux, and the mass flux of species. In general, there is no need to specify pressures; however, when obstructions are present, the elements representing the obstructions should be specified with zero pressure.

Currently, only time independent boundary conditions (except those for finite-duration releases) are allowed. Some typical boundary conditions used in a heavy gas dispersion simulation are illustrated in Fig. 3.6. If the $k-\varepsilon$ turbulence submodel is employed, it is also necessary to specify the profiles of k and ε on the inlet plane. And on the ground surface, wall functions associated with the logarithmic layer will be used in calculating the relevant quantities of turbulence fluxes. Specification of these boundary conditions begins with the command "bcongen", which is then followed by a combination of appropriate subcommands and data statements. Described below are the required input cards and available options.

First card: Boundary condition command card (A7).

Columns	Variable	Entry
1 – 7	ICMND	bcongen

Notes:

This command calls the BCONGEN module to generate the forced and natural boundary conditions for the field variables, including velocity components (u, v, w), pressure (p), temperature (θ), species concentrations (q_v and q_ℓ), and turbulence variables (k and ε). This card is to be followed by the appropriate subcommands and data statements and finally terminated by subcommand "endbc".

<u>*Forced Boundary Conditions.*</u>

Most of the forced boundary conditions for the variables mentioned above can be specified by using subcommand "plane" for specifying nodal variables on an entire plane (Option A) and/or "subdm" for specifying nodal variables within a 3-D region or a 2-D area on a plane (Option B). Alternatively, these boundary conditions can be specified separately for each field variable using the subcommands starting with "fbc" (Option C). Either a single option or a combination of them can be used to specify the necessary forced boundary conditions.

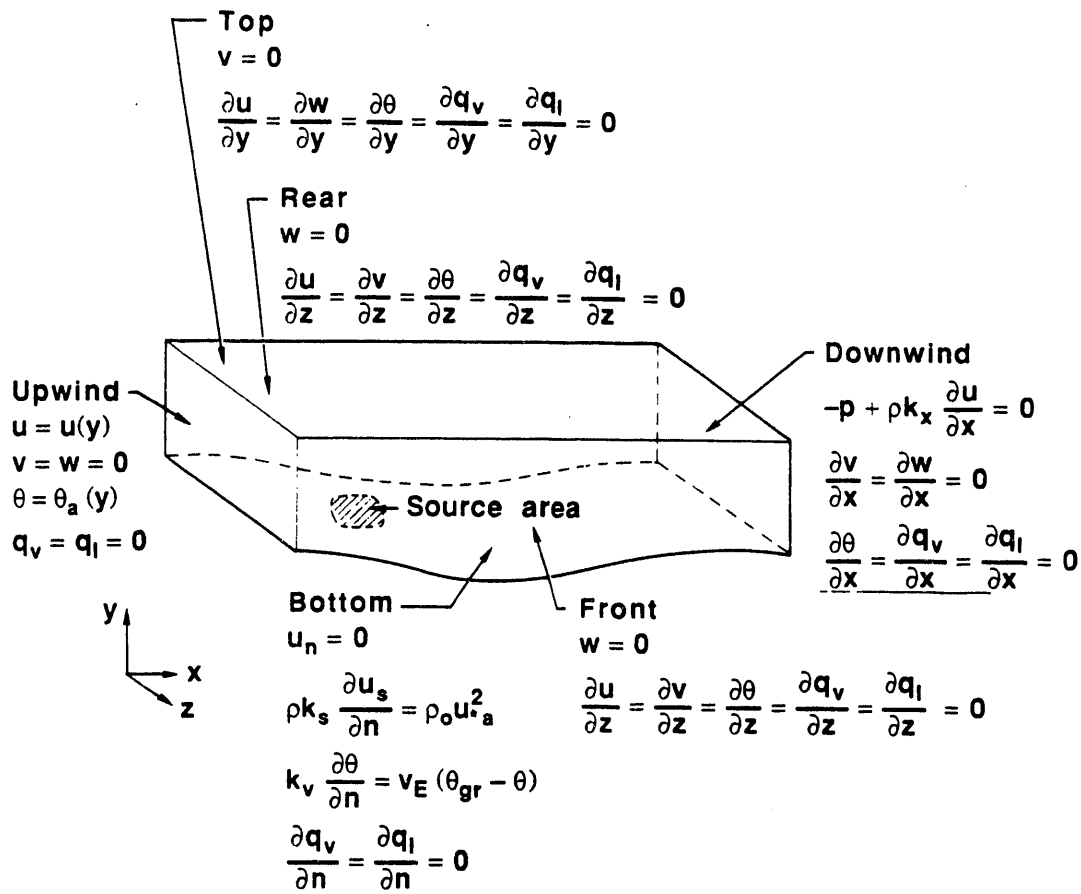

Fig. 3.6 Typical boundary conditions for the governing equations solved by the FEM3C model.

A new feature implemented in PREFEM3C is that the desired numerical values of essential boundary conditions can be obtained from the relevant fields in the initial condition files (which will be explained later) to save repetitive input otherwise required. In addition to the functions described under initial conditions data cards, two analytic functions have been implemented in the code for specifying any of the field variables, namely,

$$F(y) = C_1 + C_2 y + C_3 y^2 \ , \tag{3.5}$$

$$F(y) = C_1 \left[\ell n(y / C_2 + 1) - C_3 \right] . \tag{3.6}$$

In the above formulae, y is either the vertical coordinate (absolute height) or the height measured from the ground surface, which is to be controlled by an input parameter. The logarithmic function in Eq. (3.6) has been modified slightly with the addition of 1 to keep its argument remain positive.

Option A—plane.

This option allows a user to specify the forced boundary conditions for the selected field variables on a specified plane (or any edge of a 2-D mesh). It requires at least three cards as described below.

Card a: Plane selection subcommand (A5, A2, I3).

Columns	Variable	Entry
1– 5	ICMND	plane
6– 7	ID	The character of i, j, or k to indicate the normal direction of the plane.
8–10	IPLANE	I, J, or K value of the selected plane.

Notes:

This card defines the plane over which the forced boundary conditions described by the subsequent data statements (as many as required) will be specified. A blank card is necessary to terminate this subcommand.

Card(s) b: Variable Identification and parameters (A5, 5F10.0, I5).

Columns	Variable	Entry	Note
1–5	MNEX	Variable identifier.	(1)
6–15	C1	First coefficient.	(2)
16–25	C2	Second coefficient.	(2)
26–35	C3	Third coefficient.	(2)

36–45	YM	Height above which the function attains its maximum value.	(3)
46–55	FM	Maximum value of the specified field variable.	(3)
56–60	NDOP	Integer number indicating how the value of y is defined. >0, vertical coordinate, <0, distance measured from the ground surface.	

Notes:

(1) The variable identifier can be any of the following:

- ℓnu to specify a logarithmic u-velocity profile defined by Eq. (3.6),
- u to specify u-velocity component,
- v to specify v-velocity component,
- w to specify w-velocity component,
- t to specify deviation temperature,
- c to specify gas species concentration (in an all-vapor simulation),
- q_v to specify vapor mass fraction,
- q_ℓ to specify liquid mass fraction,
- k to specify turbulence kinetic energy,
- e to specify the dissipation rate of turbulence kinetic energy,
- p to specify pressure (usually zero) within elements,
- +p to specify p (usually zero) within elements right above the selected plane,
- -p to specify p (usually zero) within elements beneath the selected plane.

(2) If the value of C1 is 1.e20, the nodal value(s) of the relevant field variables in the initial condition arrays will be taken as the desired specified values(s). Otherwise, C1, together with C2 and C3, are the coefficients in Eq. (3.5). However, if the variable identifier is "ℓnu", they represent then the coefficients in Eq. (3.6).

(3) The default value YM is 10^{10}. A cutoff value of FM is imposed if $y \geq$ YM.

Card c: Blank card to terminate subcommand "plane."

Option B—subdm.

This option offers basically the same capabilities as those described in Option A, except that the region over which the forced boundary conditions are specified can be a block of nodes or an area on a plane (as opposed to an entire plane). To accommodate such flexibility, an additional card is required to specify the selected region. The remaining data statements are the same as those described in option A.

Card a: subdomain selection subcommand (A5).

Columns	Variable	Entry
1–5	ICMND	subdm

Card al: Subdomain specification (6I5).

Columns	Variable	Entry
1– 5	IMN	Beginning I-index.
6–10	IMX	Ending I-index.
11–15	JMN	Beginning J-index.
16–20	JMX	Ending J-index.
21–25	[KMN]	Beginning K-index.
26–30	[KMX]	Ending K-index.

Card(s) b: Variable identification and parameters (A5, 5F10.0, I5).

Same as card(s) b described in option A.

Card c: Blank card to terminate subcommand "subdm."

Notes:

To define additional subdomain(s) without terminating subcommand "subdm", a card with entry "next" can be used in place of card *a*, and then followed by cards *al* and *b* to define the desired subdomain and the specified boundary conditions, as illustrated in the section of numerical examples. In doing so, only one blank card is necessary, because "subdm" only appears once.

Option C—specification for individual variables.

Instead of specifying the forced boundary conditions from one segment of boundary to another (with the relevant variables collected under each segment of boundary), the present option uses one subcommand for each variable to collectively specify the forced boundary condition for the variable over all boundary segments. In addition to the logarithmic function of Eq. (3.6), this option allows any variable to be specified as up to a complete quadratic polynomial function as in Eq. (3.7). The following cards are required in order to use this option.

$$F(y) = C_1 + C_2\,x + C_3\,y + C_4\,z + C_5\,x^2 + C_6\,xy + C_7\,y^2 + C_8\,yz + C_9\,z^2 + C_{10}\,xz \tag{3.7}$$

Card a: Field subcommand and cut-off parameters (A5, 5X, 2F10.0).

Columns	Variable	Entry	Note
1– 5	ICMND	Forced boundary condition (FBC) identifier.	(1)
11–20	YM	Height above which the specified function attains its maximum value.	(2)
21–30	FM	Maximum value of the specified variable.	(2)

Notes:

(1) The FBC identifier can be any one of the following:

fbcfu	to specify u-velocity component,
fbcfv	to specify v-velocity component,
fbcfw	to specify w-velocity component,
fbcft	to specify deviation temperature,
fbcfc	to specify gas species concentration (in an all-vapor simulation),
fbcqv	to specify vapor mass fraction,
fbcqℓ	to specify liquid mass fraction,
fbcfk	to specify turbulence kinetic energy, and
fbcfe	to specify the dissipation rate of turbulence kinetic energy.

(2) The default value of YM is 10^{10}. A cutoff value of FM is imposed if $y \geq$ YM. It applies to all segments of boundary under this subcommand.

Card(s) b: Node numbers and function parameters (6I5, 4F10.0, I5).

Columns	Variable	Entry	Note
1– 5	IMN	Beginning I-index.	(1)
6–10	IMX	Ending I-index.	(1)
11–15	JMN	Beginning J-index.	(1)
16–20	JMX	Ending J-index.	(1)

21–25	[KMN]	Beginning K-index.	(1)
26–30	[KMX]	Ending K-index.	(1)
31–40	C1	First coefficient	(2)
41–50	C2	Second coefficient.	(2)
51–60	C3	Third coefficient.	(2)
61–70	[C4]	Fourth coefficient.	(2)
71–75	NDOP	Analytic function identifier = 0, constant, = 1 or -1, linear function, = 2 or -2, quadratic function, = 3 or -3, logarithmic function.	(3)

Notes:

(1) These indices define an enclosed region over which forced boundary conditions will be specified.

(2) If NDOP = -3 or 3, Eq. (3.6) is used and only the first three coefficients are required to define the logarithmic function. Otherwise, all four values are required to define the constant and linear terms in Eq. (3.7).

(3) A negative value of NDOP implies that the height (y) is measured from the ground surface, instead of being vertical coordinate.

Card(s) b1: Coefficients of quadratic terms (6F10.0).

Columns	Variable	Entry
1–10	C5	Fifth coefficient.
11–20	C6	Sixth coefficient.
21–30	C7	Seventh coefficient.
31–40	[C8]	Eighth coefficient.
41–50	[C9]	Ninth coefficient.
51–60	[C10]	Tenth coefficient.

Notes:

This card is required only when NDOP = 2 or -2. These coefficients define the quadratic terms in Eq. (3.7).

Card c: Blank card to terminate the current subcommand.

Notes:

Prior to the blank card, as many cards *b* as required can be used to generate the same type of forced boundary condition for various segments of the boundary.

Natural Boundary Conditions.

In the present code, natural boundary conditions for all variables can be generated as functions up to a complete linear polynomial of the coordinates, i.e.,

$$F = C_1 + C_2 x + C_3 y + C_4 z \tag{3.8}$$

in which F represents the specified stresses for momentum equations, heat flux for temperature, or mass flux for species. Note that only *nonzero* natural boundary conditions need to be specified because zero stresses or flux contribute nothing to their relevant boundary integrals. The required input cards are similar to those of Option C described above.

Card a: Field subcommand (A5).

Columns	Variable	Entry
1–5	ICMND	Natural boundary condition (NBC) identifier.

Notes:

The NBC identifier can be any one of the following:

nbcfu	to specify stress in the u-velocity direction,
nbcfv	to specify stress in the v-velocity direction,
nbcfw	to specify stress in the w-velocity direction,
nbcft	to specify heat flux,
nbcfc	to specify mass flux (all-vapor),
nbcqv	to specify mass flux in vapor phase,
nbcqℓ	to specify mass flux in liquid phase.

After each subcommand, one card is required for each group of nodes for which *nonzero* natural boundary conditions are to be applied. Again, a blank card is used to terminate each individual subcommand.

Card(s) b: Node numbers and function parameters (6I5, 4F10.0).

Columns	Variable	Entry	Note
1– 5	IMN	Beginning I-index.	(1)
6–10	IMX	Ending I-index.	(1)
11-15	JMN	Beginning J-index.	(1)
16–20	JMX	Ending J-index.	(1)
21–25	[KMN]	Beginning K-index.	(1)
26–30	[KMX]	Ending K-index.	(1)
31–40	C1	First coefficient.	(2)
41-50	C2	Second coefficient.	(2)
51–60	C3	Third coefficient.	(2)
61-70	[C4]	Fourth coefficient.	(2)

Notes:

(1) These indices define a region (an area for 3-D problems and a line segment for 2-D problems) over which the integrals related to natural boundary conditions will be evaluated.

(2) These are the coefficients in Eq. (3.8). In most cases, only the first coefficient is needed to specify a constant stress or flux. The proper signs of the specified stresses are shown in Fig. 3.7. Stresses for the hidden surfaces are normally in directions opposite to those shown on the respective opposite surface, and the sign is negative. For heat or mass flux, it is considered to be positive if the flux is coming into the computational domain; otherwise, the flux is considered to be negative. For mass flux or heat flux, the required input to the code is the initial injection velocity, i.e., $v_I = \dot{m}/\rho_o$, as illustrated in the example problems of Section 5.

Card c: Blank card to terminate the current subcommand.

Notes:

Prior to the blank card, as many cards b as required can be used to generate the same type of natural boundary condition for various segments of the boundary.

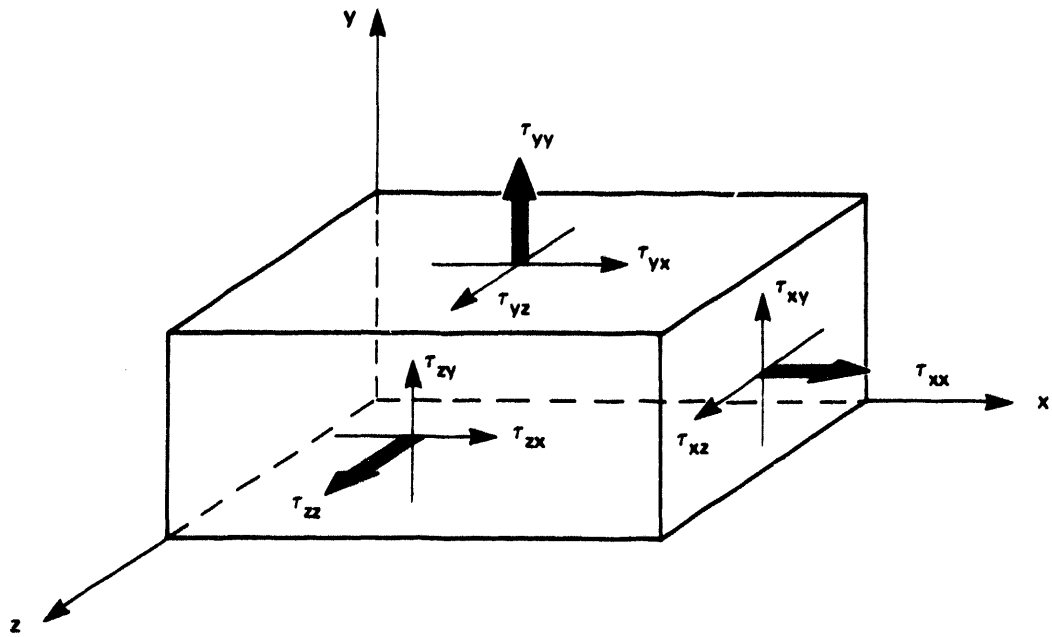

Fig. 3.7 Sketch showing specified stresses with positive sign.

Normal/Tangential Velocity Components and Shear Stresses.

In order to be able to specify zero normal velocity for cases involving variable terrain and, at the same time, apply a partial slip boundary condition (i.e., specify shear stresses) along the tangential directions (this is called mixed-type boundary conditions), the Cartesian velocity components on such a boundary must be transformed into components in the normal and tangential directions. To do so, those nodes on the "ground surface" must be identified, using the cards described below. When mixed-type boundary conditions are specified, the normal velocity is to be treated as though it were u and the tangential velocity component parallel to the x-y plane is to be treated as though it were v. For simulations involving flat terrain only, such a transformation is not required, because the mixed-type boundary conditions can be directly applied to the momentum equations written in the Cartesian coordinate system.

Card a: Ground surface nodes generation subcommand (A5).

Columns	Variable	Entry
1–5	ICMND	dicos

Notes:

This subcommand, together with the succeeding input card, causes the preprocessor to generate the local normal and tangential directions for all nodes on the ground surface. The divergence matrix is also transformed accordingly.

Card b: Surface nodes generation card (7I5, 3F10.0).

Columns	Variable	Entry	Note
1– 5	IMN	Beginning I-index.	(1)
6–10	IMX	Ending I-index.	(1)
11–15	JMN	Beginning J-index.	(1)
16–20	JMX	Ending J-index.	(1)
21-25	[KMN]	Beginning K-index.	(1)
26–30	[KMX]	Ending K-index.	(1)
31–35	ISF	Flag for selecting values of direction cosines = 0, use values computed in the code, ≠ 0, use user-supplied values of direction cosines in the last three fields.	(2)
36–45	XN	Specified value of direction cosine between the normal vector and x-axis.	(2)
46–55	YN	Specified value of direction cosine between the normal vector and y-axis.	(2)
56–65	[ZN]	Specified value of direction cosine between the normal vector and z-axis.	(2)

Notes:

(1) These indices should correspond to the nodes on the ground surface with IMN = IMX = 1, which could have been generated automatically by the preprocessor. However, the present form provides the flexibility for selecting other parts of the boundary as well.

(2) In certain cases, e.g., the edges and corners of a domain, it may be desirable to specify the direction cosines, instead of using those based on consistent-normal calculations, for the momentum equations. This group of input parameters provide such flexibility to override the values computed in the code.

Card c: Blank card to terminate the "dicos" subcommand.

Wall-Function Related Boundary Conditions

As discussed in Chan (1994), because the standard $k-\varepsilon$ turbulence model is not valid in the immediate vicinity of the wall (the viscous buffer-layer), the computational domain is terminated in the fully turbulent region at some distance Δ from the wall. Use is then made of the so-called logarithmic wall-laws to bridge the gap between the wall and the fully turbulent flow condition at Δ. Specifically, on such a boundary, the normal gradient of the turbulence kinetic energy is assumed to be zero, and the turbulent heat and momentum fluxes, together with the dissipation rate of turbulence kinetic energy, are updated each time step using the logarithmic wall-laws. The input

cards necessary to impose such boundary conditions are similar to those used for specifying natural boundary conditions.

Card a: Wall-function subcommand (A5).

Columns	Variable	Entry
1– 5	ICMND	slpbc

Cards(s) b: Node numbers and function parameters (6I5, 4F10.0).

Columns	Variable	Entry	Note
1– 5	IMN	Beginning I-index.	(1)
6–10	IMX	Ending I-index.	(1)
11–15	JMN	Beginning J-index.	(1)
16–20	JMX	Ending J-index.	(1)
21–25	[KMN]	Beginning K-index.	(1)
26–30	[KMX]	Ending K-index.	(1)
31–40	Uwall	Velocity on the wall.	(2)
41–50	Twall	Departure temperature on the wall.	(2)

Notes:

(1) These indices define a plane (or a line segment for 2-D problems) over which the wall functions are to be applied. One card is required for each plane and as many cards as necessary can be used until terminated by a blank card.

(2) These values are usually zero unless the solid wall is moving or the departure temperature is non-zero.

Card c: Blank card to terminate the current subcommand.

Last card: Boundary conditions termination subcommand (A5).

Columns	Variable	Entry
1– 5	ICMND	endbc

Notes:

This is the last card in the BCONGEN section and is always required to terminate the execution of the BCONGEN module.

3.3.5 Finite Element Integrals Generation Card

Columns	Variable	Entry
1–7	ICMND	mtrxgen

Notes:

This command calls the appropriate subroutines to generate the finite element integrals, including element volumes (or areas in 2-D), the mass matrix, and the divergence matrix. The resulting matrices are written into various disk files. This command requires no subcommands or data statements.

3.3.6 Initial Conditions Data Cards

Initial conditions for field variables of velocity, temperature, and species are generated by subroutine ICONGEN which, if called, produces an initial conditions file INITCO for the above field variables plus the density field. With an appropriate subcommand, another file named INITKE containing the initial values for the $k-\varepsilon$ fields may also be produced. While Eqs. (3.6) and (3.7) can be used to generate most profiles of the above fields, it is often appropriate and more convenient to use the well-known similarity theory and formulae established for the atmospheric boundary layer. Specifically, the vertical profiles of velocity and temperature (departure from a reference value) are defined respectively as:

$$u = \frac{u_*}{\kappa}\left[\ell n\left(\frac{y}{y_o}\right) + \psi\right], \tag{3.9}$$

and

$$\theta = \frac{\theta_*}{\kappa}\left[\ell n\left(\frac{y}{y_o}\right) + \psi_\theta\right]. \tag{3.10}$$

The associated profiles of turbulence kinetic energy (k) and its dissipation rate (ε) are defined as:

$$k = C_\mu^{-\frac{1}{2}}\ u_*^2\left(1 - \frac{Ri}{\phi}\right)^{\frac{1}{2}}, \tag{3.11}$$

and

$$\varepsilon = u_*^3(\phi - Ri)/\kappa y. \tag{3.12}$$

In the above formulae, u_* is the friction velocity, y_o is the ground surface roughness scale, θ_* is friction temperature, κ is von Karman's constant $(=0.41)$, C_μ is an empirical coefficient $(=0.09)$, Ri is the gradient Richardson number ($Ri = y/L$, in which L is the Monin-Obukhov length scale), and ψ, ψ_θ, and ϕ are the similarity functions used by Haroutunian (1987).

For instantaneous sources, constant values for the species concentration and the temperature fields are assumed within each region (usually in the shape of a box in 3-D) representing the source containment and extended by trivariate Gaussian functions in the region immediately surrounding the nodes representing the sources. Specifically, these variables are defined to be

$$F = \begin{cases} F_o & \text{within the box} \\ F_o e^{-1/2\left[\frac{(x-\bar{x})^2}{\sigma_h^2}+\frac{(y-\bar{y})^2}{\sigma_v^2}+\frac{(z-\bar{z})^2}{\sigma_h^2}\right]} & \text{outside of the box} \end{cases} \tag{3.13}$$

in which $(\bar{x},\bar{y},\bar{z})$ are on the boundary of the box defined by the location of the source center and the source dimensions.

Unless defined by the respective subcommand and input card(s), all the field variables (except density) are initialized as zero. At least two cards (the first and the last) are necessary to generate file INITCO. If any of the field variables differs from zero, one to three additional cards are required to define it.

First card: Initial condition command and material inventory (A7, I5).

Columns	Variable	Entry	Note
1– 7	ICMND	icongen	(1)
8–12	NPTS	Flag for inventory of the total amount of material for instantaneous source(s). = 0, no inventory is desired, = n, a non-negative integer to indicate how many variations of the total inventory should be taken.	(2)

Notes:

(1) This command calls ICONGEN to initialize the field variables and, if necessary, to generate nonzero initial conditions. If any of the field variables is different from zero, the following group of card(s) is required. Otherwise, all field variables except density remain zero and only the last card is required to terminate the command.

(2) For simulation involving instantaneous sources, it is often difficult to obtain the desired total amount of material due to the complexity of the source geometry and the nonlinear relationship between density and mass fraction of species. For this reason, a procedure has been implemented to vary the value of the species concentration and compute the total amount of material accordingly. If $n = 1$, the material inventory will be evaluated assuming 100% of the source strength. If $n = 2$, an additional inventory will be conducted by assuming 90% of the source strength, i.e., F_0 in Eq. (3.13) is reduced to 90%. The maximum value of n is 10, which will produce a minimum amount of material corresponding to 10% of the assumed source strength. Based on these values (and trial-and-error, if necessary), the total amount of source material can be made as close as possible to the desired amount by adjusting the source strength and/or its geometry.

The following describes the cards required to generate non-zero initial conditions for the relevant variables, using Eqs. (3.6) and (3.7).

Card a: Field identifier and parameters (A5, I5, 3F10.0).

Columns	Variable	Entry	Note
1– 7	ICMND	Field identifier.	(1)
6–10	NDOP	Analytic function identifier. = 0, constant, = 1, or -1, linear function, = 2 or -2, quadratic function, = 3 or -3, logarithmic function.	(2)
11–20	VALUE	Constant value of the field variable (when NDOP = 0).	
21–30	YM	Height above which the field variable attains its maximum value.	(3)
31–40	FM	Maximum value of the field variable.	(3)

Notes:

(1) The field identifier can be any one of the following:

iclog — for u, θ, k, and ε as defined by Eqs. (3.9) through (3.12). In such a case, only four parameter values are required in the next input line (with format 4F10.0) to define the values of u_* (friction velocity), y_o (ground surface roughness scale), L (Monin-Obukhov length scale), and θ_* (the friction temperature).

iconu — for u-velocity component,

iconv — for v-velocity component,

iconw — for w-velocity component,

icont — for departure temperature (i.e., deviation from the reference temperature),

iconc — for *mass fraction* of species (all-vapor),

icoqt — for total mass fraction of vapor/droplets (phase-change). In this case, the preprocessor will calculate the corresponding mass fractions of vapor and droplets, and the associated temperature field, based on thermodynamic equilibrium assumption.

(2) A negative value of NDOP implies that the height (y) in Eqs. (3.6) and (3.7) is measured from the ground surface, otherwise y is the vertical coordinate in those equations. If NDOP $\neq 0$, additional cards are required.

(3) The default value of YM is 10^{10}. A cut-off value of FM is applied if $y \geq YM$.

Card a1: Linear or logarithm function definition (4F10.0).

Columns	Variable	Entry
1–10	C1	First coefficient.
11–20	C2	Second coefficient.
21–30	C3	Third coefficient.
31–40	[C4]	Fourth coefficient.

Notes:

This card is required when NDOP ≠ 0. If NDOP = -3 or 3, only the first three coefficients are required to define the logarithmic function of Eq. (3.6). Otherwise, all four values are required to define the first four coefficients in Eq. (3.7).

Card a2: Coefficients of quadratic terms (6F10.0).

Columns	Variable	Entry
1–10	C5	Fifth coefficient.
11–20	C6	Sixth coefficient.
21–30	C7	Seventh coefficient.
31–40	[C8]	Eight coefficient.
41–50	[C9]	Ninth coefficient.
51–60	[C10]	Tenth coefficient.

Notes:

This card is required only if NDOP = 2 or -2. These coefficients define the quadratic terms in Eq. (3.7).

To specify initial conditions of concentration and temperature associated with instantaneous source(s) defined by Eq. (3.13), the following cards are necessary.

Card b: Field identifier and source dimensions (A5, I5, 4F10.0).

Columns	Variable	Entry	Note
1– 5	ICMND	Field identifier.	(1)
6–10	NDOP	Source dimension identifier	(2)

		= 4, source dimensions to be specified separately for each source, = 5, source dimensions are the same for all sources as specified in columns 11 through 50.	
11–20	HHW	Source half-width in the horizontal direction.	(3)
21–30	VHW	Source half-width in the vertical direction.	(3)
31–40	SIGH	Value of σ_h in Eq. (3.13).	
41–50	SIGV	Value of σ_v in Eq. (3.13).	

Notes:

(1) The field identifier can be any one of the following:

icont — for departure temperature (i.e., deviation from the reference temperature),

iconc — for mass fraction of species (all-vapor),

icoqt — for total mass fraction of vapor/droplets (phase-change). In this case, the preprocessor will calculate the appropriate mass fractions of vapor and droplets, and the corresponding temperature field, based on local thermodynamic equilibrium assumption.

(2) NDOP = 4 is designed for multiple sources with different source dimensions. In this case, the source dimensions will be defined separately for each source on the source definition card. NDOP = 5 is designed for multiple sources of identical dimensions (but source strength can vary). In this case, the source dimensions defined in Columns 11 through 50 will be used for all sources.

(3) The source is defined to be in the shape of a box, within which the species concentration (or temperature) is constant. The values of source half-width are measured from the center to the respective edges of the source.

Card(s) b1: Source definition card (8F10.0).

Columns	Variable	Entry	Note
1–10	FO	Constant value of F_0 in Eq. (3.13).	(1)
11–20	XO	x-coordinate of source center.	(1)
21–30	YO	y-coordinate of source center.	(1)
31–40	[ZO]	z-coordinate of source center.	(1)
41–50	HHW	Source half-width in the horizontal direction.	(2)
51–60	VHW	Source half-width in the vertical direction.	(2)

61–70	SIGH	Value of σ_h in Eq. (3.13).	(2)
71–80	SIGV	Value of σ_v in Eq. (3.13).	(2)

Notes:

(1) One card is required for each source. These cards can be stacked until terminated by a blank card.

(2) These values are required only when NDOP = 4. For NDOP = 5, their values are defined on Card b. The location of the source center, together with the values of source half-widths, define a box-shaped region alluded to earlier about Eq. (3.13).

Last card: Initial conditions termination card (A5).

Columns	Variable	Entry
1–5	ICMND	endic

Notes:

This card is always required if "icongen" is present in the input deck. The functions of this subcommand are to finish generating initial conditions and to write a file called INITCO for use in the main code.

3.3.7 Time-History Data Cards

In many simulations, it is often desirable to produce certain time-history data for analyzing the results. With the following group of cards, the desired nodal numbers and variables are identified and passed to the main code, which subsequently collects all the desired time-history data into file THIST for plotting by post-processor EZPLOT.

First card: time-history data selection command card (A7).

Columns	Variable	Entry
1–7	ICMND	thisgen

Notes:

This command indicates to the code that time-history data for the nodes and field variables specified in the succeeding cards are desired.

Intermediate cards: Node numbers and variables selection cards (3I5, 13A5).

Columns	Variable	Entry	Note
1– 5	I	I-index of the selected node.	(1)
6–10	J	J-index of the selected node.	(1)
11–15	[K]	K-index of the selected node.	(1)
16–20	VAR(1)	List of selected variables.	(2)
21–25	VAR(2)		(2)
26–30	VAR(3)		(2)
•			(2)
•			(2)
•			(2)
•			(2)
71–75	VAR(12)		(2)
76–80	VAR(13)		(2)

Notes:

(1) The values of (I, J, K) define the nodal point for which time-history data are to be collected. One card is required for each nodal point.

(2) These are (right-justified) variable names. Up to thirteen variables in the following list can be selected, but the total number of time history plots must not exceed 99 as presently configured in the code:

u	for u-velocity component,
v	for v-velocity component,
w	for w-velocity component,
t	for temperature of the mixture (in °C in output file),
c	for volumetric fraction of vapor material,
qv	for mass fraction of material in vapor phase,
$q\ell$	for mass fraction of liquid material,
rho	for density of the mixture,
p	for dynamic pressure computed in the code,
dos	for dosage,
k	for turbulence kinetic energy,
e	for dissipation rate of turbulence kinetic energy,
vk	for turbulent diffusivity in the vertical direction.

Last card: Blank card to terminate the thisgen command.

3.3.8 Pressure Matrix Generation and Decomposition Card (A7)

Columns	Variable	Entry
1–7	ICMND	callfis

Notes:

This command calls FISSLE (a package for solving linear system of equations via Gaussian elimination) to generate the pressure matrix and then decompose it into the form of LDL^T for use in the main code. Also, it generates a disk file AICCG containing the matrices necessary for the iterative solver-ICCG (an alternative solution package for linear system of equations, see Kershaw, 1978).

3.3.9 End-of-Input Deck Card (A7)

Columns	Variable	Entry
1–7	ICMND	endfile

Notes:

This command indicates to the code that there are no more commands to read in PREPIN. A sequential file named FEMCIN will be written as part of the input to the main code. Also, a file called FEM3INDF is generated, which can be edited to make the FEM3IN file necessary in running FEM3C.

4. FEM3C USER'S GUIDE

4.1 Introduction

FEM3C is the main code for solving numerically the coupled system of conservation equations. A modified Galerkin finite element method with eight-node isoparametric hexahedrons (four-node quadrilaterals in two dimensions) is used for spatial discretization, and a modified forward Euler method is employed to integrate in time all primary variables except pressure, which is solved either directly by a skyline solver or iteratively by a preconditioned conjugate gradient method. The code can be used to solve both two- and three-dimensional problems. It also handles variable terrain and obstructions. Like PREFEM3C, the code is dynamically dimensioned to fit individual problem size.

Before running FEM3C, the preprocessor must be executed to produce the necessary files. A short additional file named FEM3IN is also required to specify certain run-time parameters. After the run is completed, the resulting data in THIST and POLYPLOT files can then be plotted by postprocessors EZPLOT and PLOTRDM, respectively (unfortunately, these postprocessors are not readily exportable but are available to LLNL users).

The input and output files of FEM3C are described in the next subsection, and instructions for preparing FEM3IN are given in the last subsection.

4.2 Input and Output Files

As stated earlier, most FEM3C input data are generated by PREFEM3C and written into a number of disk files. In most situations, only a short, additional file FEM3IN (described in Section 4.3) has to be prepared in order to run FEM3C. Figure 4.1 is a sketch showing the file names and Table 4.1 is a brief description of these files. A typical run usually requires six files to provide the necessary input data, namely, CTRANS1, FEM3IN, FEMCIN, INITCO, POLYPLOT, and either AICCG or DECOML (depending on the equation solver being selected). When the $k-\varepsilon$ turbulence submodel is selected, file INITKE is also required for specifying the initial values of the k and ε fields. For restart runs with initial conditions contained in POLYPLOT, file INITCO is not required. As indicated in Fig. 4.1, CTRANS and INITFL are also optional. File CTRANS is necessary if mixed-type boundary conditions are used or, for 3-D problems, variable terrain is present (and with LQR = 3 in PREPIN). The flow field file (arbitrarily designated as INITFL) is required only when the flow field in INITCO or POLYPLOT has to be replaced.

The output files from this code include FEM3OT, POLYPLOT, RMSERR, and THIST. FEM3OT is an ASCII file containing the essential input data and parameters, the computed variables at selected times, and also the error messages if the run is aborted. POLYPLOT is a binary file containing mainly solution of the field variables at preselected times and THIST is an ASCII file containing data for time-history plots. The RMSERR file contains information on the time truncation errors of the field variables being computed and data pertaining to subcycling. It also contains the maximum speed (qmax) within the entire computational domain which, along with the dynamic time step (deltd), is an indication of the dynamical behavior of the system. For example, if the maximum speed varies rapidly and the dynamic time step is small, they indicate that the system is changing fast in time. On the other hand, if the maximum speed is nearly independent of time and the dynamic time step is increasing monotonically, these are indications that the system is approaching a steady state. When the $k-\varepsilon$ turbulence submodel is used, the code also produces KEFILE, which can be edited to yield INITKE for a restart run.

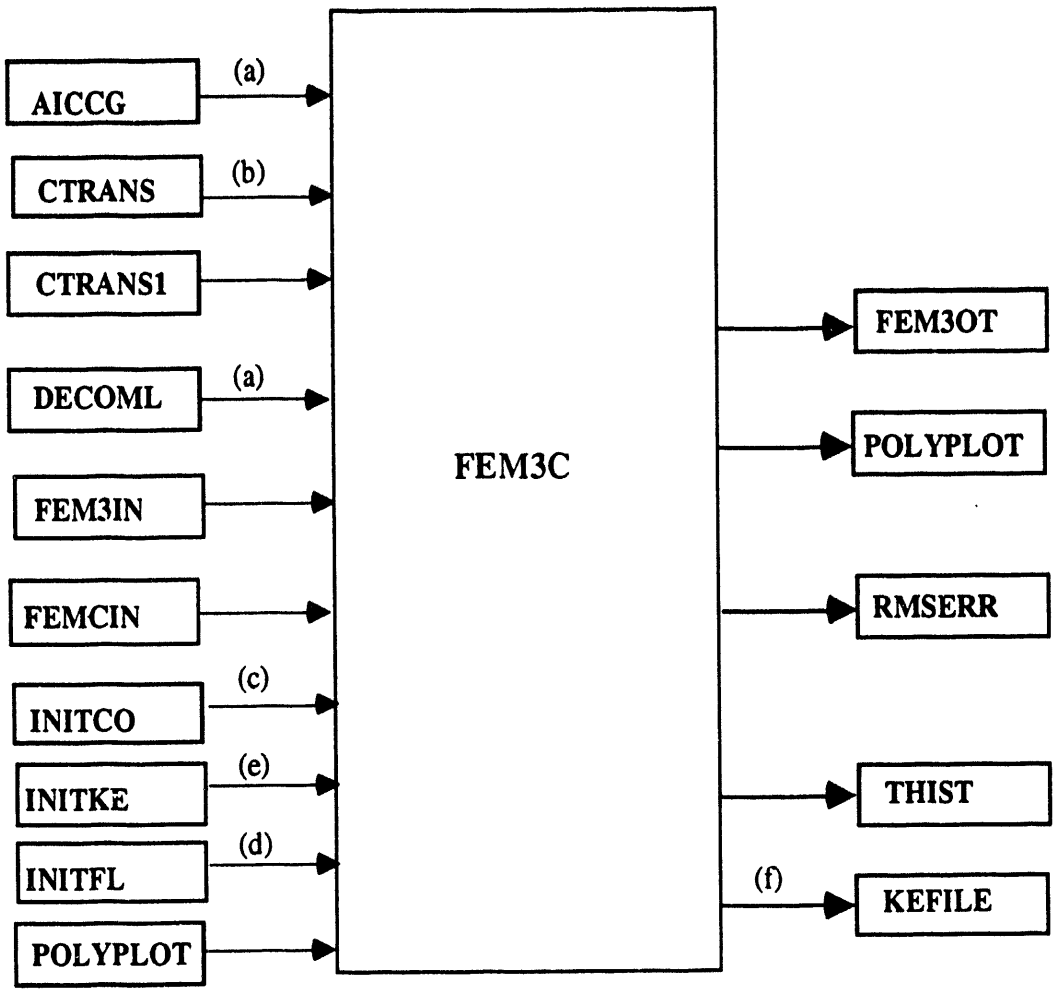

Fig. 4.1. Input and output files associated with FEM3C.

(a) AICCG is required if iterative equation solver is selected; otherwise, DECOML is required for the direct solver FISSLE.

(b) File is required if problem involves variable terrain (LQR=3 in PREPIN file) or mixed-type boundary conditions (DICOS is present in PREPIN file).

(c) File is required if NDS = 0 in FEM3IN File.

(d) File is required if the flow field in INITCO or POLYPLOT file has to be replaced.

(e) File is required if $k-\varepsilon$ turbulence submodel is selected (i.e., KFLG = –2 in FEM3IN).

(f) File is produced if $k-\varepsilon$ turbulence submodel is used in the run.

Table 4.1. FEM3C input and output files.

Unit No.	File name	Description	File type	File access
5	FEM3IN	First program input file	ASCII	Sequential
6	FEM3OT	Program output file	ASCII	Sequential
7	INITCO	Initial conditions file	ASCII	Sequential
7	INITFL*	Initial flow field file	ASCII	Sequential
8	DECOML	Decomposed pressure matrix file	Binary	Random
9	CTRANS	Divergence Matrix file	Binary	Sequential
9	CTRANS1	Half of the entries of the divergence matrix obtained with one-point quadrature	Binary	Sequential
10	POLYPLOT	Input and output file containing results for graphical displays	Binary	Random
11	FEMCIN	Second program input file	Binary	Sequential
12	THIST	Time history data file	ASCII	Sequential
14	AICCG	File containing matrices associated with the iterative equation solvers	Binary	Sequential
15	RMSERR	RMS errors and subcycling information	ASCII	Sequential
19	INITKE	Initial conditions file for the $k-\varepsilon$ fields	ASCII	Sequential
20	KEFILE	Solution at selected times for the $k-\varepsilon$ fields	ASCII	Sequential

* File name specified in line 3 of FEM3IN.

4.3 Preparation of FEM3IN File

FEM3IN is an input file to FEM3C, in addition to other files generated by the preprocessor, to define certain parameters in running the main code. This file can be conveniently constructed by editing the appropriate entries of FEM3INDF, which is always generated by the preprocessor. The entire file is composed of 24 lines.

In FEM3IN, each line has four fields, of which only the second field is read by the code. The first field (columns 1 through 4) is the sequential line number. The second field (columns 5 through 12) defines the numerical value or parameter associated with the input variable defined in the third field (columns 13 through 24). The fourth field is a brief description of the input variable. Except lines 3 and 15, which uses formats (4X, A8) and (4X, 4A4), respectively, the usual FORTRAN conventions (i.e., integers begin with I through N and floating-point numbers begin with the remaining alphabetical characters) are used in naming the variables and the corresponding formats are (4X, I8) and (4X, F8.0), respectively.

The following is a description of the input variables and the choices available.

Line 1: NEQS—Number of conservation equations (4X, I8).

NEQS is the total number of conservation equations to be solved, including the equations for momentum, energy, and species, but excluding the equation of continuity. Specifically, in three-dimensional simulations, NEQS is equal to 3 for flow field calculations only, 4 for thermal flows (without species), 5 for dispersion simulations involving vapor only, and 6 for dispersion simulations involving phase-change. In the case of pure vapor dispersion simulations with the gas temperature equal to that of the ambient atmosphere (i.e., isothermal case), a value of -5 can be used to save the time otherwise required in updating a constant temperature field. For two-dimensional problems, the value of NEQS is reduced by one, because the number of momentum equations is two instead of three.

Line 2: NDS—Indicator of initial conditions (4X, I8).

NDS is a non-negative integer number indicating how initial conditions are provided to the code. If NDS = 0, FEM3C will read the initial conditions from INITCO, which must have been generated by PREFEM3C or been constructed, for a restart run, from the ASCII output file (FEM3OT) of an earlier run. Alternatively, the initial conditions can be read from the binary file POLYPLOT. In such a case, NDS is the desired data set number in POLYPLOT.

Line 3: NFLOW—File name of initial flow field (4X, A8).

This is a flexibility designed to provide initial conditions to FEM3C using two separate files, namely, flow field from the file specified herein and the remaining fields (temperature and species concentrations) from the file defined above. Specifically, the initial conditions (for all field variables) defined by Line 2 are read in first and, if Line 3 contains a file name (up to 8 right-justified characters) in columns 5 through 12, the code will read the velocity components from such designated file and replace the velocity field already read in. This option is often necessary in starting a gas dispersion simulation involving instantaneous source(s) and/or obstructions, when the flow field and the file defined by Line 2 does not properly account for the presence of source containment(s) and/or obstructions. For restart runs, however, it is unnecessary to exercise such an option, because a compatible flow field has already been established in the earlier simulation. In such a case, the field should be left as "……".

Line 4: ICCGFLG—Method of solving the pressure field (4X, I8).

There are three methods available in the present code for solving the linear system of equations associated with the pressure field (and the Lagrange multipliers in mass adjustment): a direct method and two iterative methods. The direct method implemented in the code is an out-of-core, skyline solver called FISSLE (Taylor *et al.*, 1981), which is most efficient when the decomposed pressure matrix can be stored in memory. For large-scale problems where the decomposed matrix can not fit in memory (for a 3-D mesh with ℓ, m, n elements in the I-, J- and K-direction, respectively, the memory size required to store the decomposed pressure matrix is approximately $\ell^2 m^2 n$ decimal words), the iterative methods, i.e., the Incomplete Cholesky Conjugate Gradient (ICCG) or the Diagonally Scaled Conjugate Gradient (DSCG) method, are recommended because of the significant reduction in I/O costs and their less demand on storage requirements. Of the two iterative methods, ICCG has been tested more extensively than DSCG and is recommended whenever storage permits. The solution method is selected by setting the value of ICCGFLG as:

ICCGFLG = 0, FISSLE,
= 1, DSCG,
= 2, ICCG.

Line 5: ISTOP—Maximum number of iterations for ICCG or DSCG (4X, I8).

ISTOP is the maximum number of iterations allowed when ICCG or DSCG is being used to solve the pressure field (and the Lagrange Multipliers as well in mass adjustment). Its default value is 200. When the actual number of iterations exceeds the value of ISTOP, the run will abort with an error message printed in FEM3OT. The required number of iterations generally increases with the size(or number of elements) of the problem and the tolerance in solution convergence specified in the next input line. In most cases, for a problem of 10,000 elements, the number of iterations required for the ICCG solver with a convergence criterion of 0.0001 is on the order of 100. For DSCG, the required number of iterations may be 5 to 10 times more; however, the cost for each iteration is much lower.

Line 6: E3—Convergence tolerance for the pressure solution (4X, F8.0).

When ICCG or DSCG is used to solve the pressure field, convergence criteria must be specified to stop the iterations. The convergence criteria used currently are the norm of the solution change between two consecutive iterates and the norm of the residuals of the linear system, both of which must not exceed the specified value for convergence. The present code has a default value of 0.0001, which has been found to be satisfactory in most applications. Other values can be specified if necessary. However, too large a value of E3 could give inaccurate and "strange" results, e.g., the number of iterations may behave erratically, even though the pressure solution appears to vary smoothly in time. Such an anomaly is not completely understood, but is probably due to the randomness of small errors (allowed by the loose convergence tolerance) in the divergence of the velocity field.

Line 7: NSC—Subcycling flag (4X, I8).

This is one of the cost-effective measures available in the code to allow less frequent update of the pressure field. If subcycling is requested, the pressure field will be updated only at the end of the major time steps determined by accuracy requirements; within the next major time step, linear extrapolation in time is used to construct the approximate pressure gradients in the momentum equations. The subcycling option has been found especially cost-effective when FISSLE is used to solve the pressure field. For the iterative methods (ICCG or DSCG), numerical experiments seem to suggest that subcycling may not be cost-effective enough (or even be cost ineffective sometimes) due to the high cost usually associated with mass adjustment. For these reasons, the subcycling

option is available only when FISSLE is used and can be turned on by specifying NSC equal to -1. If subcycling is not desired, the value of NSC should be set equal to 1 (which is set in the code for the iterative methods).

Line 8: TIMEF—Stop time of the run (4X, F8.0).

TIMEF is the final simulation time of the run. When the value of TIMEF is less than or equal to the value of TIME (which is read from the initial conditions file), only mass adjustment of the velocity field will be performed.

Line 9: DELTCR—Time step to be used (4X, F8.0).

This is the time step to be used in integrating the conservation equations based on estimated stability requirements. For guidelines, see Gresho, *et al.*, 1984. Should the input time step exceed the stability limit of the equations being solved, the run will abort as soon as the maximum velocity becomes unreasonably large (arbitrarily set to be 100 in the current code), together with an error message printed in FEM3OT. In such a case, the run should be retried with a smaller time step, after making sure the instability is not caused by incorrect input data.

Line 10: TINJOFF—Time to turn off source injection (4X, F8.0).

This is the time at which the material injection, which may involve vapor and/or liquid droplets, is to be turned off. It pertains only to simulations of continuos or finite-duration releases and is irrelevant for instantaneous releases.

Line 11: CHM—Coefficient of the hourglass matrix (4X, F8.0).

Due to the use of one-point quadrature in evaluating the diffusion terms, hourglass correction terms must be supplemented to control the possible growth of $2\Delta X$ wave components (hourglass modes) in the solution of the field variables. The near-optimal coefficient (to yield approximately the same physical diffusion for all wave numbers) for the hourglass matrix is 1.0 in two dimensions. For three-dimensional problems, the selection of the appropriate scalar multipliers for the four hour-glass correction matrices is not nearly so straight forward (see Gresho *et al.*, 1984). As a rule-of-thumb, a coefficient approximately equal to the average element length, say, $L = \left(\sum_{i=1}^{3} L_i/N_i \right)/3$ in which L_i and N_i are the total length and the number of elements in the i-direction, is often adequate.

Line 12: DTPBCD—Output frequency to FEM3OT (4X, F8.0).

This is the time interval for which ASCII data output to FEM3OT file is desired. Results of the last time step are always written into FEM3OT if the run terminates properly.

Line 13: DTPBIN—Output frequency to POLYPLOT (4X, F8.0).

This is the time interval for which data output to POLYPLOT file is desired. Results of the last time step are always written into POLYPLOT if the run terminates properly. Values of the velocity components and density are always written into POLYPLOT. In addition, temperature and species concentration are also written into the file if these variables are being computed.

Line 14: DTPTH—Output frequency to THIST (4X, F8.0).

This is the time interval for which output to the ASCII file THIST is desired. In addition to results for the times requested herein, data corresponding to the end of a major time step after mass adjustment are also written into THIST. The default value of DTPTH is five times that of DELTCR.

Line 15: IPVA(1), IPVA(2), IPVA(3), IPVA(4)—Optional output variables (4X, 4A4).

For analysis/diagnosis purposes, four optional field variables (in addition to those discussed earlier) are allowed to be written into POLYPLOT. Four variables can be selected from the following: pressure (p), Richardson number (ri), inverse prandtl number (prti), dosage (dos), turbulence kinetic energy (k), turbulence dissipate rate (e), and eddy viscosity (vk). The variables must be right-justified with format A4 but the order of the selected variables is arbitrary.

Line 16: KFLG—Turbulence submodel flag (4X, I8).

There are basically three turbulence submodels available in FEM3C: constant diffusivities, algebraic K-theory based on similarity functions, and K-theory based on the $k-\varepsilon$ transport equations. To invoke one of the submodels, KFLG should be set according to the following and followed by lines 17 through 22 with the relevant input parameters:

KFLG = 0, constant diffusivities,
2 or 1, K-theory using similarity functions,
– 2, K-theory based on $k-\varepsilon$ transport equations.

The first option is the simplest among all three submodels and is mainly for exploratory and testing purposes. It requires six input values in the following order: horizontal momentum diffusivity, vertical momentum diffusivity, horizontal thermal diffusivity, vertical thermal diffusivity, horizontal species diffusivity, and vertical species diffusivity.

The algebraic K-theory submodel is activated by setting KFLG=2 or 1. In general, KFLG=2 should be used. However, if heavy-gas effects are not present, e.g., when establishing the initial flow field prior to a heavy gas release, it is more efficient to use the KFLG=1 option. Described in the following are the six input parameters required by the algebraic K-theory submodel, of which the last three are also required by the turbulence submodel based on the $k-\varepsilon$ transport equations.

Line 17: USTARA—Friction velocity of the ambient atmosphere (4X, F8.0).

The value of this parameter is either obtained from the experiment being simulated or inferred from other experiments which have ambient conditions similar to those of the current simulation. This parameter has the dimension of velocity.

Line 18: RMOL—Monin-Obukhov length scale (4X, F8.0).

RMOL is also a parameter, which must be inferred from relevant experiments to reflect the stability class of the ambient atmosphere. It has the dimension of length.

Line 19: ETV—Effective energy transfer velocity (4X, F8.0).

This is a bulk coefficient used to parameterize the ground heat transfer effects on turbulence and on the energy conservation equation, respectively. Its value generally depends on the dispersed

material and the site. For the Burro series of LNG spill experiments, its value was estimated to be 0.0125 m/s.

Line 20: TGRD—Ambient ground temperature (4X, F8.0).

This is a variable used in calculating the in-cloud "convection velocity" and the ground heat transfer between the vapor cloud and the bottom boundary. Its default value is the reference temperature.

Line 21: HKMIN—Lower limit of the horizontal diffusivities (4X, F8.0).

Line 22: VKMIN—Lower limit of the vertical diffusivities (4X, F8.0).

The above limits are sometimes required to circumvent certain numerical difficulties (wiggles in the solution) caused by insufficient spatial resolution in some flow regions. The desired cutoff values are generally problem- and mesh-dependent. As a rule-of-thumb, these values should be set such that the maximum grid Reynolds number are reasonably small, say, order of 100.

For the K-theory submodel based on the $k - \varepsilon$ equations, input parameters are again defined in lines 17–22, of which lines 20–22 have already been described. Actually, the value defined in line 20 is not used currently but this extra line is kept for the convenience of switching between submodels. Described in the following are the first three parameters required by this submodel.

Line 17: DYN—Distance from computational boundary to solid wall(s) (4X, F8.0)

This is the standoff distance between the computational boundary and the solid wall(s). Its value should be so selected that the wall-laws are valid on the computational boundary in order to assure the quality of the numerical solution. Typically its value should lead to y^+ between 30 and 200 ($y^+ = u_* \Delta / \nu$, in which u_* is the friction velocity, Δ is the standoff distance, and ν is the molecular viscosity of the fluid). As a check on the validity of Δ, one should make sure the value of $k^{1/2} \Delta / \nu$ (k is the value of turbulence kinetic energy) on the boundary as given by the numerical solution is much greater than unity.

Line 18: C3—Coefficient of the buoyancy term in the ε-equation (4X, F8.0).

Lacking better estimate, a value of 2.15 is recommended. However, due to its controversial nature, this coefficient is currently treated as an input parameter for possible numerical tuning.

Line 19: BETAH—Parameter for anisotropic turbulence (4X, F8.0).

This is a parameter used to introduce anisotropic turbulence via modifying (typically increasing) the diffusivities in the streamwise and transverse directions (which are, in the present code, the horizontal directions). A value of 1.0 yields isotropic turbulence and a value other than unity corresponds to anisotropic turbulence.

In addition to the parameters defined in lines 17–22, the $k - \varepsilon$ equation submodel also requires a file named INITKE, which contains the initial conditions for the k, ε fields. Such a file is often generated by PREFEM3C; for a restart run, it should be constructed from KEFILE generated in the earlier run.

Line 23: CSH—Superheating coefficient (4X, F8.0).

This parameterization has been devised to account for the superheating effects when a cryogenic liquid such as LNG is spilled on water in a confined environment. (see UCRL-XXXX, Section x.y for more details). For most applications, superheating of the source material is probably absent or insignificant. In such cases, the value of CSH should be set equal to "0."

Line 24: MCFLG—Mass conservation flag (4X, I8).

This flag selects the desired option for mass conservation and can have one of the following two values:

MCFLG = 1, conserving mass of individual species,
2, conserving species and global mass.

Its value should be set equal to 1 except for certain special cases wherein the global mass is time-independent such as instantaneous release in an enclosed domain.

5. NUMERICAL EXAMPLES

In this section, three examples are presented to demonstrate some of the features available in the FEM3C model: instantaneous and continuous sources, flat and/or sloping terrain, 2D and 3D simulations, and different turbulence submodels. Selected input and output files plus sample results are used as illustrations. Other applications of the model, such as dispersion simulations involving material phase-change and multiple sources, can be found in UCRL-21043.

5.1 *Two-Dimensional Simulation With A Continuous Source*

The following example is a simulation of one of the three laboratory tests conducted by McQuaid (1976), which were designed to investigate the structure of shear flows with stable density stratification. The experiments were conducted in a wind tunnel with a fully developed rectangular channel flow of air into which carbon dioxide was introduced through a 'line' source at ground level. The particular test being simulated is No. 3 and has the following test conditions: source rate of 0.0227 kg/s, average flow velocity of 1.28 m/s, and a source Richardson No. of 17.8. In this simulation, the initial flow field prior to the beginning of vapor dispersion is assumed to have a logarithmic profile. The complete PREPIN file needed to run PREFEM3C and the FEM3IN file needed to run FEM3C are listed on the next two pages.

It is recommended these input files be studied line-by-line with respect to the User's Guides given in sections 3.3 and 4.3. Described below are only several main features of the files. The 'mappx' option, with two blocks, is conveniently used to generate a graded mesh. Due to the fact that wall functions are not valid on the ground surface, the bottom boundary has been 'moved' up by 0.01 m. The continuous source, with the desired source rate, is modeled via appropriate boundary conditions, i.e., an injection velocity of 0.175 m/s over the source area ($x = -0.06$ to 0.02). Those forced (Dirichlet) boundary conditions which are to be obtained from the given initial conditions are designated by a big number, 1.e+20. The nodes for which wall functions are to be invoked are generated with subcommand slpbc and two associated input lines. Finally, initial conditions for u, v, k, and ε, are generated using the iclog option associated with Eqs. (3.9)–(3.12).

After running PFEFEM3C, the vapor dispersion simulation is started using the FEM3IN file, in addition to those files already generated by PREFEM3C. As seen in FEM3IN, the $k-\varepsilon$ turbulence submodel is to be used. Appended at the end of the file are also the necessary replacements if the turbulence submodel based on similarity functions is desired.

PREPIN

```
pbsetup
 mq3--Quaid's experiment No. 3, kflg=-2
    2   49   99    1    5
  293.0     293.0     44.00     1005.    101325.    28.96     1005.     9.806
meshgen
mappx
    1   50    1   51  1.040     1.000
 -0.820    1.1800    1.1800    -0.820
  0.010     0.010     0.500     0.500
    1   50   51  100  1.040     1.030
  1.180     6.000     6.000     1.180
  0.010     0.010     0.500     0.500

endms
bcongen
plane j  1
    u    1.e+20
    v    0.000
    c    0.000
    k    1.e+20
    e    1.e+20

subdm
   50   50    2  100
    v  0.000
 next
    1    1    2  100
    v  0.000
 next
    1    1   20   22
    u  0.000
    v  0.175

nbcfc
    1    1   20   22  0.175

slpbc
    1    1    1  100

endbc
icongen
iclog
 0.0528    1.e-05    10000.
endic
thisgen
    1   27    c
    1   34    c
    1   47    c
    1   66    c
    1   78    c
    1   87    c
    1   94    c
    1  100    c

mtrxgen
callfis
```

FEM3IN

```
 1     1.      -4  neqs      no. of equations (u,v,w,t,c,qv,ql) to solve
 2     2.       0  nds       0 (initco) or data-set no. (in polyplot)
 3     3.  ......  nflow     file to replace flow field in i.c.
 4     4.       0  iccgflg   p solver: 0 (fissle); 1 or 2 (iccg)
 5     5.     200  istop     max. no. of iterations for p solution
 6     6.   .0001  e3        convergence criterion for p with iccg
 7     7.      -1  nsc       subcycling - fissle only; -1 (yes) or 1 (no)
 8     8.    20.0  timef     stop time for run
 9     9.   0.005  deltcr    max. time step based on stability limits
10    10.   999.0  tinjoff   time to turn off source injection
11    11.     1.0  chm       coefficient for hourglass matricies
12    12.    20.0  dtpbcd    output frequency to bcd file (fem3ot)
13    13.    10.0  dtpbin    output frequency to binary file (polyplot)
14    14.    0.25  dtpth     output frequency to time history file (thist)
15    15.prti  vk   k   e    optional fields to put in polyplot
16    16.      -2  kflg      k-model flag (-2, 0, 1, or 2)
17    17.    0.01  dyn       distance from boundary to apply wall function
18    18.    2.15  c3        parameter for buoyancy term in e-equation
19    19.    1.00  betah     parameter for anisotropy model
20    20.   293.0  tgrd      ambient ground temperature (in kelvin)
21    21.  0.0001  hkmin     lower limit of horizontal diffusivities
22    22.  1.0e-6  vkmin     lower limit of vertical diffusivities
23    23.    0.00  csh       coefficient of superheating
24    24.       1  mcflg     mass conservation options (1 or 2)
25
26
27    15.  vk  ri            optional fields to put in polyplot
28    16.       2  kflg      k-model flag (-2, 0, 1, or 2)
29    17.  0.0528  ustara    friction velocity of the ambient atmosphere
30    18.  10000.  rmol      monin-obukhov length scale
31    19.    0.00  etv       effective energy transfer velocity
32    20.   293.0  tgrd      ambient ground temperature (in kelvin)
33    21.  0.0001  hkmin     lower limit of horizontal diffusivities
34    22.  1.0e-6  vkmin     lower limit of vertical diffusivities
35    23.    0.00  csh       coefficient of superheating
36    24.       1  mcflg     mass conservation options (1 or 2)
```

Upon completion of a run, a number of output files are produced. One of such files is THIST, which collects the time history data for certain preselected mesh points. An edited file containing its beginning and ending portions is listed below. Following the problem identification, the value of 15 in line 2 indicates the number of entries per data set (14 variables plus time). Lines 4 through 18 are the identifiers for the collected data. For instance, symbol 'c' denotes volumetric concentration and is followed by the node number behind @, delt is the dynamic time step calculated in the code for subcycling option, qmax is the maximum velocity within the entire domain, Tinin and Tmax are the minimum and maximum values of temperature, gmass is the global mass, and cmass is the total amount of species mass. At LLNL, a post-processor named EZPLOT is available for plotting the time series data on the Sun workstation. Another file produced for graphical processing is POLYPLOT, a binary file used as input to a post-processing code named PLOTRDM available at LLNL. The contents of POLYPLOT are described in Appendix A for possible adaptation by the users of the FEM3C model.

THIST

```
mq3--Quaid's experiment No. 3, kflg=-2
  15

' Time'
' c    @ 1301'
' c    @ 1651'
' c    @ 2301'
' c    @ 3251'
' c    @ 3851'
' c    @ 4301'
' c    @ 4651'
' c    @ 4951'
' delt'
' qmax'
' Tmax'
' Tmin'
' gmass'
' cmass'

  0.0000000E+00
  0.0000000E+00   0.0000000E+00   0.0000000E+00   0.0000000E+00   0.0000000E+00
  0.0000000E+00   0.0000000E+00   0.0000000E+00   5.0000000E-03   1.3934179E+00
  2.0000000E+01   2.0000000E+01   4.0253655E+00   0.0000000E+00

  5.0000000E-03
  0.0000000E+00   0.0000000E+00   0.0000000E+00   0.0000000E+00   0.0000000E+00
  0.0000000E+00   0.0000000E+00   0.0000000E+00   5.0000000E-03   1.4362852E+00
  2.0000000E+01   2.0000000E+01   4.0253943E+00   8.4320965E-05

  1.0000000E-02
  0.0000000E+00   0.0000000E+00   0.0000000E+00   0.0000000E+00   0.0000000E+00
  0.0000000E+00   0.0000000E+00   0.0000000E+00   1.1104866E-03   1.4351269E+00
  2.0000000E+01   2.0000000E+01   4.0254248E+00   1.7368283E-04

  1.5000000E-02
  0.0000000E+00   0.0000000E+00   0.0000000E+00   0.0000000E+00   0.0000000E+00
  0.0000000E+00   0.0000000E+00   0.0000000E+00   1.8586385E-03   1.4342135E+00
  2.0000000E+01   2.0000000E+01   4.0254556E+00   2.6394112E-04

  2.0000000E-02
  0.0000000E+00   0.0000000E+00   0.0000000E+00   0.0000000E+00   0.0000000E+00
  0.0000000E+00   0.0000000E+00   0.0000000E+00   2.2118510E-03   1.4334686E+00
  2.0000000E+01   2.0000000E+01   4.0254869E+00   3.5568299E-04

  2.5000000E-02
  0.0000000E+00   0.0000000E+00   0.0000000E+00   0.0000000E+00   0.0000000E+00
  0.0000000E+00   0.0000000E+00   0.0000000E+00   2.8528464E-03   1.4328418E+00
  2.0000000E+01   2.0000000E+01   4.0255186E+00   4.4849398E-04

  3.0000000E-02
 -3.2065564E-07   0.0000000E+00   0.0000000E+00   0.0000000E+00   0.0000000E+00
  0.0000000E+00   0.0000000E+00   0.0000000E+00   3.7858908E-03   1.4323008E+00
  2.0000000E+01   2.0000000E+01   4.0255507E+00   5.4233733E-04


  1.9980000E+01
  8.6366451E-01   6.6859391E-01   5.0282747E-01   3.6898569E-01   3.0108788E-01
  2.5649887E-01   2.2524431E-01   2.0082531E-01   6.4619318E-02   1.4792741E+00
  2.0000000E+01   2.0000000E+01   4.0901758E+00   1.8960829E-01

  2.0000000E+01
  8.6366420E-01   6.6858930E-01   5.0283119E-01   3.6898428E-01   3.0108816E-01
  2.5649913E-01   2.2524486E-01   2.0082654E-01   2.0000000E-02   1.4793336E+00
  2.0000000E+01   2.0000000E+01   4.0901758E+00   1.8960840E-01
```

Some of the results from the present run are depicted in Figs. 5.1 through 5.3. Owing to negative buoyancy and the suppression of turbulence within the vapor cloud, a very low cloud is produced as indicated by Fig. 5.1 (note the factor of 10 scaling in the vertical coordinate). Despite the presence of some wiggles near the upwind edge of the vapor cloud (caused by insufficient mesh resolution in such a region), the present results obtained have been found to compare quite well with the measured data.

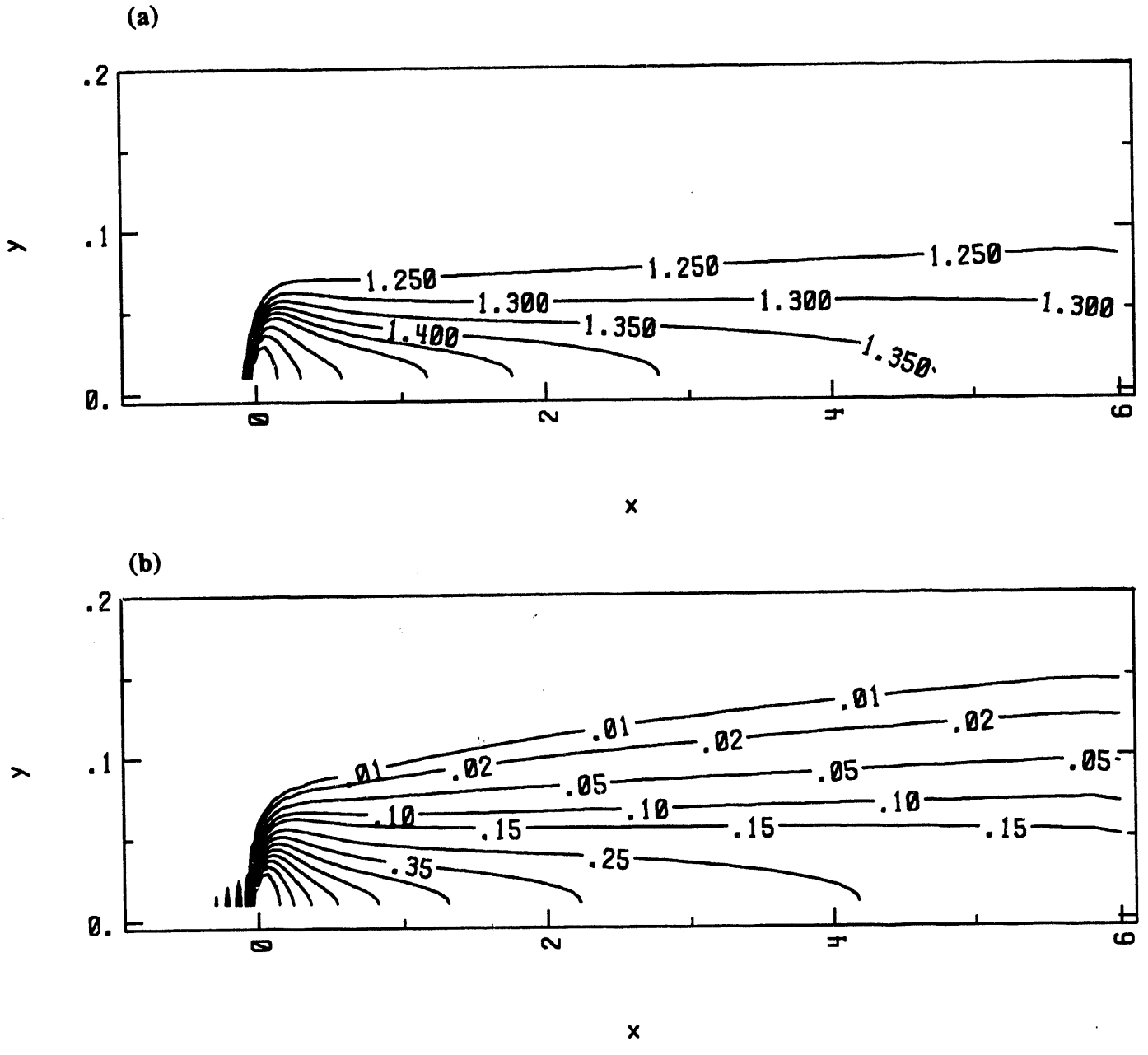

Fig. 5.1 Simulated results for McQuaid's experiment No. 3:
(a) contours of density (in kg/m^3), and
(b) contours of volumetric concentration.

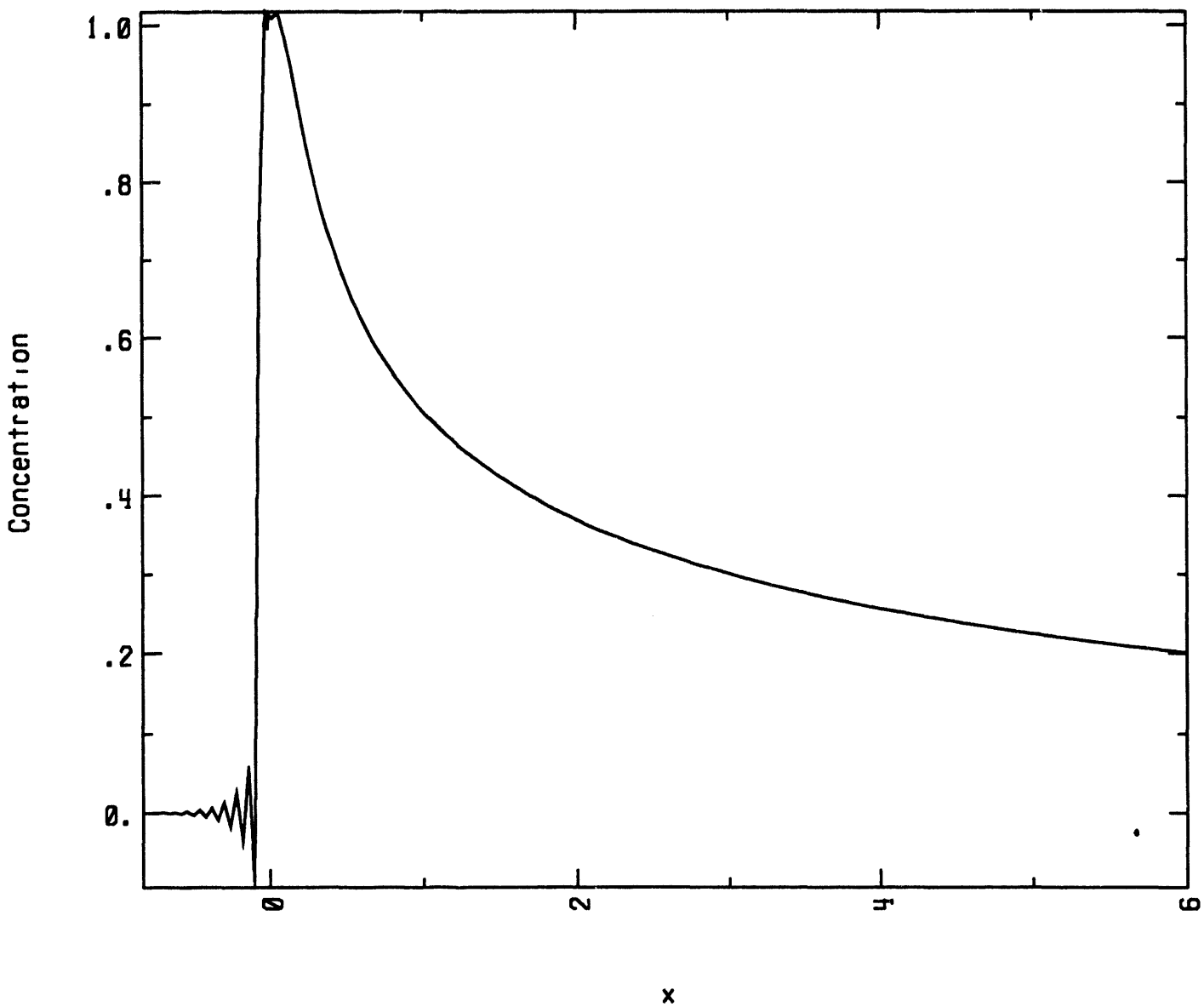

Fig. 5.2 Ground level concentration of CO_2 for McQuaid's experiment No. 3.

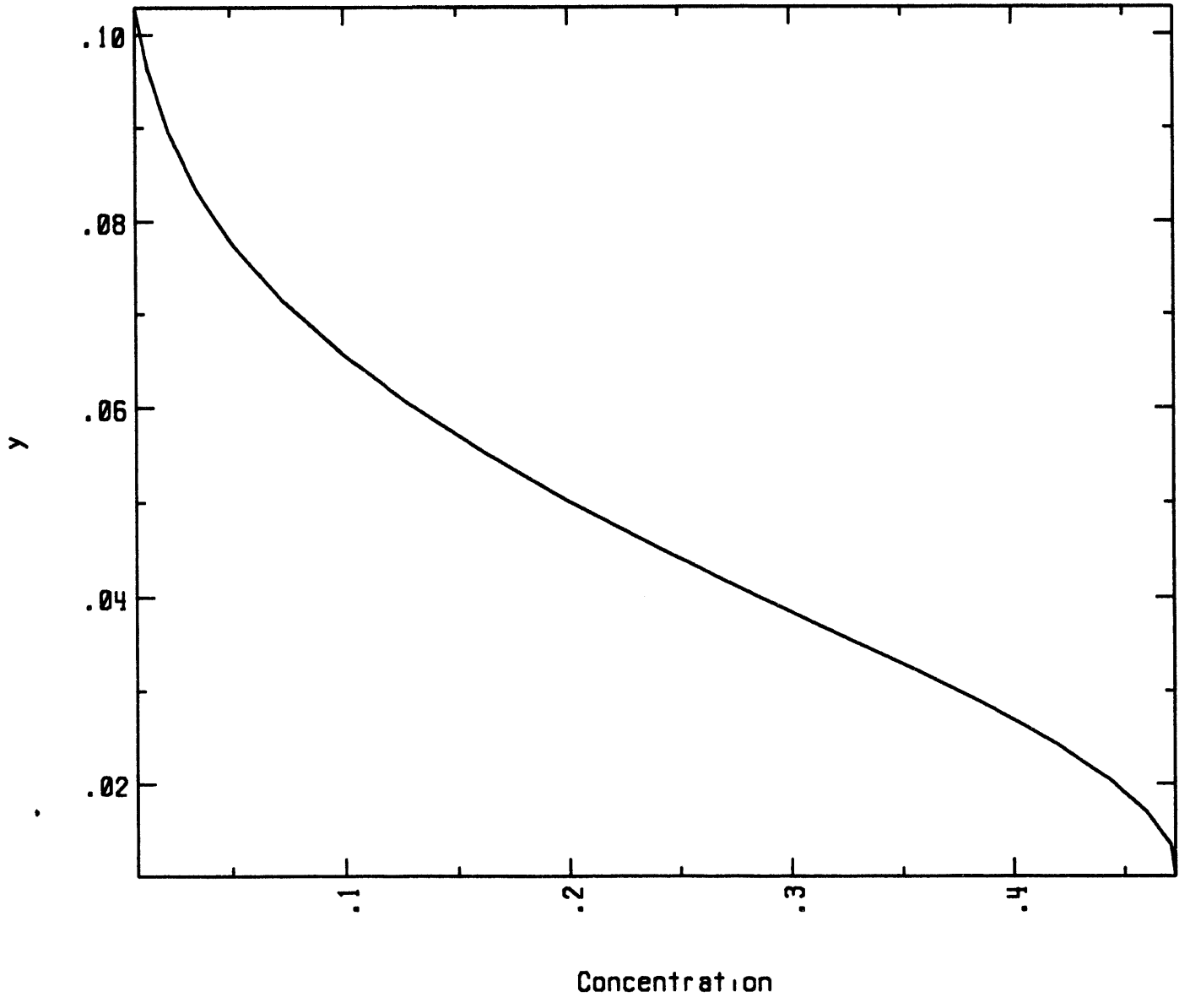

Fig. 5.3 Predicted concentration profile at $x = 1.18$ m for McQuaid's experiment No. 3.

5.2 Vapor Cloud Dispersion Over A Ramp

This example involves the dispersion simulation of an instantaneous release of 485–kg SO_2 near a ramp, such as the topography near a shoreline. The following atmospheric conditions are assumed: an average wind speed of $2\,m/s$ blowing toward the ramp, a moderate temperature of 20°C, and a slightly stable atmosphere with roughness length = 0.01 cm and friction velocity = 6.88 cm/s. A vertical profile of the terrain and computational domain are shown in Fig. 5.4 (a). Lateral symmetry is assumed and the half-width of the mesh is taken to be 120 m. The source is centered at a distance 80 m downwind of the inlet plane. The ramp starts at 40 m downwind of the source and rises to a height of 20 m over a horizontal distance of 100 m. The outlet plane of the mesh is 80 m downwind of the top of the ramp and the upper boundary of the mesh is 60 m above the lowest ground level. A graded mesh consisting of 8100 nodes, with 12 nodes in the vertical, 15 nodes in the lateral, and 45 nodes in the longitudinal directions respectively, was used in the simulation.

A complete simulation of the vapor dispersion in this case is a two-step process: first a flow field consistent with the terrain is generated, then the dispersion simulation is made using such a flow field as initial condition. In the following, we list and briefly comment on some of the files used and produced from the two parts of simulation.

Listed below are the PREPIN, FEM3IN, and an edited THIST files from the flow field calculation. Under command 'bcongen', a block of nodes with zero velocity and pressure are defined using the 'subdm' command to model the blocking effects of the source region. Subcommand 'dicos' is used to treat the sloping terrain and to invoke mixed types of boundary conditions. Defined by lines 57–59 is the turbulent shear stress ($=\rho u_*^2$) to be applied on the ground surface, with the '–' sign indicating its direction being opposite to the prevailing wind. The value of –3 following 'iconu' indicates that initial condition for the velocity field is to be generated using the logarithmic profile formula with vertical distance measured from the local ground level. Note that line 33 under 'bcongen' is not really needed in the flow field calculation but is needed in the vapor dispersion simulation. The 'iconc' subcommand and corresponding input lines under 'icongen' are included in this run for the purpose of establishing the sizes and strength of the instantaneous source. The value of 6 in line 62 requests PREFEM3C to evaluate the inventory of material mass based on 50, 60, ..., and 100% of the source strength specified in line 66. These results are then used as the basis to adjust, if necessary, the strength and/or sizes of the source to yield the desired amount of source material. Lines 5 and 6 are used to define the physical properties of the dispersed material, which are necessary for calculating the amount of source material.

PREPIN

```
pbsetup
flow -- flow field over sea-land interface with a ramp
    3   11   14   44    5    2
  293.2     293.2     64.06     617.2     101325.    28.96     1005.     9.806
matprob
  so2
meshgen
mappx
    1   12    1   15    1   14   1.15      1.05      0.95
  0.00      0.00      80.0      80.0      0.00      0.00      80.0      80.0
  0.00      0.00      0.00      0.00      60.0      60.0      60.0      60.0
  0.00      120.      120.      0.00      0.00      120.      120.      0.00
    1   12    1   15   14   22   1.15      1.05      1.05
  80.0      80.0      120.      120.      80.0      80.0      120.      120.
  0.00      0.00      0.00      0.00      60.0      60.0      60.0      60.0
  0.00      120.      120.      0.00      0.00      120.      120.      0.00
    1   12    1   15   22   36   1.15      1.05      1.00
  120.      120.      220.      220.      120.      120.      220.      220.
  0.00      0.00      20.0      20.0      60.0      60.0      60.0      60.0
  0.00      120.      120.      0.00      0.00      120.      120.      0.00
    1   12    1   15   36   45   1.15      1.05      1.05
  220.      220.      300.      300.      220.      220.      300.      300.
  20.0      20.0      20.0      20.0      60.0      60.0      60.0      60.0
  0.00      120.      120.      0.00      0.00      120.      120.      0.00

endms
bcongen
plane k  1
    u  1.0e20
    v  1.0e20
    w  1.0e20
    t  1.0e20
    c  1.0e20

plane i 12
    v  0.000

plane j  1
    w  0.000

plane j 15
    w  0.000

subdm
    1    2    1    3   12   16
    u  0.000
    v  0.000
    w  0.000
    p  0.000

dicos
    1    1    1   15    1   45

plane i  1
    u  0.000

nbcfv
    1    1    1   15    1   45  -0.0057

endbc
mtrxgen
icongen    6
iconu   -3            60.00     2.669
  0.1996    0.0001    -0.2686
iconc    5  0.1000    0.1000    6.0000    2.0000
  1.0000    80.000    0.0000    0.0000

endic
thisgen
    5    8   22    u    v    w
    5    8   36    u    v    w
    5    8   45    u    v    w

callfis
endfile
```

FEM3IN

1	1.	3	neqs	no. of equations (u,v,w,t,c,qv,ql) to solve
2	2.	0	nds	0 (initco) or data-set no. (in polyplot)
3	3.	.....	nflow	file to replace flow field in i.c.
4	4.	0	iccgflg	p solver: 0 (fissle); 1 or 2 (iccg)
5	5.	200	istop	max. no. of iterations for p solution
6	6.	.00001	e3	convergence criterion for p with iccg
7	7.	-1	nsc	subcycling - fissle only; -1 (yes) or 1 (no)
8	8.	120.0	timef	stop time for run
9	9.	0.40	deltcr	max. time step based on stability limits
10	10.	999.	tinjoff	time to turn off source injection
11	11.	1.0	chm	coefficient for hourglass matricies
12	12.	120.0	dtpbcd	output frequency to bcd file (fem3ot)
13	13.	60.0	dtpbin	output frequency to binary file (polyplot)
14	14.	1.0	dtpth	output frequency to time history file (thist)
15	15.	vk	p	optional fields to put in polyplot
16	16.	2	kflg	k-model flag (-2, 0, 1, or 2)
17	17.	0.0688	ustara	friction velocity of the ambient atmosphere
18	18.	35.0	rmol	monin-obukhov length scale
19	19.	0.01	etv	effective energy transfer velocity
20	20.	293.2	tgrd	ambient ground temperature (in kelvin)
21	21.	1.00	hkmin	lower limit of horizontal diffusivities
22	22.	0.05	vkmin	lower limit of vertical diffusivities
23	23.	0.00	csh	coefficient of superheating
24	24.	1	mcflg	mass conservation options (1 or 2)

THIST

```
flow -- flow field over sea-land interface with a ramp
   16

 ' Time'
 ' u    @ 3869'
 ' v    @ 3869'
 ' w    @ 3869'
 ' u    @ 6389'
 ' v    @ 6389'
 ' w    @ 6389'
 ' u    @ 8009'
 ' v    @ 8009'
 ' w    @ 8009'
 ' delt'
 ' qmax'
 ' Tmax'
 ' Tmin'
 ' qmass'
 ' cmass'

   0.0000000E+00
   2.3031228E+00   1.9099150E-01  -4.6579996E-03   3.6841957E+00   2.6567565E-01
  -2.6934858E-04   3.6763428E+00   3.2483169E-02  -8.6075404E-06   4.0000000E-01
   2.7092280E+00   2.0200000E+01   2.0200000E+01   2.2153582E+06   0.0000000E+00

   4.0000000E-01
   2.3036033E+00   1.8893078E-01  -4.7134666E-03   3.6833679E+00   2.6903328E-01
  -2.7104271E-04   3.6754989E+00   3.4608123E-02  -1.6771360E-06   4.0000000E-01
   3.9569856E+00   2.0200000E+01   2.0200000E+01   2.2153582E+06   0.0000000E+00

   8.0000000E-01
   2.3041250E+00   1.8685212E-01  -4.7723677E-03   3.6824924E+00   2.7206565E-01
  -2.7277796E-04   3.6747445E+00   3.6728657E-02   5.4199312E-06   7.4540571E-01
   3.9583924E+00   2.0200000E+01   2.0200000E+01   2.2153585E+06   0.0000000E+00

   1.2000000E+00
   2.3046767E+00   1.8477560E-01  -4.8333142E-03   3.6815746E+00   2.7473333E-01
  -2.7451261E-04   3.6740741E+00   3.8843219E-02   1.2695983E-05   8.0261643E-01
   3.9598019E+00   2.0200000E+01   2.0200000E+01   2.2153586E+06   0.0000000E+00

   1.6000000E+00
   2.3052551E+00   1.8271455E-01  -4.8962312E-03   3.6806334E+00   2.7701882E-01
  -2.7622742E-04   3.6734842E+00   4.0949572E-02   2.0161432E-05   8.2090847E-01
   3.9612118E+00   2.0200000E+01   2.0200000E+01   2.2153588E+06   0.0000000E+00

   2.0000000E+00
   2.3058574E+00   1.8068172E-01  -4.9610442E-03   3.6796873E+00   2.7891394E-01
  -2.7790084E-04   3.6729718E+00   4.3045379E-02   2.7826219E-05   8.3911417E-01
   3.9626175E+00   2.0200000E+01   2.0200000E+01   2.2153589E+06   0.0000000E+00


   1.1880000E+02
   2.3369920E+00   1.8171167E-01  -9.7605994E-03   3.7000166E+00   2.5574992E-01
  -1.1737350E-03   3.6859218E+00   1.3502580E-01   1.0813625E-03   2.0000000E+00
   3.9164698E+00   2.0200000E+01   2.0200000E+01   2.2153616E+06   0.0000000E+00

   1.1960000E+02
   2.3369020E+00   1.8164098E-01  -9.7152871E-03   3.7000329E+00   2.5577976E-01
  -1.1853636E-03   3.6859431E+00   1.3501731E-01   1.0749667E-03   2.0000000E+00
   3.9164698E+00   2.0200000E+01   2.0200000E+01   2.2153616E+06   0.0000000E+00

   1.2000000E+02
   2.3368584E+00   1.8160113E-01  -9.6913607E-03   3.7000413E+00   2.5579271E-01
  -1.1907341E-03   3.6859531E+00   1.3501313E-01   1.0713260E-03   2.0000000E+00
   3.9164698E+00   2.0200000E+01   2.0200000E+01   2.2153616E+06   0.0000000E+00
```

In the following, the corresponding PREPIN, FEM3IN, and THIST files from the vapor dispersion simulation are listed. The contents of the present PREPIN files are the same as the previous one except in the following areas: the removal of the boundary conditions associated with the source region, the deletion of those lines related to generating the initial velocity (which is to be provided through the flow field calculation), and the changes regarding nodal points and variables to be put into the THIST file. Since the source strength and dimensions have already been determined in the first part of the simulation, lines 5 and 6 are really not needed for the present isothermal simulation (but it would be required if the dispersion involved phase-change). In the FEM3IN file, the value of –5 in line 1 means that the dispersion process is isothermal, thus eliminating the need to solve the temperature equation. The word "flowuv" in line 3 is the file name containing the initial velocity field obtained from the flow field calculation. The "–1" in line 7 requests that direct solver FISSLE be used with subcycling in solving the pressure field, which is often the most cost-effective way to perform a simulation, provided sufficient memory is available for storing the entire decomposed pressure matrix.

PREPIN

```
pbsetup
disp -- SO2 vapor dispersion over a plane and up a ramp
    3   11   14   44    5    2
  293.2     293.2     64.06     617.2     101325.    28.96     1005.     9.806
matprob
  so2
meshgen
mappx
    1   12    1   15    1   14   1.15      1.05      0.95
  0.00      0.00      80.0      80.0      0.00      0.00      80.0      80.0
  0.00      0.00      0.00      0.00      60.0      60.0      60.0      60.0
  0.00      120.      120.      0.00      0.00      120.      120.      0.00
    1   12    1   15   14   22   1.15      1.05      1.05
  80.0      80.0      120.      120.      80.0      80.0      120.      120.
  0.00      0.00      0.00      0.00      60.0      60.0      60.0      60.0
  0.00      120.      120.      0.00      0.00      120.      120.      0.00
    1   12    1   15   22   36   1.15      1.05      1.00
  120.      120.      220.      220.      120.      120.      220.      220.
  0.00      0.00      20.0      20.0      60.0      60.0      60.0      60.0
  0.00      120.      120.      0.00      0.00      120.      120.      0.00
    1   12    1   15   36   45   1.15      1.05      1.05
  220.      220.      300.      300.      220.      220.      300.      300.
  20.0      20.0      20.0      20.0      60.0      60.0      60.0      60.0
  0.00      120.      120.      0.00      0.00      120.      120.      0.00

endms
bcongen
plane k  1
    u  1.0e20
    v  1.0e20
    w  1.0e20
    t  1.0e20
    c  1.0e20

plane i 12
    v  0.000

plane j  1
    w  0.000

plane j 15
    w  0.000

dicos
    1    1    1   15    1   45

plane i  1
    u  0.000

nbcfv
    1    1    1   15    1   45  -0.0057

endbc
mtrxgen
icongen    6
iconc    5  0.1000    0.1000    6.0000    2.0000
  1.0000    80.000    0.0000    0.0000

endic
thisgen
    2    1   22    u    v  rho    c
    2    1   36    u    v  rho    c

callfis
endfile
```

FEM3IN

1	1.	-5	neqs	no. of equations (u,v,w,t,c,qv,ql) to solve
2	2.	0	nds	0 (initco) or data-set no. (in polyplot)
3	3.	flowuv	nflow	file to replace flow field in i.c.
4	4.	0	iccgflg	p solver: 0 (fissle); 1 or 2 (iccg)
5	5.	200	istop	max. no. of iterations for p solution
6	6.	.00001	e3	convergence criterion for p with iccg
7	7.	-1	nsc	subcycling - fissle only; -1 (yes) or 1 (no)
8	8.	120.0	timef	stop time for run
9	9.	0.40	deltcr	max. time step based on stability limits
10	10.	999.	tinjoff	time to turn off source injection
11	11.	1.0	chm	coefficient for hourglass matricies
12	12.	120.0	dtpbcd	output frequency to bcd file (fem3ot)
13	13.	60.0	dtpbin	output frequency to binary file (polyplot)
14	14.	1.0	dtpth	output frequency to time history file (thist)
15	15.	vk	p	optional fields to put in polyplot
16	16.	2	kflg	k-model flag (-2, 0, 1, or 2)
17	17.	0.0688	ustara	friction velocity of the ambient atmosphere
18	18.	35.0	rmol	monin-obukhov length scale
19	19.	0.01	etv	effective energy transfer velocity
20	20.	293.2	tgrd	ambient ground temperature (in kelvin)
21	21.	1.00	hkmin	lower limit of horizontal diffusivities
22	22.	0.05	vkmin	lower limit of vertical diffusivities
23	23.	0.00	csh	coefficient of superheating
24	24.	1	mcflg	mass conservation options (1 or 2)

THIST

```
disp -- SO2 vapor dispersion over a plane and up a ramp
   15

 ' Time'
 ' u   @ 3782'
 ' v   @ 3782'
 ' rho @ 3782'
 ' c   @ 3782'
 ' u   @ 6302'
 ' v   @ 6302'
 ' rho @ 6302'
 ' c   @ 6302'
 ' delt'
 ' qmax'
 ' Tmax'
 ' Tmin'
 ' gmass'
 ' cmass'

   0.0000000E+00
   1.0895880E+00   2.2247604E-03   1.2034792E+00   0.0000000E+00   3.6060890E+00
   3.0942995E-01   1.2007272E+00   0.0000000E+00   4.0000000E-01   3.9167970E+00
   2.0200000E+01   2.0200000E+01   2.2162095E+06   4.8529348E+02

   4.0000000E-01
   1.0891429E+00   2.3258339E-03   1.2034792E+00   0.0000000E+00   3.6059350E+00
   3.0940965E-01   1.2007272E+00   0.0000000E+00   4.0000000E-01   3.9166200E+00
   2.0200000E+01   2.0200000E+01   2.2162095E+06   4.8529348E+02

   8.0000000E-01
   1.0887038E+00   2.4287808E-03   1.2034794E+00   0.0000000E+00   3.6058090E+00
   3.0939700E-01   1.2007272E+00   0.0000000E+00   5.8201197E-01   3.9167035E+00
   2.0200000E+01   2.0200000E+01   2.2162096E+06   4.8529348E+02

   1.2000000E+00
   1.0882602E+00   2.5342363E-03   1.2034794E+00   7.2190783E-09   3.6056841E+00
   3.0938421E-01   1.2007272E+00   0.0000000E+00   5.6452040E-01   3.9167832E+00
   2.0200000E+01   2.0200000E+01   2.2162096E+06   4.8529348E+02

   1.6000000E+00
   1.0878122E+00   2.6418360E-03   1.2034794E+00   3.4069509E-08   3.6055602E+00
   3.0937128E-01   1.2007272E+00   0.0000000E+00   5.4812392E-01   3.9168657E+00
   2.0200000E+01   2.0200000E+01   2.2162096E+06   4.8529348E+02

   2.0000000E+00
   1.0873609E+00   2.7518672E-03   1.2034795E+00   9.9534371E-08   3.6054376E+00
   3.0935817E-01   1.2007272E+00   0.0000000E+00   5.3465632E-01   3.9169510E+00
   2.0200000E+01   2.0200000E+01   2.2162096E+06   4.8529348E+02


   1.1920000E+02
   5.4382352E-01  -3.9015514E-02   1.2340768E+00   2.0978111E-02   3.3531148E+00
   3.0118494E-01   1.2051108E+00   3.0116368E-03   2.5750913E+00   3.9320770E+00
   2.0200000E+01   2.0200000E+01   2.2161633E+06   3.9977752E+02

   1.1960000E+02
   5.4783909E-01  -3.6373755E-02   1.2338267E+00   2.0806612E-02   3.3527160E+00
   3.0106716E-01   1.2051140E+00   3.0138150E-03   8.0000000E-01   3.9262637E+00
   2.0200000E+01   2.0200000E+01   2.2161625E+06   3.9825789E+02

   1.2000000E+02
   5.5200720E-01  -3.3689745E-02   1.2335704E+00   2.0630826E-02   3.3523476E+00
   3.0094824E-01   1.2051174E+00   3.0161608E-03   4.0000000E-01   3.9251004E+00
   2.0200000E+01   2.0200000E+01   2.2161616E+06   3.9673582E+02
```

A sample of the results are presented in Figs. 5.4 through 5.6. Shown in Fig. 5.4 are the fields of SO_2 concentration and velocity projection on the vertical plane of symmetry at the beginning of the dispersion simulation. In Fig. 5.5, the SO_2 concentration contours on the ground surface for two different times are illustrated, which indicate a very wide and ground-hugging cloud. In Fig. 5.6, the time series of concentration at two representative locations, one near the foot of the ramp and the other near the top of the ramp, are displayed. These plots illustrate clearly the persistency of the vapor cloud, in marked contrast to the characteristics normally observed in the dispersal of a neutrally buoyant gas cloud.

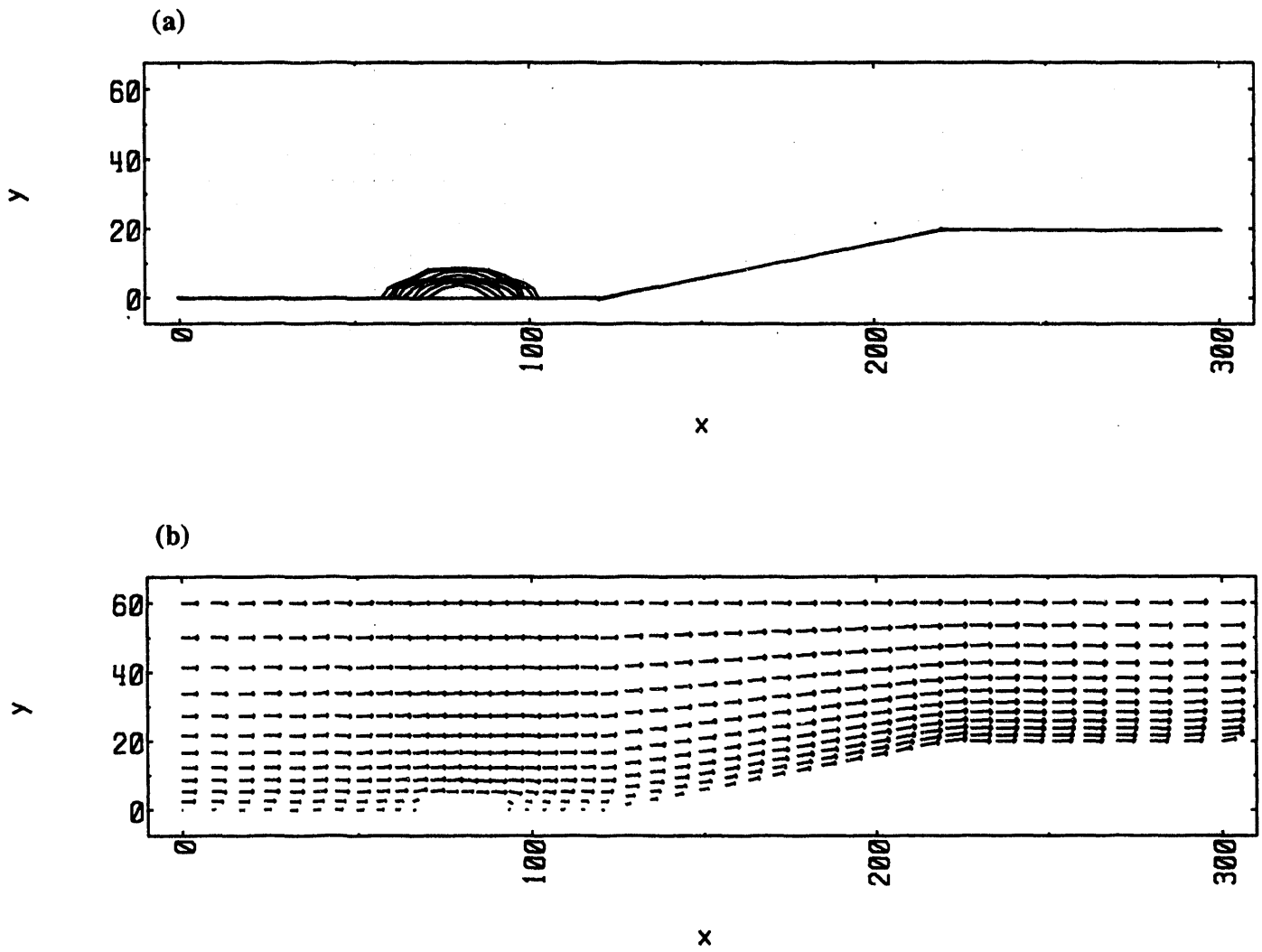

Fig. 5.4 Initial conditions on the plane of symmetry for the SO_2 dispersion simulation over a sloping terrain:
(a) volumetric concentration, and
(b) velocity projection.

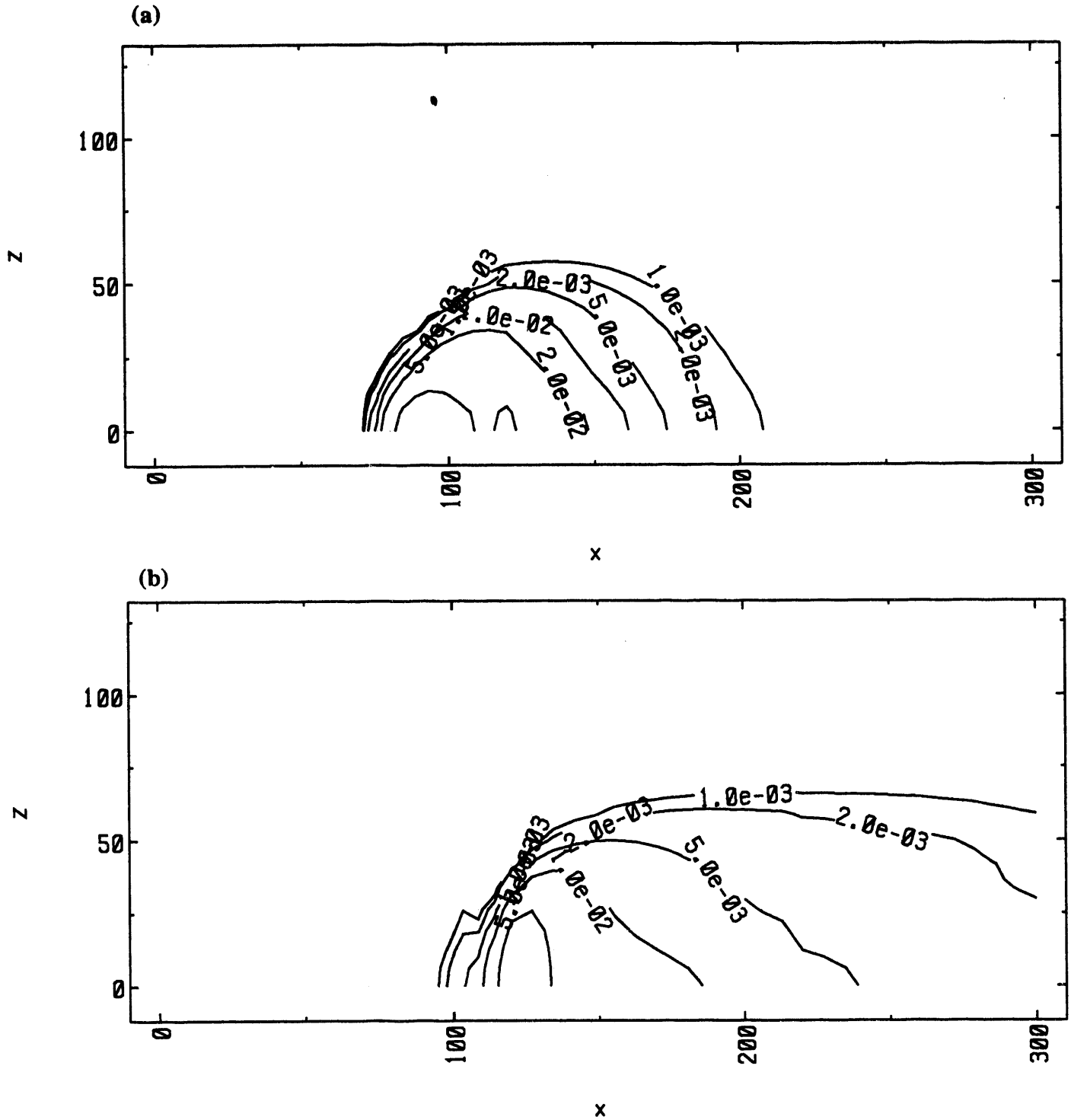

Fig. 5.5 Predicted contours of concentration on the ground surface at two different times:
(a) $t = 60$ s, and
(b) $t = 120$ s.

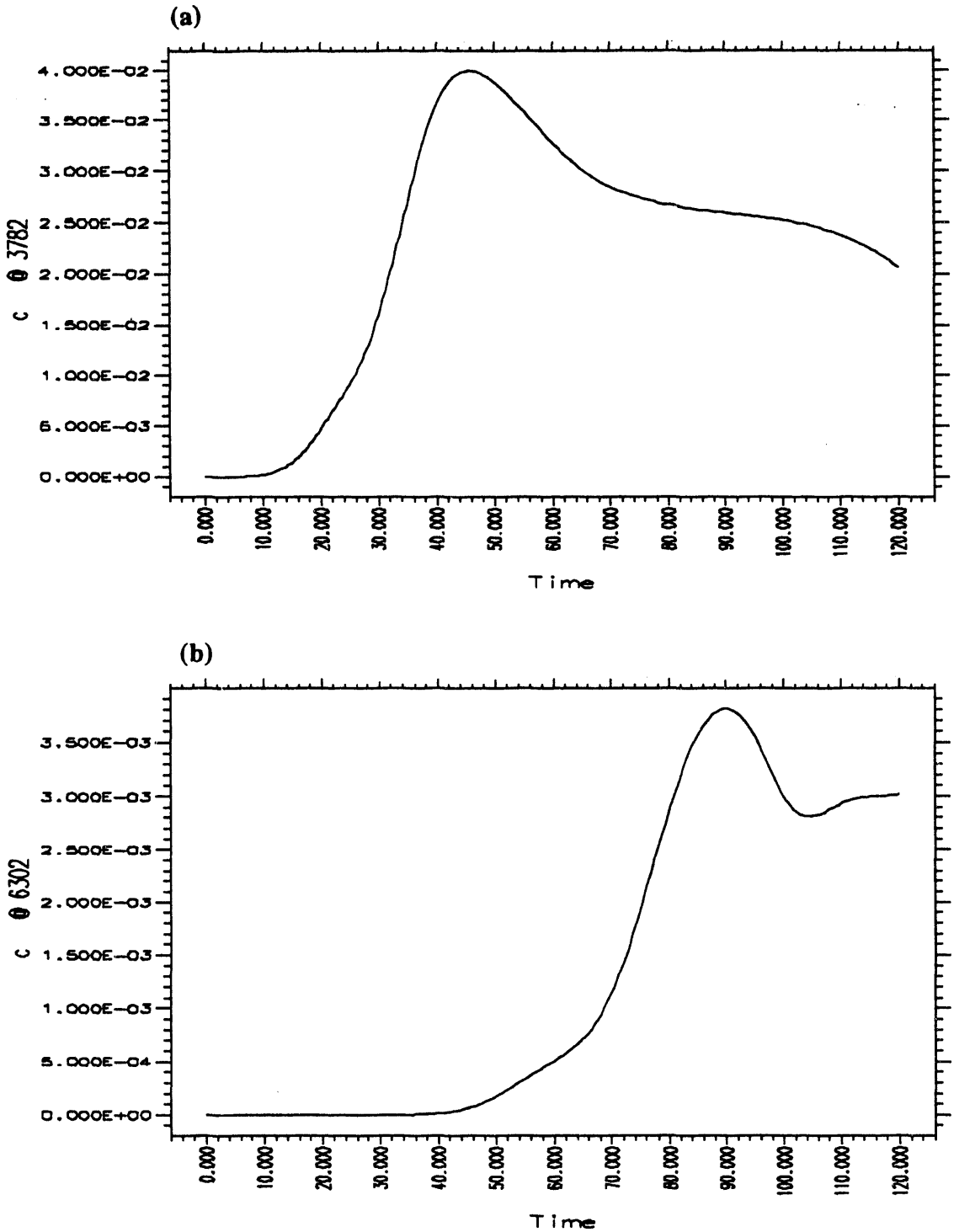

Fig. 5.6 Time series of concentration at two selected locations on the plane of symmetry:
(a) at the foot of the ramp (height = 2.46 m), and
(b) at the top of the ramp (height = 21.64 m).

5.3 Vapor Dispersion Simulation Of An LNG Spill

This example is a simulation of one of the Burro series LNG (liquefied natural gas) vapor dispersion experiments conducted by LLNL in 1980 (Koopman, *et al.*, 1982). The experiment being simulated is Burro-8, a test conducted under very low wind speed and stable atmospheric conditions. During the test, 28 m^3 of LNG was piped onto the spill pond at a rate of 16 m^3/min. The atmospheric conditions include an average wind speed of 1.8 m/s at 2 m height, an estimated friction velocity of 0.074 m/s, a Monin-Obukhov length scale of 16.5 m, and an adiabatic lapse rate of approximately -0.02 °C/m. Unlike the previous cases, the present simulation involves a cryogenic material, for which temperature also plays an important role in the fluid dynamics and dispersion process. Hence, the temperature field is solved in this case concurrently with the pressure and velocity fields.

Listed below are the PREPIN, FEM3IN, and an edited THIST files from the simulation. In this simulation, the ambient velocity profile is assumed to be logarithmic and the vapor cloud is assumed to be symmetric about the vertical plane bisecting the spill area and along the prevailing wind direction, thus allowing only one-half of the vapor cloud to be simulated. The 'digix' option is used to discretize the computational domain into a graded mesh of 8,100 zones. The spilled LNG is modelled as NG vapor going into the computational domain via appropriate boundary conditions. More specifically, vaporized LNG is injected over a source area of 25.6 m by 12.8 m (for one-half of the source) with an injection velocity of 0.13 m/s (defined by lines 53–56 for the vertical velocity and by lines 57–59 for the species equation in the PREPIN file) and over a period of 108 s (see line 10 of FEM3IN). For dispersion simulation involving a cryogenic gas, heat transfer between the ground surface and the gas cloud is also important. Such a process is modelled in FEM3C via a bulk heat transfer submodel and parameterized with an effective heat transfer velocity of 0.0125 m/s (defined by lines 48–52 of PREPIN for the entire bottom boundary except the source area). Because the $k-\varepsilon$ turbulence submodel is being used, the bottom boundary is defined at 0.05 m (see the first entry of line 14 of PREPIN and line 17 of FEM3IN) above the ground surface so that wall functions can be appropriately applied. Lines 45–47 of PREPIN are used to generate the nodal points over which wall functions are being applied. The FEM3IN file is similar to the one used in the previous case except the present case is non-isothermal and the $k-\varepsilon$ turbulence submodel is employed. Again, the necessary replacements for the alternative turbulence submodel (based on similarity functions) is appended at the end of the file, if such a turbulence submodel is desired.

A sample of the simulation results are contained in the edited THIST file and also depicted in two succeeding figures. In Fig. 5.7, concentration contours and velocity projection on the plane 1 m above the ground surface at 120 s after the beginning of spill are displayed. Profound changes of the velocity field, which was originally unidirectional, are apparent. The concentration contours manifest clearly the gravity spreading of the vapor cloud in the lateral and upwind directions. They also show a bifurcated vapor cloud, as evidenced by concentration levels of 0.25 and above. In Fig. 5.8, the predicted time series of concentration and temperature at a downwind location of 60 m from the center of spill are displayed. The predicted results have been compared with experimental data and very good agreement was observed (Chan, 1994).

PREPIN

```
pbsetup
 B8FM -- Burro 8 with flat terrain, k-e model
    3   12   15   45    5    1           -0.02
  306.0     111.0     16.88     2180.    95347.0    28.96     1005.     9.806
meshgen
digix
    1   46    1   13    1   16
 -100.0    -90.00    -80.00    -70.00    -60.00    -50.00    -42.00    -35.00
 -29.00    -24.00    -19.50    -16.00    -12.80    -9.600    -6.400    -3.200
  0.000     3.200     6.400     9.600     12.80     16.00     20.00     25.00
  31.00     38.00     45.00     52.00     60.00     70.00     82.00     95.00
  110.0     125.0     140.0     155.0     170.0     190.0     215.0     240.0
  265.0     290.0     315.0     340.0     370.0     400.0
  0.050     0.300     0.600     1.000     1.500     2.200     3.100     4.200
  5.500     7.000     9.000     11.50     15.00
  0.000     3.200     6.400     9.600     12.80     16.00     20.00     25.00
  32.00     40.00     50.00     60.00     71.00     84.00     100.0     120.0

endms
bcongen
plane i 13
    v    0.000
    w    0.000
    u    1.e+20
    t    1.e+20
    k    1.e+20
    e    1.e+20

subdm
    1   12    1   16    1    1
    v    0.000
    w    0.000
    u    1.e+20
    t    1.e+20
    k    1.e+20
    e    1.e+20
    c    0.000

plane j  1
    w   0.000

plane i  1
    v    0.000

slpbc
    1    1    1   16    1   46

nbcft
    1    1    1   16    1   13  0.0125
    1    1    5   16   13   21  0.0125
    1    1    1   16   21   46  0.0125

subdm
    1    1    1    5   13   21
    v    0.130

nbcfc
    1    1    1    5   13   21   0.130

endbc
icongen
iclog
  0.074     .0002     16.50
icont    1
  0.000     0.000     0.020
endic
thisgen
    4    1   29    t    c
    4    1   35    t    c
    4    1   46    c

mtrxgen
callfis
endfile
```

FEM3IN

```
 1    1.       5  neqs      no. of equations (u,v,w,t,c,qv,ql) to solve
 2    2.       0  nds       0 (initco) or data-set no. (polyplot)
 3    3.  ......  nflow     file to replace flow field in i.c.
 4    4.       0  iccgflg   p solver: 0 (fissle); 1 or 2 (iccg)
 5    5.     200  istop     max. no. of iterations for p solution
 6    6.   .0001  e3        convergence criterion for p with iccg
 7    7.      -1  nsc       subcycling - fissle only; -1 (yes) or 1 (no)
 8    8.   240.0  timef     stop time for run
 9    9.   0.100  deltcr    max. time step based on stability limits
10   10.   108.0  tinjoff   time to turn off source injection
11   11.     2.0  chm       coefficient for hourglass matricies
12   12.   240.0  dtpbcd    output frequency to bcd file (fem3ot)
13   13.    60.0  dtpbin    output frequency to binary file (polyplot)
14   14.     1.0  dtpth     output frequency to time history file (thist)
15   15.    prti  vk   k    optional fields to put in polyplot
16   16.      -2  kflg      k-model flag (-2, 0, 1, or 2)
17   17.    0.05  dyn       distance from boundary to apply wall function
18   18.    2.15  c3        parameter for buoyancy term in e-equation
19   19.    1.00  betah     parameter for anisotropy model
20   20.    306.  tgrd      ambient ground temperature (in kelvin)
21   21.    1.00  hkmin     lower limit of horizontal diffusivities
22   22.    0.01  vkmin     lower limit of vertical diffusivities
23   23.    0.00  csh       coefficient of superheating
24   24.       1  mcflg     mass conservation options     (1 or 2)
25
26
27   15.      vk  ri        optional fields to put in polyplot: ri and p
28   16.       2  kflg      k-model flag (-2, 0, 1, or 2)
29   17.   0.074  ustara    friction velocity of the ambient atmosphere
30   18.   16.50  rmol      monin-obukhov length scale
31   19.   .0125  etv       effective energy transfer velocity
32   20.   306.0  tgrd      ambient ground temperature (in kelvin)
33   21.    1.00  hkmin     lower limit of horizontal diffusivities
34   22.    0.01  vkmin     lower limit of vertical diffusivities
35   23.    0.00  csh       coefficient of superheating
36   24.       1  mcflg     mass conservation options     (1 or 2)
```

THIST

```
B8FM -- Burro 8 with flat terrain, k-e model
  12

' Time'
' t    @ 5828'
' c    @ 5828'
' t    @ 7076'
' c    @ 7076'
' c    @ 9364'
' delt'
' qmax'
' Tmax'
' Tmin'
' gmass'
' cmass'

  0.0000000E+00
  3.3020000E+01   0.0000000E+00   3.3020000E+01   0.0000000E+00   0.0000000E+00
  1.0000000E-01   3.0843344E+00   3.3300000E+01   3.3001000E+01   9.7227365E+05
  0.0000000E+00

  1.0000000E-01
  3.3020008E+01   0.0000000E+00   3.3020008E+01   0.0000000E+00   0.0000000E+00
  1.0000000E-01   3.0843324E+00   3.3300000E+01  -1.0990026E+01   9.7227766E+05
  4.6234635E+00

  2.0000000E-01
  3.3020026E+01   0.0000000E+00   3.3020026E+01   0.0000000E+00   0.0000000E+00
  1.3384039E-01   3.0843344E+00   3.3648183E+01  -4.3871163E+01   9.7228209E+05
  9.2745072E+00

  3.0000000E-01
  3.3020041E+01   0.0000000E+00   3.3020041E+01   0.0000000E+00   0.0000000E+00
  1.5213918E-01   3.0843345E+00   3.4568996E+01  -6.9610245E+01   9.7228686E+05
  1.3951820E+01

  4.0000000E-01
  3.3020057E+01   0.0000000E+00   3.3020057E+01   0.0000000E+00   0.0000000E+00
  1.7328262E-01   3.0843343E+00   3.5531560E+01  -9.0451797E+01   9.7229188E+05
  1.8653493E+01

  5.0000000E-01
  3.3020073E+01   0.0000000E+00   3.3020073E+01   0.0000000E+00   0.0000000E+00
  2.0193935E-01   3.0843293E+00   3.6399596E+01  -1.0775568E+02   9.7229715E+05
  2.3377551E+01

  6.0000000E-01
  3.3020091E+01   0.0000000E+00   3.3020091E+01   0.0000000E+00   0.0000000E+00
  2.3644944E-01   3.0843359E+00   3.7105600E+01  -1.2239750E+02   9.7230263E+05
  2.8122118E+01

  9.0000000E-01
  3.3020152E+01  -2.4248951E-13   3.3020152E+01   0.0000000E+00   0.0000000E+00
  2.7283127E-01   3.0843359E+00   3.8057736E+01  -1.5542107E+02   9.7232027E+05
  4.2454723E+01


  2.3990000E+02
  3.2783724E+01   1.6333357E-03   2.6593144E+01   7.7563322E-02   1.2082569E-02
  2.0000000E-01   3.5072241E+00   3.5737738E+01   2.5392872E+01   9.7055685E+05
  6.1570534E+03

  2.4000000E+02
  3.2778366E+01   1.7256927E-03   2.6594294E+01   7.7627611E-02   1.2127277E-02
  1.0000000E-01   3.5086268E+00   3.5730975E+01   2.5405631E+01   9.7055665E+05
  6.1549846E+03
```

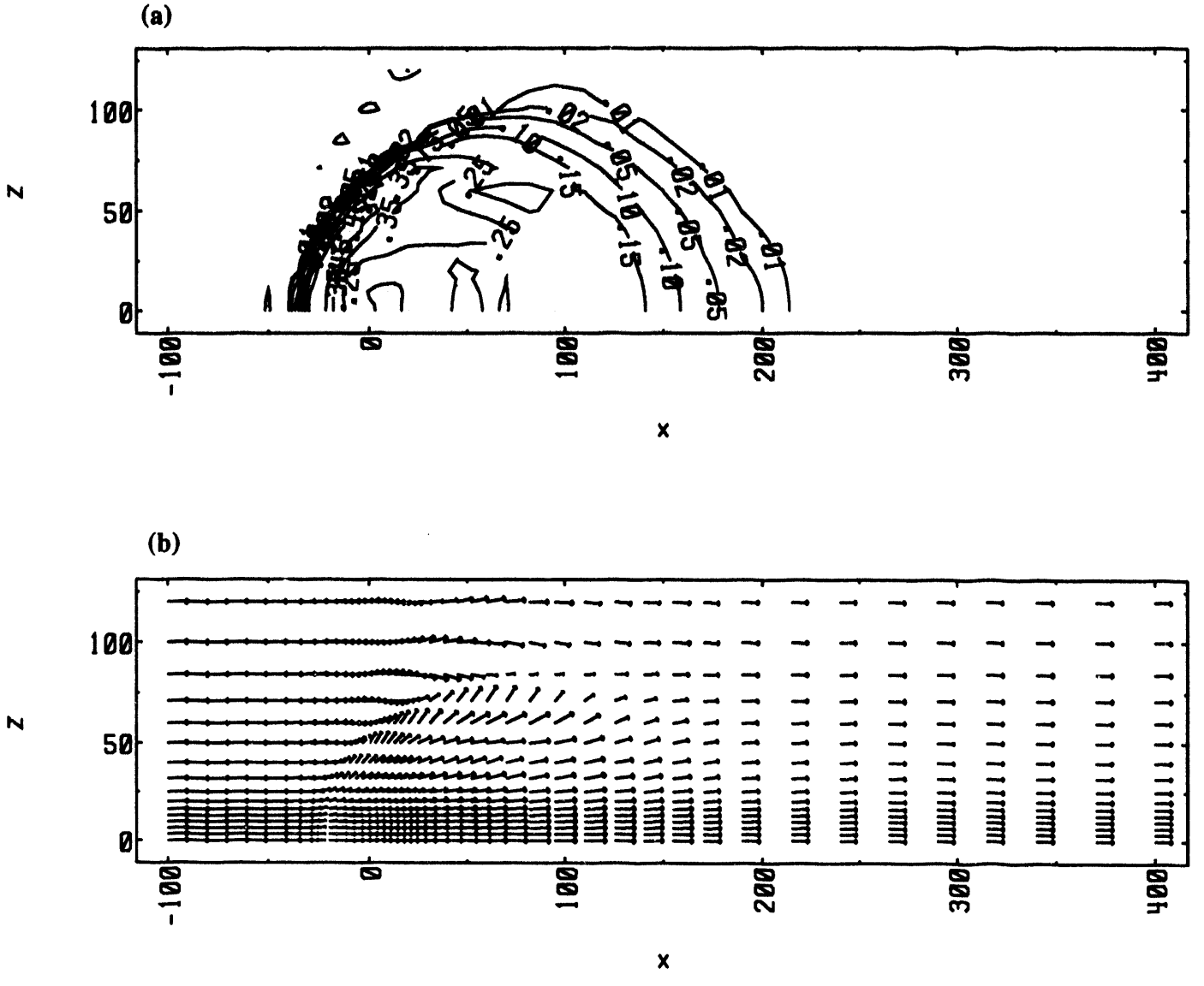

Fig. 5.7 Burro-8 simulated results on the plane 1 m above ground at 120 s after spill starts:
(a) contours of volumetric concentration of NG, and
(b) velocity projection.

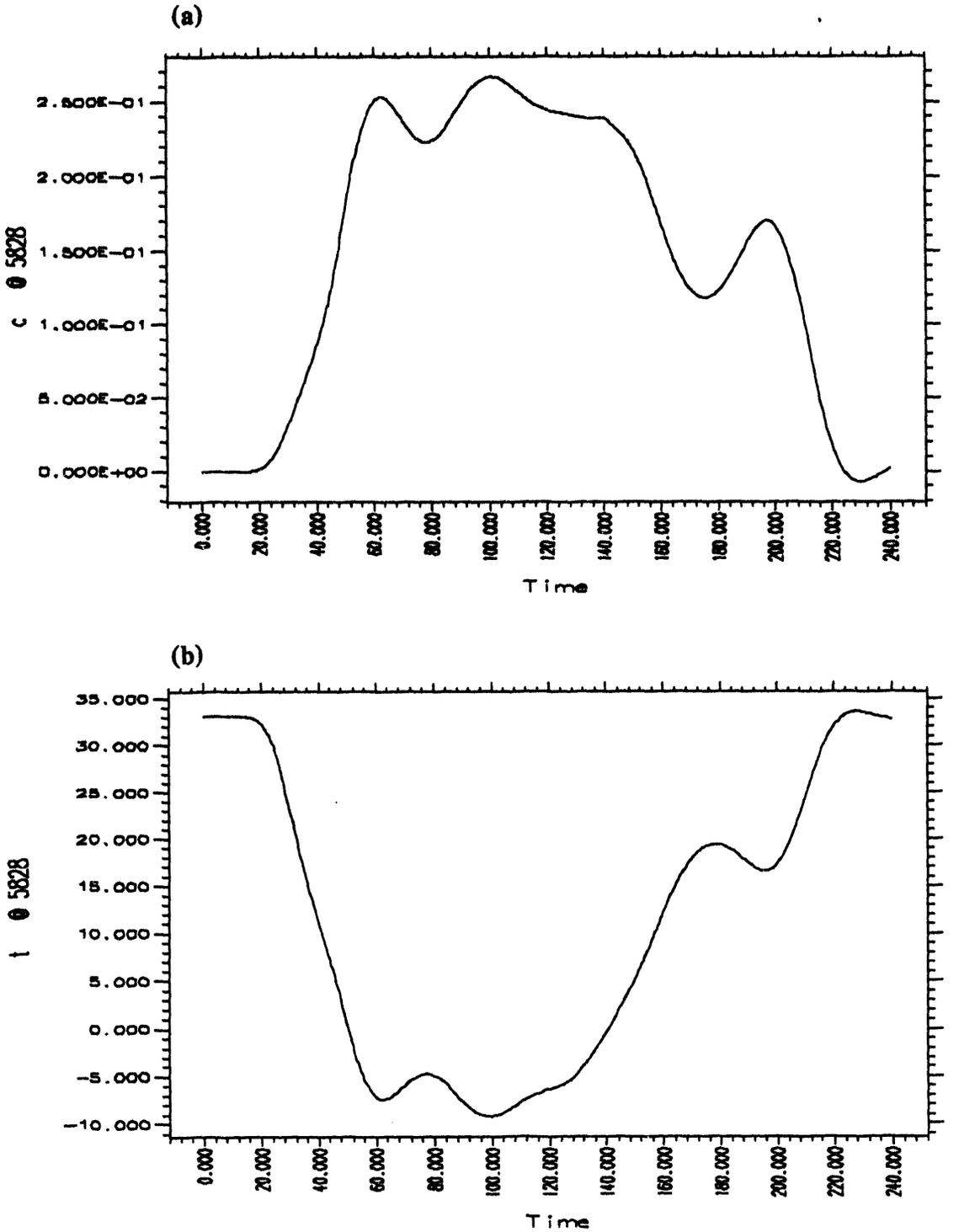

Fig. 5.8 Time series of concentration and temperature at a selected location which is on the cloud center line, 60 m downwind, and 1 m above the ground surface:
(a) volumetric concentration, and
(b) temperature (in °C).

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Appendix A. *Contents of POLYPLOT File*

POLYPLOT is a binary file containing primarily solutions of the field variables at preselected times, which are to be postprocessed graphically by PLOTRDM. Because the graphics library used by PLOTRDM is not readily exportable, the contents of POLYPLOT are described herein for possible adaptation by the user's own postprocessing code. If necessary, the user could tailor the contents of the file to suit his own need by modifying subroutines GRAFOUT and PLOTPARA. Currently POLYPLOT is composed of three parts: a header section containing problem identification, problem size, and labels for graphical output, a section on nodal locations and the connectivity of elements (i.e., nodes connected to each element), and solution of the field variables at preselected times.

The relevant entries of the 64-word header section being used by PLOTRDM are the following:

W(1) through W(10)	=	TITLE, problem identification as given in PREPIN file.
W(15)	=	NFIXV, number of variables whose nodal solution are put in POLYPLOT. These variables may include temperature (T), volumetric fraction of gas species (C), mass fraction of vapor material (q_v), mass fraction of liquid material (q_ℓ), density of the mixture (ρ), and the velocity components (u, v, w).
W(16)	=	NDIM, number of spatial dimensions of the problem (2 for 2-D and 3 for 3-D problems).
W(17)	=	NUMNP, total number of nodal points.
W(24)	-	NUMEL, total number of elements.
W(25)	=	IMAX + 1, number of nodes in the I-direction.
W(26)	=	JMAX + 1, number of nodes in the J-direction.
W(27)	=	KMAX + 1, number of nodes in the K-direction (1 for 2-D problems)
W(28)	=	IJKXYZ, an ASCII word to indicate how the (I, J, K) system is related to the Cartesian coordinate system (x, y, z). For the logical grids presently used, it is "YX" for 2-D problems and "YZX" for 3-D problems.
W(29)	=	NGDS, total number of data sets in POLYPLOT file.
W(30)	=	NVARPN, total number of variables (per node) whose nodal solutions are put in POLYPLOT. The value of NVARPN could be up to four greater than the value of NFIXV for possible inclusion of four optional variables defined in line 15 of the FEM3IN file.
W(35) to W(64)	=	IPVF, array storing the labels for identifying the variables in graphical output.

The middle section of the file starts at word W(65) and contains in its first part the nodal coordinates, i.e., x_1, y_1, [z_1], x_2, y_2, [z_2], ..., x_n, y_n, [z_n], in which items in [ ] are present for 3-D problems only and n is the total number of nodal points. The second part of this section contains the connectivity of elements, namely, {[IX (I, J), I = 1, NPE + 1], J = 1, NUMEL}. The value of NPE is 4 for 2-D problems and is 8 for 3-D problems. The last row of array IX currently has a constant value of "1" to indicate that only linear elements are used.

In the last section, data from preselected times (by input in FEM3IN file) are written into POLYPLOT when they become available. For each data set, the value of time is first written, which is immediately followed by the nodal values of the optional variables, such as p, ri, dos, vk, k, etc. The nodal values of other computed field variables including T (temperature in °C), C(volumetric fraction of species in vapor phase), q_v (mass fraction of vapor material), and q_ℓ (mass fraction of liquid material) are then written (one field variable after another). Finally, the velocity components are written as the last part of a data set.

Appendix B. *Material Properties for Twelve Selected Materials*

Table B1. Coefficients for the Antoine equation given below for twelve selected hazardous materials. The data source is Ref. 1 and the values of the coefficients are such that temperature (T) is in Kelvins and pressure (p_v) is in N/m^2 in

$$\log\ p_v = A - B/\,(T + C)\ .$$

No.	Formula	Name	A	B	C
1	H_2S	hydrogen sulfide	9.1188	768.14	-26.06
2	C_3H_6	propylene	8.9445	785.01	-26.15
3	C_3H_8	propane	8.9546	813.20	-25.16
4	$C\ell_2$	chlorine	9.0567	859.18	-27.01
5	NH_3	ammonia	9.4854	926.14	-32.98
6	$C_2H_3C\ell$	vinyl chloride	8.6220	783.40	-43.15
7	SO_2	sulfur dioxide	9.4072	999.90	-35.97
8	$COC\ell_2$	phosgene	8.9679	941.26	-43.15
9	C_2H_4O	ethylene oxide	9.3950	1115.10	-29.01
10	HF	hydrogen fluoride	9.8101	1478.56	15.06
11	N_2O_4	nitrogen tetroxide	11.0420	1798.54	3.65
12	HCN	hydrogen cyanide	9.2968	1123.00	-37.15

Table B2. Coefficients for the Watson relation below for twelve selected hazardous materials. The data source is Ref. 1 except as noted for the exponents n. The heat of vaporization (λ_v) is in J/kg and the temperature (T) is in Kelvins in

$$\lambda_v = \lambda_{vb}\left(\frac{T_c - T}{T_c - T_b}\right)^n\ .$$

No.	Formula	Name	$\lambda_{vb}x10^{-5}$	T_c	T_b	n[Ref.]
1	H_2S	hydrogen sulfide	5.4755	373.2	212.8	0.374 [2]
2	C_3H_6	propylene	4.3748	365.0	225.4	0.386 [2]
3	C_3H_8	propane	4.2573	369.8	231.1	0.384 [2]
4	$C\ell_2$	chlorine	2.8796	417.	238.7	0.259 [2]
5	NH_3	ammonia	13.7084	405.6	239.7	0.396 [2]
6	$C_2H_3C\ell$	vinyl chloride	3.5621	429.7	259.8	0.38 [1, default]
7	SO_2	sulfur dioxide	3.8893	430.8	263.	0.399 [2]
8	$COC\ell_2$	phosgene	2.4660	455.	280.8	0.38 [1, default]
9	C_2H_4O	ethylene oxide	5.8124	469.	283.5	0.466 [2]
10	HF	hydrogen fluoride	3.3462	461.	292.7	0.01 [3, see note]
11	N_2O_4	nitrogen tetroxide	4.1425	431.4	294.3	0.01 [see note]
12	HCN	hydrogen cyanide	9.3306	456.8	298.9	0.38 [1, default]

Note: The plot in Ref. 3 shows that λ_v first increases and then decreases with temperature in the case of HF; the value of n = 0.01 results in an almost constant value of λ_v near and above the boiling point which is a better approximation than n = 0.38. The value of n = 0.01 for N_2O_4 was selected in analogy to HF.

Table B3. Coefficients for the equation below for the vapor specific heat for twelve selected hazardous materials. The data source is Ref. 1. The specific heat (C_{pv}) is in J/kg and the temperature (T) is in Kelvins in

$$C_{pv} = a_v + b_v T + c_v T^2 + d_v T^3 \ .$$

No.	Formula	Name	a_v	$b_v \times 10^3$	$c_v \times 10^6$	$d_v \times 10^9$
1	H_2S	hydrogen sulfide	936.6	42.12	713.2	-345.0
2	C_3H_6	propylene	88.09	5570.0	-2755.0	523.6
3	C_3H_8	propane	-95.74	6941.0	-3595.0	728.5
4	$C\ell_2$	chlorine	379.5	476.9	-545.3	218.0
5	NH_3	ammonia	1602.7	1398.4	1001.8	-695.2
6	$C_2H_3C\ell$	vinyl chloride	95.13	3229.0	-2456.0	763.2
7	SO_2	sulfur dioxide	372.1	1045.0	-773.9	207.2
8	$COC\ell_2$	phosgene	283.8	1374.7	-1387.8	512.2
9	C_2H_4O	ethylene oxide	-170.76	5041.0	-2850.0	587.9
10	HF	hydrogen fluoride	1451.6	33.02	-101.52	125.06
11	N_2O_4	nitrogen tetroxide	526.4	1050.4	-452.0	6.366
12	HCN	hydrogen cyanide	808.4	2242.0	-1834.5	671.3

Table B4. Coefficients for the equation below for the liquid specific heat for twelve selected hazardous materials. The data sources are indicated by [ ]. The specific heat $(C_{p\ell})$ is in J/kg and the temperature (T) is in Kelvins in

$$C_{p\ell} = a_\ell + b_\ell T + c_\ell T^2 + d_\ell T^3 \ .$$

No.	Formula	Name	a_ℓ	b_ℓ	c_ℓ	d_ℓ
1	H_2S	hydrogen sulfide [3]	2010.	0	0	0
2	C_3H_6	propylene [4]	2180.	0	0	0
3	C_3H_8	propane [4]	2230.	0	0	0
4	$C\ell_2$	chlorine [3]	927.	0	0	0
5	NH_3	ammonia [3] (see note)	7015.	-22.5	0.05	0
6	$C_2H_3C\ell$	vinyl chloride [5]	1170.	0	0	0
7	SO_2	sulfur dioxide [3]	1360.	0	0	0
8	$COC\ell_2$	phosgene [6]	1020.	0	0	0
9	C_2H_4O	ethylene oxide [7]	1970.	0	0	0
10	HF	hydrogen fluoride [3]	2500.	0	0	0
11	N_2O_4	nitrogen tetroxide [8]	1540.	0	0	0
12	HCN	hydrogen cyanide [3]	2620.	0	0	0

Note: The values of a_ℓ, b_ℓ, and c_ℓ for ammonia were fitted to the plot in Ref. 3 for -40°C < T < 40°C.

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Appendix C. *Consistent Units*

The following list provides examples of consistent units for quantities encountered in the use of FEM3C.

Quantity	English	Metric	SI
Length	Foot (ft)	Centimeter (cm)	Meter (m)
Time	Second (s)	Second (s)	Second (s)
Mass	lb_m	Gram (g)	Kilogram (kg)
Force	lb_m -ft/s^2	g-cm/s^2	Newton (N)
Energy	Btu	Calorie (cal)	Joule (J)
Temperature	Fahrenheit (F)	Centigrade (C)	Kelvin (K)
	or Rankin (R)	or Kelvin (K)	
Gravitational acceleration	ft/s^2	cm/s^2	m/s^2
Density	lb_m/ft^3	g/cm^3	kg/m^3
Velocity	ft/s	cm/s	m/s
Stress (pressure)	lb_m/ft-s^2	g/cm-s^2	Pascal (N/m^2)
Viscosity	lb_m/ft-s	g/cm-s	Pascal-s
Specific heat	Btu/lb_m-F	cal/g-C	J/kg-K
Power	Btu/s	cal/s	J/s (W)
Heat flux	Btu/ft^2-s	cal/cm^2-s	J/m^2-s
Heat-transfer coefficient	Btu/ft^2-s-F	cal/cm^2-s-C	J/m^2-s-K
Thermal conductivity	Btu/ft-s-F	cal/cm-s-C	J/m-s-K

Appendix D. *Troubleshooting*

This appendix is intended to assist the user in understanding and dealing with certain errors issued by the model. Discussed below are a number of commonly encountered errors, their meaning, and suggested corrective actions. The first groups of errors are from the preprocessor PREFEM3C and the second group of messages pertain to the main code FEM3C.

No. 1 ierr=xxx from hpalloc.

The code was trying to allocate a block of memory from the heap using the Cray system routine hpalloc and an error code xxx (-1 or -2) was encountered. xxx=-1 means the requested length is not an integer greater than 0; xxx=-2 means no more memory is available from the system.

If xxx=-1, try to determine why the requested length is not positive. Make sure the values of numnp (total number of grid points) and numel (total number of elements) have been generated correctly. If xxx=-2, check and see if the problem is really too big for the system. The problem sometimes can be solved just by decreasing the storage (the value of n1024 on card No. 3) requested for FISSLE. Otherwise, special arrangement might have to be made with the system manager to accommodate a big run.

No. 2 xxxxxxxx is not a valid command.

The input item xxxxxxxx is an unrecognizable command word to the main routine prefem3c.

Make sure the input command word is spelled correctly and is one of the following:

pbsetup, tdmprop, matprob, meshgen, bcongen, icongen, mtrxgen, callfis, thisgen, endfile.

Also, make sure each section under a command has ended properly.

No. 3 xxxxxxxx is not a valid bcongen subcommand.

The input item xxxxxxxx is an unrecognizable subcommand word to the bcongen subroutine.

Make sure the input subcommand word is spelled correctly and is one of the following:

fbcfu, fbcfv, fbcfw, fbcft, fbcfc, fbcqv, fbcql, nbcfu, nbcfv, nbcfw, nbcft, nbcfc, nbcqv, nbcql, fbcfk, fbcfe, nbcfk, nbcfe, dicos, plane, subdm, slpbc, endbc.

Also, make sure each subcommand has been supplemented with appropriate input line(s) and ended properly, e.g., with a blank line.

No. 4 xxxxxxxx is not a valid icongen subcommand.

The input item xxxxxxxx is an unrecognizable subcommand word to the icongen subroutine.

Make sure the input subcommand word is spelled correctly and is one of the following:

iconu, iconv, iconw, icont, iconc, icoqv, icoql, icoqt, iconk, icone, iclog, endic.

Also, make sure each subcommand has been supplemented with appropriate input line(s) and ended properly.

No. 5 xxxxxxxx is not a meshgen subcommand.

The input item xxxxxxxx is an unrecognizable subcommand word to the meshgen subroutine.

Make sure the input subcommand word is spelled correctly and is one of the following:

coord, digix, mappx, terra, endms.

Also, make sure each subcommand has been supplemented with appropriate input line(s) and ended properly, e.g., with a blank line.

No. 6 error in jacobian, xsj=xxxx.

In the above, xxxx is the value of Jacobian evaluated at a Gauss point. This error is issued when the value of xxxx is less than 10^{-12}.

Make sure the coordinate values of the control points for the selected option(s) are entered correctly or, when they are contained in a file such as TERRAIN or COORDS, make sure there is no bad data in the file.

No. 7 error encountered in meshgen-option terra.

The 'terra' option used to generate the coordinates of the mesh points has problem with convergence. This could happen if the topography data contained in TERRAIN file are not read in properly and/or there is error in the vertical coordinates generation card.

Examine the TERRAIN file and make sure data for the bottom topography are correct. Also check and make sure the input values on the vertical coordinates generation card are correct.

No. 8 improper ndop=xxx.

This message is produced by the icongen module when it encounters an inappropriate input value for ndop, which is supposed to be an integer with value between -3 and 5.

Make sure the input value of ndop is correct and confirms to the required format.

No. 9 time history plots exceed limit of 999.

More than 999 variables under 'thisgen' has been requested by the user, which exceed the size of the arrays designated for storing the nodal information and the requested variables.

Delete some of the requested nodes/variables so that the limit is not exceeded, or increase the size of arrays inod and icmp in common block 'this' to accommodate the request.

Once the preprocessor PREFEM3C has been run successfully and input file FEM3IN has been correctly prepared, there is a very good chance that FEM3C will run smoothly to the desired time. However, a number of possibilities still exist which could cause the code to abort. When such a situation arises, an error message is written into the FEM3OT file before the run terminates itself.

No. 1 ierr=xxx from hpalloc.

The code was trying to allocate a block of memory from the heap using the Cray system routine hpalloc and an error code xxx (-1 or -2) was encountered. xxx=-1 means the requested length is not an integer greater than 0; xxx=-2 means no more memory is available from the system.

The case with xxx=-1 normally should not occur because the problem presumably has been set up properly by PREFEM3C. When xxx=-2, selecting either ICCG or DSCG as the pressure solver normally can relieve much of the memory requirements (but at the expense of more CPU cost). If the problem in still too big, make arrangement with the system manager to accommodate your needs.

No. 2 can't open polyplot file.

This message appears if the POLYPLOT file is missing when the run starts. POLYPLOT file is for storing certain calculated results for post-processing and is sometimes used to provide the initial conditions for a restart run.

Make sure the POLYPLOT file is available, or rerun PREFEM3C to generate one, before executing FEM3C.

No. 3 run aborted due to ct*u after mass adjustment is greater than xxxx.

In the above, xxxx is the input value of e3 (line 6 of FEM3IN). This problem may arise if the specified boundary conditions violate global mass conservation.

Examine closely the specified boundary conditions, regarding their locations and specified values and make sure the inflow flux is in balance with the outflow flux.

No. 4 run terminated because velocity is blowing up.

The maximum speed of the run is constantly monitored and when it exceeds a limit, which is currently data-loaded as 100, the code will print out the results for closer examination and stop. The problem is often caused by violating one of the stability limits as the flow evolves.

Re-examine the estimated time step size, and, if necessary, reduce it, e.g., by a factor of two and resubmit the run. For complex problems a few trials may be needed to find a satisfactory time step size to use. However, if the required time step size is getting unreasonably small, for instance below the most conservative estimates using a combination of the largest expected velocity (and diffusivity as well) and the smallest grid size, it may imply the problem is not well-defined, such as inconsistent specifications of boundary conditions and/or errors in specifying the physical properties of the problem.

No. 5 run aborted because of too many iccg iterations.

The iterative solver (ICCG or DSCG) is sometimes used to solve the linear system for the pressure equation and DSCG is always used to solve the linear systems for the momentum and other transport equations. If the number of iterations reaches the value of istop (line 5 of FEM3IN) but the solution fails to satisfy the selected convergence criteria, the code will print out the above message and abort.

Increase the value if istop and retry. Also make sure the value of e3 in line 6 of FEM3IN is adequate but not too small (the required number of iterations usually increases faster than linear with the reduction in e3).

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