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3DFATMIC

Three-Dimensional Subsurface Flow, Fate and Transport of Microbes and Chemicals Model

User's Manual
Version 1.0

3DFATMIC: User's Manual of a Three-Dimensional Subsurface Flow, Fate and Transport of Microbes and Chemicals Model
Version 1.0

by

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DISCLAIMER

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FOREWORD

The U.S. Environmental Protection Agency is charged by Congress with protecting the Nation's land, air, and water resources. Under a mandate of national environmental laws, the Agency strives to formulate and implement actions leading to a compatible balance between human activities and the ability of natural systems to support and nurture life. To meet these mandates, EPA's research program is providing data and technical support for solving environmental problems today and building a science knowledge base necessary to manage our ecological resources wisely, understand how pollutants affect our health, and prevent or reduce environmental risks in the future.

The National Risk Management Research Laboratory is the Agency's center for investigation of technological and management approaches for reducing risks from threats to human health and the environment. The focus of the Laboratory's research program is on methods for the prevention and control of pollution to air, land, water, and subsurface resources; protection of water quality in public water systems; remediation of contaminated sites and ground water, and prevention and control of indoor air pollution. The goal of this research effort is to catalyze development and implementation of innovative, cost-effective environmental technologies; develop scientific and engineering information needed by EPA to support regulatory and policy decisions; and provide technical support and information transfer to ensure effective implementation of environmental regulations and strategies.

Bioremediation is unique among remediation technologies in that it degrades or transforms contaminants through the use, possibly with manipulative enhancement, of indigenous microorganisms. Bioremediation can be used in many ways - degradation on concentrated organic contaminants near their sources, as a secondary remediation strategy following physical or chemical treatment methods, for sequestration of metals through microbially mediated transformation processes, and for remediating large plumes of dilute contaminants that are broadly dispersed in the environment. Thus, bioremediation has the potential to be one of the most cost-effective technologies for dealing with environmental remediation problems. Yet, realistically quantitative predictions and assessments of bioremediation technologies appear lacking. In order to meet the objectives of having a realistic tool for predicting and assessing if a bioremediation technology can be successfully implemented, the 3DFATMIC model has been developed. This numerical model simulates 1) the fate and transport of multiple microbes, electron acceptors, substrates, and nutrients and density-dependent fluid flow in saturated-unsaturated subsurface media under either steady-state or transient conditions; 2) multiple distributed and point sources/sinks as well as boundary sources; and, 3) processes which degrade and transform contaminants, cause the growth and death of microbes, and control the fluid flow.

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ABSTRACT

This document is the user's manual of 3DFATMIC, a 3-Dimensional Subsurface Flow, FAte and Transport of MIcrobes and Chemicals Model using a Lagrangian-Eulerian adapted zooming and peak capturing (LEZOOMPC) algorithm. This 3-dimensional model can completely eliminate peak clipping, spurious oscillation, and numerical diffusion; i.e., solve the advective transport problems exactly, within any prescribed error tolerance, using very large mesh Courant numbers. The size of mesh Courant number is limited only by the accuracy requirement of the Eulerian step. Since this model also includes diffusion zooming in solving diffusion elemental matrix, the accuracy is improved by specifying the number of local subelements in every global element. In other words, the more subelements zoomed in diffusion step, the more accuracy at Eulerian step. To sum up, a better solution with respect to advection transport can be obtained with larger time-step sizes; the time-step sizes are only limited by the accuracy requirement with respect to diffusion/dispersion transport and chemical reaction terms. However, the limitation of time-step size imposed by diffusion/dispersion transport is normally not a very severe restriction.

The model, 3DFATMIC, is designed to obtain the density-dependent fluid velocity field, and to solve the advective-dispersive transport equation coupled with biodegradation and microbial biomass production. Water flow through saturated-unsaturated media and the fate and transport of seven components (one substrate, two electron acceptors, one trace element, and three microbial populations) are modeled. For each specific application, 74 maximal control-integers must be assigned using PARAMETER statements in the MAIN program. In addition, if a user uses different analytical forms of boundary conditions, source/sink strength value functions, and soil property functions from those used in this program, he is instructed to modify subroutines ESSFCT, WSSFCT, VBVFCT, DBVFCT, NBVFCT, CBVFCT, and SPFUNC, respectively. The input data to the program include the control indices, properties of the media either in tabular or analytical form, the geometry in the form of elements and nodes, initial conditions and boundary conditions for flow and transport, and microbe-chemical interaction constants. Principal output includes the spatial distribution of pressure head, total head, moisture content, Darcy velocity component, concentrations, and material fluxes at any desired time step. Fluxes through various types of boundaries are shown in the mass balance table. In addition, diagnostic variables, such as the number of non-convergent nodes and residuals, may be printed, if desired, for debugging purposes.

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1. INTRODUCTION

3DFATMIC (A 3-Dimensional Subsurface Flow, FAte and Transport of MIcrobes and Chemicals Model) can be used to investigate saturated-unsaturated flow alone, contaminant transport alone, combined flow and transport, or the fate and transport of microbes and chemicals in ground-water environment. For the flow module, the Galerkin finite element method is used to discretize the Richards' equation and for the transport module, the hybrid Lagrangian-Eulerian approach with an adapted zooming and peak capturing algorithm is used to discretize the transport equation. This approach can completely eliminate spurious oscillation, numerical dispersion, and peak clipping due to advection transport. Large time-step sizes as well as large spatial-grid sizes can be used and still yield accurate simulations. The only limitation on the size of time steps is the requirement of accuracy with respect to dispersion transport, which does not pose much severe restrictions.

The purpose of this manual is to provide guidance to users of the computer code for their specific applications. Section 2.1 lists the governing equations, initial conditions, and boundary conditions for which 3DFATMIC is designed to solve. Section 2.2 describes the numerical procedure used to simulate the governing equations. Section 2.3 contains the description of all subroutines in 3DFATMIC. Since occasions may arise that require the user to modify the code, this section should help the user to trace the code so the user can make necessary adjustments for individual purposes. Section 3.1 contains the parameter specification. For each application, the user needs to assign 74 maximal control-integers in the MAIN program. Section 3.2 describes the required modification of the code so that one might use a different analytical form of soil property function from the ones used in this report. Section 3.3 describes files required for the execution of 3DFATMIC. Appendix A contains the data input guide that is essential for any specific application.

The users may choose whatever consistent set of units. Units of mass (M), length (L), and time (T) are indicated in the input description.

The special features of 3DFATMIC are its flexibility and versatility in modeling as wide a range of problems as possible. This model can handle: (1) heterogeneous and anisotropic media consisting of as many geologic formations as desired; (2) both spatially distributed and point sources/sinks that are spatially and temporally dependent; (3) the prescribed initial conditions by input or by simulating a steady state version of the system under consideration; (4) the prescribed transient concentration over Dirichlet nodes; (5) time dependent fluxes over Neumann nodes; (6) time dependent total fluxes over Cauchy nodes; (7) variable boundary conditions of evaporation, infiltration, or seepage on the soil-air interface for the flow module and variable boundary conditions of inflow and outflow for the transport module automatically; (8) two options of treating the mass matrix - consistent and lumping; (9) three options (exact relaxation, under- and over-relaxation) for estimating the nonlinear matrix; (10) automatically time step size reset when boundary conditions or sources/sinks changed abruptly; (11) two options, Galerkin weighting or upstream weighting for advection term in transport module; (12) two options for the Lagrangian numerical scheme in transport module, which are enabling and disabling adapted zooming scheme; (13) two options for solving Eulerian step including the enable and disable of diffusion zooming; (14) the mass balance checking over the entire region for every time step; and, (15) modification of program if different conditions are used.

2. DESCRIPTION OF 3DFATMIC MODEL

2.1 Mathematical Statement of 3DFATMIC

3DFATMIC is designed to solve the following system of governing equations, along with initial and boundary conditions, which describe flow and transport through saturated-unsaturated media. The governing equations for flow (detailed derivation shown in Appendix B.), which describes the flow of variable-density fluid, are basically the Richards' equation.

Governing Flow Equation

$$\frac{\rho}{\rho_w}\frac{d\theta}{dh}\frac{\partial h}{\partial t} = \nabla\cdot\left[\mathbf{K_s}K_r\cdot(\nabla h + \frac{\rho}{\rho_w}\nabla z)\right] + \frac{\rho^*}{\rho_w}q(\text{or } -\frac{\rho}{\rho_w}q) \qquad (2.1)$$

The saturated hydraulic conductivity $\mathbf{K_s}$ is given by

$$\mathbf{K_s} = \mathbf{K_{sw}}\frac{(\rho/\rho_w)}{(\mu/\mu_w)} \qquad (2.2a)$$

where h is the referenced pressure head defined as $p/\rho_w g$ in which p is pressure (M/LT^2), t is time (T), $\mathbf{K_s}$ is the saturated hydraulic conductivity tensor (L/T), K_r is the relative hydraulic conductivity or relative permeability, z is the potential head (L), q is the source and/or sink (L^3/T), and θ is the moisture content, ρ and μ are the density (M/L^3) and dynamic viscosity (M/LT) at microbial concentrations C_1, C_2, C_3, and chemical concentrations C_s, C_o, C_n, and C_p (M/L^3); and $\mathbf{K_{sw}}$, ρ_w and μ_w are the referenced saturated hydraulic conductivity tensor, density, and dynamic viscosity, respectively. The strength of the source/sink is the discharge or withdraw flow rate q, and ρ^* is the density of the injected fluid. These referenced values are usually taken as the saturated hydraulic conductivity at zero microbial and chemical concentrations. The density and dynamic viscosity of fluid are functions of microbial and chemical concentrations and are assumed to take the following form

$$\frac{\rho}{\rho_w} = 1 + \sum_i \left(\frac{1}{\rho_w} - \frac{1}{\rho_i} \right) C_i; \quad i = 1,\ 2,\ 3,\ s,\ o,\ n,\ p \tag{2.2b}$$

$$\frac{\mu}{\mu_w} = 1 + \beta_s C_s + \beta_o C_o + \beta_n C_n + \beta_p C_p + \beta_1 C_1 + \beta_2 C_2 + \beta_3 C_3 \tag{2.2c}$$

where C_s and ρ_s are dissolved concentration and intrinsic density of substrate, respectively (M/L^3); C_o and ρ_o are dissolved concentration and intrinsic density of oxygen (M/L^3), respectively; C_n and ρ_n are dissolved concentration and intrinsic density of nitrate (M/L^3), respectively; C_p and ρ_p are dissolved concentration and intrinsic density of nutrient (M/L^3), respectively; C_1 and ρ_1 are dissolved concentration and intrinsic density of microbe #1 (M/L^3), respectively; C_2 and ρ_2 are dissolved concentration and intrinsic density of microbe #2 (M/L^3), respectively; C_3 and ρ_3 are dissolved concentration and intrinsic density of microbe #3 (M/L^3), respectively; and β_s, β_o, β_n, β_p, β_1, β_2, and β_3 are viscosity-effecting factor of associated species (L^3/M). It is assumed that microbe #1 utilizes substrate under aerobic conditions, microbe #2 utilizes substrate under anaerobic conditions, and microbe #3 utilizes substrate under both aerobic and anaerobic conditions.

The Darcy velocity is calculated as follows:

$$\mathbf{V} = -\mathbf{K_s} K_r \cdot \left(\frac{\rho_w}{\rho} \nabla h + \nabla z \right) \tag{2.3}$$

Initial Conditions for Flow Equation

$$h = h_i(x, y, z) \qquad \text{in } R \tag{2.4}$$

where R is the region of interest and h_i is the prescribed initial condition, which can be obtained by either field measurement or by solving the steady-state version of Eq.(2.1).

Boundary Conditions for Flow Equation

Dirichlet Conditions:

$$h = h_d(x_b, y_b, z_b, t) \qquad \text{on } B_d \tag{2.5}$$

Neumann Conditions (gradient condition) :

$$-\mathbf{n}\cdot\mathbf{K}_s K_r \cdot \frac{\rho_w}{\rho}\nabla h = q_n(x_b, y_b, z_b, t) \qquad \text{on } B_n \tag{2.6}$$

Cauchy Conditions (flux condition) :

$$-\mathbf{n}\cdot\mathbf{K}_s K_r \cdot \left(\frac{\rho_w}{\rho}\nabla h + \nabla z\right) = q_c(x_b, y_b, z_b, t) \qquad \text{on } B_c \tag{2.7}$$

Variable Conditions - During Precipitation Period:

$$h = h_p(x_b, y_b, z_b, t) \quad \textit{iff} \quad -\mathbf{n}\cdot\mathbf{K}_s K_r \cdot \left(\frac{\rho_w}{\rho}\nabla h + \nabla z\right) \geq q_p \qquad \text{on } B_v \tag{2.8a}$$

or

$$-\mathbf{n}\cdot\mathbf{K}_s K_r \cdot \left(\frac{\rho_w}{\rho}\nabla h + \nabla z\right) = q_p(x_b, y_b, z_b, t) \quad \textit{iff} \quad h \leq h_p \qquad \text{on } B_v \tag{2.8b}$$

Variable Conditions - During Non-precipitation period:

$$h = h_p(x_b, y_b, z_b, t) \quad \textit{iff} \quad \mathbf{n}\cdot\mathbf{K}_s K_r \cdot \left(\frac{\rho_w}{\rho}\nabla h + \nabla z\right) \geq 0 \qquad \text{on } B_v \tag{2.8c}$$

or

$$h = h_m(x_b, y_b, z_b, t) \quad \textit{iff} \quad \mathbf{n}\cdot\mathbf{K}_s K_r \cdot \left(\frac{\rho_w}{\rho}\nabla h + \nabla z\right) \leq q_e \qquad \text{on } B_v \tag{2.8d}$$

or

$$-\mathbf{n}\cdot\mathbf{K}_s K_r \cdot \left(\frac{\rho_w}{\rho}\nabla h + \nabla z\right) = q_e(x_b, y_b, z_b, t) \quad \textit{iff} \quad h \geq h_m \qquad \text{on } B_v \tag{2.8e}$$

where (x_b, y_b, z_b) is the spatial coordinate on the boundary; **n** is an outward unit vector normal to the boundary; h_d, q_n, and q_c are the prescribed Dirichlet functional value, Neumann flux, and Cauchy flux, respectively; B_d, B_n, and B_c are the Dirichlet, Neumann, and Cauchy boundaries, respectively; B_v is the variable boundary; h_p is the allowed ponding depth and q_p is the throughfall of precipitation on the variable boundary; h_m is the allowed minimum pressure, and q_e is the allowed maximum evaporation rate on the variable boundary, which is the potential evaporation.

Only one of Eqs. (2.8a) through (2.8e) is used at any point on the variable boundary at any time. It normally occurs at air-soil interface. During precipitation period, it is assumed that only seepage or infiltration can occur for any point on the air-soil interface. No evapotranspiration is allowed. If seepage happens, the Dirichlet boundary condition, Eq. (2.8a), must be imposed. On the other hand, if infiltration occurs, either the Dirichlet boundary condition, Eq. (2.8a), or the Cauchy boundary condition, Eq. (2.8b), may be specified depending on the soil property and throughfall rate q_p in Eq. (2.8b). The problem is which equation, Eq. (2.8a) or Eq. (2.8b), should be prescribed for a point on the boundary. This problem is settled by iteration. The procedure adopted is as follows. At each iteration, the solution is examined at each node along the variable boundary and test whether the existing boundary condition is still consistent. Specifically, if the existing condition is Eq. (2.8b) (Cauchy boundary condition), the pressure head at the boundary node is computed. If the head is greater than the allowed ponding depth h_p in Eq. (2.8a), too much water has been forced into the region through the node. In other words, the throughfall rate is greater than that which the media can absorb. To account for this, the boundary condition is changed to Eq. (2.8a), which in practice should result in infiltration at a rate less than that q_p in Eq. (2.8b) or result in seepage. If the computed head is less than the ponding depth, the media is capable of absorbing all throughfall and no change of boundary condition is required. On the other hand, if the existing boundary condition is Eq. (2.8a) (Dirichlet boundary condition), Darcy's flux at the node is computed. If the computed Darcy's flux is going out of the region (seepage) or into the region (infiltration) but its magnitude is less than q_p in Eq. (2.8b), no change of boundary condition is needed. However, if the computed Darcy's flux is directed into the region (infiltration) with a rate greater than the throughfall rate q_p, a change of boundary condition to Eq. (2.8b) is required since Eq. (2.8a) would force more water than available into the region. By changing the boundary condition to Eq. (2.8b), it should in practice result in a pressure head less than h_p. The iteration outlined above is discontinued when no change-over of boundary condition is encountered along the entire boundary.

Similarly, during non-precipitation period, it is assumed that only evapotranspiration or seepage can occur and no infiltration is allowed. If seepage actually occurs at a node, Eq. (2.8c) (Dirichlet boundary condition) must be specified at the node. On the other hand, if evapotranspiration happens, either Eq. (2.8d) (Dirichlet boundary condition) or Eq. (2.8e) (Cauchy boundary condition) may be imposed at the node. The problem is again to determine which of the three equations should be used as boundary conditions. Iteration procedure is used to solve the problem. If the existing boundary condition is Eq. (2.8c), the Darcy's flux is calculated. When the computed Darcy's flux is going out of the region, the existing boundary condition is consistent and no change on boundary condition is necessary. When the Darcy's flux is directed into the region (remember no infiltration is allowed), the application of Eq. (2.8c) implies the infiltration and prohibits evapotranspiration. Hence, the boundary condition is changed to Eq. (2.8e), which in practice would generate evapotranspiration and would result in a pressure head lower than the ponding depth in Eq. (2.8c). If the existing boundary condition is Eq. (2.8d), the Darcy's flux is computed. Since the minimum pressure is prescribed on the boundary, it is unlikely that this computed Darcy's flux will be directed into the region. Thus, when the computed outgoing Darcy's flux is less than q_e in Eq. (2.8e), the existing boundary condition is consistent and no change on boundary condition is needed. When the computed Darcy's flux is greater than q_e in Eq. (2.8e), the application of Eq. (2.8d) implies the imposition of too much suction at the node. Hence, the boundary condition is changed to Eq. (2.8e), which in practice should result in a pressure greater than h_m in Eq. (2.8d). If the existing boundary condition is Eq. (2.8e), pressure head at the node is calculated. If this computed pressure head is not lower than h_m in Eq. (2.8d), the boundary condition is consistent and no change is required. However, if the computed head is lower than h_m in Eq. (2.8d), the application of Eq. (2.8e) implies too much water is removed through the node yielding a too low pressure head. Hence, the boundary condition is changed to Eq. (2.8d), which should yield an evapotranspiration rate less than q_e in Eq. (2.8e). This iteration process is completed only when consistent boundary conditions have been applied to all nodes on the variable boundary.

The governing equations for transport are derived based on the continuity of mass and flux laws. The major processes are advection, dispersion/diffusion, adsorption, decay, source/sink, and microbial-chemical interactions.

Governing Equations for Transport

Transport of the carbonaceous substrate, oxygen, nitrate, and nutrient in the bulk pore fluid is expressed by advection-dispersion equations coupling sink terms that account for biodegradation. The four nonlinear transport and fate equations are (derivation shown in Appendix B)

$$\underbrace{\left(\theta+\rho_b K_{ds}\right)\frac{\partial C_s}{\partial t}}_{(1)} + \underbrace{\mathbf{V}\cdot\nabla C_s}_{(2)} = \underbrace{\nabla\cdot\theta\mathbf{D}\cdot\nabla C_s}_{(3)} - \underbrace{\Lambda_s(\theta+\rho_b K_{ds})C_s}_{(4)} + \underbrace{q_{in}C_{sin}}_{(5)} + \underbrace{\left(\frac{\rho_w}{\rho}\mathbf{V}\cdot\nabla(\frac{\rho}{\rho_w}) - \frac{\rho^*}{\rho}q_{in}\right)C_s}_{(6)}$$

$$- \underbrace{\left[\left(\theta+\rho_b K_{d1}\right)C_1\right]\left\{\frac{\mu_o^{(1)}}{Y_o^{(1)}}\left[\frac{C_s}{K_{so}^{(1)}+C_s}\right]\left[\frac{C_o}{K_o^{(1)}+C_o}\right]\left[\frac{C_p}{K_{po}^{(1)}+C_p}\right]\right\}}_{(7)}$$

$$- \underbrace{\left[\left(\theta+\rho_b K_{d2}\right)C_2\right]\left\{\frac{\mu_n^{(2)}}{Y_n^{(2)}}\left[\frac{C_s}{K_{sn}^{(2)}+C_s}\right]\left[\frac{C_n}{K_n^{(2)}+C_n}\right]\left[\frac{C_p}{K_{pn}^{(2)}+C_p}\right]\right\}}_{(8)} \qquad (2.9)$$

$$-\left[\left(\theta+\rho_b K_{d3}\right)C_3\right]\left\{\begin{array}{l}\underbrace{\frac{\mu_o^{(3)}}{Y_o^{(3)}}\left[\frac{C_s}{K_{so}^{(3)}+C_s}\right]\left[\frac{C_o}{K_o^{(3)}+C_o}\right]\left[\frac{C_p}{K_{po}^{(3)}+C_p}\right]}_{(9)} \\ + \underbrace{\frac{\mu_n^{(3)}}{Y_n^{(3)}}\left[\frac{C_s}{K_{sn}^{(3)}+C_s}\right]\left[\frac{C_n}{K_n^{(3)}+C_n}\right]\left[\frac{C_p}{K_{pn}^{(3)}+C_p}\right]I(C_o)}_{(10)}\end{array}\right\}$$

$$\underset{(1)}{\left(\theta+\rho_b K_{do}\right)\frac{\partial C_o}{\partial t}} \;+\; \underset{(2)}{\mathbf{V}\cdot\nabla C_o} \;=\; \underset{(3)}{\nabla\cdot\theta\mathbf{D}\cdot\nabla C_o} \;-\; \underset{(4)}{\Lambda_o(\theta+\rho_b K_{do})C_o} \;+\; \underset{(5)}{q_{in}C_{oin}} \;+\; \underset{(6)}{\left(\frac{\rho_w}{\rho}\mathbf{V}\cdot\nabla(\frac{\rho}{\rho_w})-\frac{\rho^*}{\rho}q_{in}\right)C_o}$$

$$-\left[\left(\theta+\rho_b K_{d1}\right)C_1\right]\left\{\underset{(7)}{\gamma_o^{(1)}\mu_o^{(1)}\left[\frac{C_s}{K_{so}^{(1)}+C_s}\right]\left[\frac{C_o}{K_o^{(1)}+C_o}\right]\left[\frac{C_p}{K_{po}^{(1)}+C_p}\right]} \;+\; \underset{(8)}{\alpha_o^{(1)}\lambda_o^{(1)}\left[\frac{C_o}{\Gamma_o^{(1)}+C_o}\right]}\right\} \qquad (2.10)$$

$$-\left[\left(\theta+\rho_b K_{d3}\right)C_3\right]\left\{\underset{(9)}{\gamma_o^{(3)}\mu_o^{(3)}\left[\frac{C_s}{K_{so}^{(3)}+C_s}\right]\left[\frac{C_o}{K_o^{(3)}+C_o}\right]\left[\frac{C_p}{K_{po}^{(3)}+C_p}\right]} \;+\; \underset{(10)}{\alpha_o^{(3)}\lambda_o^{(3)}\left[\frac{C_o}{\Gamma_o^{(3)}+C_o}\right]}\right\}$$

$$\underset{(1)}{\left(\theta+\rho_b K_{dn}\right)\frac{\partial C_n}{\partial t}} \;+\; \underset{(2)}{\mathbf{V}\cdot\nabla C_n} \;=\; \underset{(3)}{\nabla\cdot\theta\mathbf{D}\cdot\nabla C_n} \;-\; \underset{(4)}{\Lambda_n(\theta+\rho_b K_{dn})C_n} \;+\; \underset{(5)}{q_{in}C_{nin}} \;+\; \underset{(6)}{\left(\frac{\rho_w}{\rho}\mathbf{V}\cdot\nabla(\frac{\rho}{\rho_w})-\frac{\rho^*}{\rho}q_{in}\right)C_r}$$

$$-\left[\left(\theta+\rho_b K_{d2}\right)C_2\right]\left\{\underset{(7)}{\gamma_n^{(2)}\mu_n^{(2)}\left[\frac{C_s}{K_{sn}^{(2)}+C_s}\right]\left[\frac{C_n}{K_n^{(2)}+C_n}\right]\left[\frac{C_p}{K_{pn}^{(2)}+C_p}\right]} \;+\; \underset{(8)}{\alpha_n^{(2)}\lambda_n^{(2)}\left[\frac{C_n}{\Gamma_n^{(2)}+C_n}\right]}\right\} \qquad (2.11)$$

$$-\left[\left(\theta+\rho_b K_{d3}\right)C_3\right]\left\{\underset{(9)}{\gamma_n^{(3)}\mu_n^{(3)}\left[\frac{C_s}{K_{sn}^{(3)}+C_s}\right]\left[\frac{C_n}{K_n^{(3)}+C_n}\right]\left[\frac{C_p}{K_{pn}^{(3)}+C_p}\right]} \;+\; \underset{(10)}{\alpha_n^{(3)}\lambda_n^{(3)}\left[\frac{C_n}{\Gamma_n^{(3)}+C_n}\right]}\right\}$$

$$\underbrace{(\theta+\rho_b K_{dp})\frac{\partial C_p}{\partial t}}_{(1)} + \underbrace{\mathbf{V}\cdot\nabla C_p}_{(2)} = \underbrace{\nabla\cdot\theta\mathbf{D}\cdot\nabla C_p}_{(3)} - \underbrace{\Lambda_p(\theta+\rho_b K_{dp})C_p}_{(4)} + \underbrace{q_{in}C_{pin}}_{(5)} + \underbrace{\left(\frac{\rho_w}{\rho}\mathbf{V}\cdot\nabla(\frac{\rho}{\rho_w}) - \frac{\rho^*}{\rho}q_{in}\right)C_p}_{(6)}$$

$$- \underbrace{\left[(\theta+\rho_b K_{d1})C_1\right]\left\{\epsilon_o^{(1)}\frac{\mu_o^{(1)}}{Y_o^{(1)}}\left[\frac{C_s}{K_{so}^{(1)}+C_s}\right]\left[\frac{C_o}{K_o^{(1)}+C_o}\right]\left[\frac{C_p}{K_{po}^{(1)}+C_p}\right]\right\}}_{(7)}$$

$$- \underbrace{\left[(\theta+\rho_b K_{d2})C_2\right]\left\{\epsilon_n^{(2)}\frac{\mu_n^{(2)}}{Y_n^{(2)}}\left[\frac{C_s}{K_{sn}^{(2)}+C_s}\right]\left[\frac{C_n}{K_n^{(2)}+C_n}\right]\left[\frac{C_p}{K_{pn}^{(2)}+C_p}\right]\right\}}_{(8)} \qquad (2.12)$$

$$- \left[(\theta+\rho_b K_{d3})C_3\right]\left\{\begin{array}{l} \underbrace{\epsilon_o^{(3)}\frac{\mu_o^{(3)}}{Y_o^{(3)}}\left[\frac{C_s}{K_{so}^{(3)}+C_s}\right]\left[\frac{C_o}{K_o^{(3)}+C_o}\right]\left[\frac{C_p}{K_{po}^{(3)}+C_p}\right]}_{(9)} \\ + \underbrace{\epsilon_n^{(3)}\frac{\mu_n^{(3)}}{Y_n^{(3)}}\left[\frac{C_s}{K_{sn}^{(3)}+C_s}\right]\left[\frac{C_n}{K_n^{(3)}+C_n}\right]\left[\frac{C_p}{K_{pn}^{(3)}+C_p}\right]I(C_o)}_{(10)} \end{array}\right\}$$

The transport equations for the three microbes are

$$\underbrace{(\theta+\rho_b K_{d1})\frac{\partial C_1}{\partial t}}_{(1)} + \underbrace{\mathbf{V}\cdot\nabla C_1}_{(2)} = \underbrace{\nabla\cdot\theta\mathbf{D}\cdot\nabla C_1}_{(3)} - \underbrace{\Lambda_1(\theta+\rho_b K_{d1})C_1}_{(4)} + \underbrace{q_{in}C_{1in}}_{(5)} + \underbrace{\left(\frac{\rho_w}{\rho}\mathbf{V}\cdot\nabla(\frac{\rho}{\rho_w}) - \frac{\rho^*}{\rho}q_{in}\right)C_1}_{(6)}$$

$$+ \underbrace{(\theta+\rho_b K_{d1})C_1}\left\{\underbrace{\mu_o^{(1)}\left[\frac{C_s}{K_{so}^{(1)}+C_s}\right]\left[\frac{C_o}{K_o^{(1)}+C_o}\right]\left[\frac{C_p}{K_{po}^{(1)}+C_p}\right]}_{(7)} - \underbrace{\lambda_o^{(1)}}_{(8)}\right\} \qquad (2.13)$$

$$\underset{(1)}{\left(\theta+\rho_b K_{d2}\right)\frac{\partial C_2}{\partial t}} + \underset{(2)}{\mathbf{V}\cdot\nabla C_2} = \underset{(3)}{\nabla\cdot\theta\mathbf{D}\cdot\nabla C_2} - \underset{(4)}{\Lambda_2(\theta+\rho_b K_{d2})C_2} + \underset{(5)}{q_{in}C_{2in}} + \underset{(6)}{\left(\frac{\rho_w}{\rho}\mathbf{V}\cdot\nabla(\frac{\rho}{\rho_w}) - \frac{\rho^*}{\rho}q_{in}\right)C_2}$$

$$+\left(\theta+\rho_b K_{d2}\right)C_2\left\{\underset{(7)}{\mu_n^{(2)}\left[\frac{C_s}{K_{sn}^{(2)}+C_s}\right]\left[\frac{C_n}{K_n^{(2)}+C_n}\right]\left[\frac{C_p}{K_{pn}^{(2)}+C_p}\right]} - \underset{(8)}{\lambda_n^{(2)}}\right\} \tag{2.14}$$

$$\underset{(1)}{\left(\theta+\rho_b K_{d3}\right)\frac{\partial C_3}{\partial t}} + \underset{(2)}{\mathbf{V}\cdot\nabla C_3} = \underset{(3)}{\nabla\cdot\theta\mathbf{D}\cdot\nabla C_3} - \underset{(4)}{\Lambda_3(\theta+\rho_b K_{d3})C_3} + \underset{(5)}{q_{in}C_{3in}} + \underset{(6)}{\left(\frac{\rho_w}{\rho}\mathbf{V}\cdot\nabla(\frac{\rho}{\rho_w}) - \frac{\rho^*}{\rho}q_{in}\right)C_3}$$

$$+\left(\theta+\rho_b K_{d3}\right)C_3\left\{\begin{array}{l}\underset{(7)}{\mu_o^{(3)}\left[\frac{C_s}{K_{so}^{(3)}+C_s}\right]\left[\frac{C_o}{K_o^{(3)}+C_o}\right]\left[\frac{C_p}{K_{pn}^{(3)}+C_p}\right]} - \underset{(8)}{\lambda_o^{(3)}} \\ + \underset{(9)}{\mu_n^{(3)}\left[\frac{C_s}{K_{sn}^{(3)}+C_s}\right]\left[\frac{C_n}{K_n^{(3)}+C_n}\right]\left[\frac{C_p}{K_{pn}^{(3)}+C_p}\right]I(C_o)} - \underset{(10)}{\lambda_n^{(3)}I(C_o)}\end{array}\right\} \tag{2.15}$$

where θ is the moisture content, ρ_b is the bulk density of the medium (M/L^3), t is time, **V** is the discharge (L/T), ∇ is the del operator, **D** is the dispersion coefficient tensor (L^2/T). The Λ_s, Λ_o, Λ_p, Λ_n, Λ_1, Λ_2, Λ_3 and K_{ds}, K_{do}, K_{dn}, K_{dp}, K_{d1}, K_{d2}, K_{d3} are transformation rate constants and distribution coefficients of dissolved substrate, oxygen, nitrate, nutrient, microbe #1, microbe #2, and microbe #3, respectively; q_{in} is the source rate of water; and $C_{sin,}$ $C_{oin,}$ $C_{nin,}$ $C_{pin,}$ $C_{1in,}$ $C_{2in,}$ and $C_{3in,}$ are the concentrations of substrate, oxygen, nitrogen, nutrient, microbe #1, microbe #2 and microbe #3 in the source, respectively.

In each of Eqs. (2.9) through (2.15), term (1) represents the rate of material increase per unit medium volume, term (2) is the rate of transport by advection, term (3) is the rate of transport by dispersion-diffusion, term (4) represents the rate of first order transformation, term (5) is due to the rate of artificial injection, and term (6) is the rate due to the rewriting of the transport equation from conservative form to advective form. In Eq. (2.9), term (7) through term (10) are the substrate removal rates under aerobic condition of microbe #1,

anaerobic condition of microbe #2, aerobic condition of microbe #3, and anaerobic condition of microbe #3, respectively. In Eq. (2.10), term (7) through term (10) represent the oxygen utilization rates resulting from the energy requirement for the growth of microbe #1, the energy maintenance of microbe #1, the energy requirement of microbe #3, and the energy maintenance of microbe #3, respectively. In Eq. (2.11), term (7) through term (10) are the nitrate utilization rates resulting from the energy requirement for the growth of microbe #2, the energy maintenance of microbe #2, the energy requirement of microbe #3, and the energy maintenance of microbe #3, respectively. In Eq. (2.12), term (7) through term (10) represent the nutrient removal for the synthesis of microbe #1 under aerobic condition, microbe #2 under anaerobic condition, microbe #3 under aerobic condition, and microbe #3 under anaerobic condition, respectively. Term (7) and term (8) in Eqs. (2.13) through (2.15) are growth rate and decay rate of microbe #1 under aerobic condition, microbe #2 under anaerobic condition, and microbe #3 under aerobic condition, respectively. Term (9) and term (10) in Eq. (2.15) represent the growth rate and decay rate of microbe #3 under anaerobic condition, respectively.

The dispersion coefficient tensor **D** in Eq. (2.9) to Eq.(2.15) is given by

$$\theta \mathbf{D} = a_T |\mathbf{V}| \delta + (a_L - a_T)\mathbf{V}\mathbf{V}/|\mathbf{V}| + \theta a_m \tau \delta \qquad (2.16)$$

where $|\boldsymbol{V}|$ is the magnitude of $\boldsymbol{V}$, δ is the Kronecker delta tensor, a_T is lateral dispersivity, a_L is the longitudinal dispersivity, a_m is the molecular diffusion coefficient, and τ is the tortuosity. $I(C_o) = \left[1 + \frac{C_o}{K_c}\right]^{-1}$ is an inhibition function which is under the assumption that denitrifying enzyme inhibition is reversible and noncompetitive, where K_c is the inhibition coefficient (M/L^3). $\mu_o^{(1)}$, $\mu_n^{(2)}$, $\mu_o^{(3)}$ and $\mu_n^{(3)}$ are the maximum specific oxygen-based growth rates for microbe #1, the maximum specific nitrate-based growth rate for microbe #2, the maximum specific oxygen-based growth rate for microbe #3, and the maximum specific nitrate-based growth rate for microbe #3 (1/T), respectively; $Y_o^{(1)}$, $Y_n^{(2)}$, $Y_o^{(3)}$, and $Y_n^{(3)}$ are the yield coefficient for microbe #1 utilizing oxygen, the yielding coefficient for microbe #2 utilizing nitrate, the

yielding coefficient for microbe #3 utilizing oxygen and nitrate, in mass of microbe per unit mass of substrate (M/M); $K_{so}^{(1)}$, $K_{so}^{(3)}$, $K_{sn}^{(2)}$, $K_{sn}^{(3)}$, $K_{po}^{(1)}$, $K_{po}^{(3)}$, $K_{pn}^{(2)}$, $K_{pn}^{(3)}$ are the retarded substrate saturation constants under aerobic conditions with respect to microbe #1, microbe #3, the retarded substrate saturation constants under anaerobic conditions with respect to microbe #2, microbe #3, the retarded nutrient saturation constants under aerobic conditions with respect to microbe #1, microbe #3, and the retarded nutrient saturation constants under anaerobic conditions with respect to microbe #2, microbe #3, respectively; $K_o^{(1)}$, $K_o^{(3)}$, $K_n^{(2)}$, $K_n^{(3)}$ are the retarded oxygen saturation constants under aerobic conditions with respect to microbe #1, microbe #3, and the retarded nitrate saturation constant under anaerobic conditions with respect to microbe #2 and microbe #3 (M/L^3), respectively. $\lambda_o^{(1)}$, $\lambda_o^{(3)}$, $\lambda_n^{(2)}$, and $\lambda_n^{(3)}$ are the microbial decay constants of aerobic respiration of microbe #1 and microbe #3, and the microbial decay constants of anaerobic respiration of microbe #2 and microbe #3 (1/T), respectively; $\gamma_o^{(1)}$, $\gamma_o^{(3)}$, $\gamma_n^{(2)}$, and $\gamma_n^{(3)}$ are the oxygen-use or nitrate-use for syntheses by microbe #1, microbe #2, or microbe #3, respectively; $\alpha_o^{(1)}$, $\alpha_o^{(3)}$, $\alpha_n^{(2)}$, and $\alpha_n^{(3)}$ are the oxygen-use or nitrate-use coefficient for energy by microbe #1, microbe #2, or microbe #3, respectively; $\Gamma_o^{(1)}$, $\Gamma_o^{(3)}$, $\Gamma_n^{(2)}$, and $\Gamma_n^{(3)}$ are the oxygen or nitrate saturation constants for decay with respect to microbe #1, microbe #2, or microbe #3 (M/L^3), respectively; and $\epsilon_o^{(1)}$, $\epsilon_o^{(3)}$, $\epsilon_n^{(2)}$, and $\epsilon_n^{(3)}$ are the nutrient-use coefficients for the production of microbe #1, microbe #2, or microbe #3 with respect to aerobic or anaerobic respiration, respectively.

Initial Conditions of Transport

$$
\begin{aligned}
C_s &= C_{si}(x,y,z) \\
C_o &= C_{oi}(x,y,z) \\
C_n &= C_{ni}(x,y,z) \\
C_p &= C_{pi}(x,y,z) \qquad in \quad R \\
C_1 &= C_{1i}(x,y,z) \\
C_2 &= C_{2i}(x,y,z) \\
C_3 &= C_{3i}(x,y,z)
\end{aligned}
\tag{2.17}
$$

Prescribed Concentration (Dirichlet) Boundary Conditions

$$
\begin{aligned}
C_s &= C_{sd}(x_b,y_b,z_b,t) \\
C_o &= C_{od}(x_b,y_b,z_b,t) \\
C_n &= C_{nd}(x_b,y_b,z_b,t) \\
C_p &= C_{pd}(x_b,y_b,z_b,t) \qquad on \ B_d \\
C_1 &= C_{1d}(x_b,y_b,z_b,t) \\
C_2 &= C_{2d}(x_b,y_b,z_b,t) \\
C_3 &= C_{3d}(x_b,y_b,z_b,t)
\end{aligned}
\tag{2.18}
$$

Variable Boundary Conditions

$$\mathbf{n}\cdot(\mathbf{V}C_s - \theta\mathbf{D}\cdot\nabla C_s) = \mathbf{n}\cdot\mathbf{V}C_{sv}(x_b, y_b, z_b, t)$$
$$\mathbf{n}\cdot(\mathbf{V}C_o - \theta\mathbf{D}\cdot\nabla C_o) = \mathbf{n}\cdot\mathbf{V}C_{ov}(x_b, y_b, z_b, t)$$
$$\mathbf{n}\cdot(\mathbf{V}C_n - \theta\mathbf{D}\cdot\nabla C_n) = \mathbf{n}\cdot\mathbf{V}C_{nv}(x_b, y_b, z_b, t)$$
$$\mathbf{n}\cdot(\mathbf{V}C_p - \theta\mathbf{D}\cdot\nabla C_p) = \mathbf{n}\cdot\mathbf{V}C_{pv}(x_b, y_b, z_b, t) \qquad \textit{if } \boldsymbol{n}\cdot\mathbf{V} \le 0 \qquad (2.19a)$$
$$\mathbf{n}\cdot(\mathbf{V}C_1 - \theta\mathbf{D}\cdot\nabla C_1) = \mathbf{n}\cdot\mathbf{V}C_{1v}(x_b, y_b, z_b, t)$$
$$\mathbf{n}\cdot(\mathbf{V}C_2 - \theta\mathbf{D}\cdot\nabla C_2) = \mathbf{n}\cdot\mathbf{V}C_{2v}(x_b, y_b, z_b, t)$$
$$\mathbf{n}\cdot(\mathbf{V}C_3 - \theta\mathbf{D}\cdot\nabla C_3) = \mathbf{n}\cdot\mathbf{V}C_{3v}(x_b, y_b, z_b, t)$$

$$\mathbf{n}\cdot(-\theta\mathbf{D}\cdot\nabla C_s) = 0$$
$$\mathbf{n}\cdot(-\theta\mathbf{D}\cdot\nabla C_p) = 0$$
$$\mathbf{n}\cdot(-\theta\mathbf{D}\cdot\nabla C_n) = 0$$
$$\mathbf{n}\cdot(-\theta\mathbf{D}\cdot\nabla C_p) = 0 \qquad \textit{if } \boldsymbol{n}\cdot\mathbf{V} > 0 \qquad (2.19b)$$
$$\mathbf{n}\cdot(-\theta\mathbf{D}\cdot\nabla C_1) = 0$$
$$\mathbf{n}\cdot(-\theta\mathbf{D}\cdot\nabla C_2) = 0$$
$$\mathbf{n}\cdot(-\theta\mathbf{D}\cdot\nabla C_3) = 0$$

Cauchy Boundary Conditions

$$
\begin{aligned}
\mathbf{n}\cdot(\mathbf{V}C_s - \theta\mathbf{D}\cdot\nabla C_s) &= q_{sc}(x_b, y_b, z_b, t) \\
\mathbf{n}\cdot(\mathbf{V}C_o - \theta\mathbf{D}\cdot\nabla C_o) &= q_{oc}(x_b, y_b, z_b, t) \\
\mathbf{n}\cdot(\mathbf{V}C_n - \theta\mathbf{D}\cdot\nabla C_n) &= q_{nc}(x_b, y_b, z_b, t) \\
\mathbf{n}\cdot(\mathbf{V}C_p - \theta\mathbf{D}\cdot\nabla C_p) &= q_{pc}(x_b, y_b, z_b, t) \qquad on \quad B_c \\
\mathbf{n}\cdot(\mathbf{V}C_1 - \theta\mathbf{D}\cdot\nabla C_1) &= q_{1c}(x_b, y_b, z_b, t) \\
\mathbf{n}\cdot(\mathbf{V}C_2 - \theta\mathbf{D}\cdot\nabla C_2) &= q_{2c}(x_b, y_b, z_b, t) \\
\mathbf{n}\cdot(\mathbf{V}C_3 - \theta\mathbf{D}\cdot\nabla C_3) &= q_{3c}(x_b, y_b, z_b, t)
\end{aligned}
\tag{2.20}
$$

Neumann Boundary Conditions

$$
\begin{aligned}
\mathbf{n}\cdot(-\theta\mathbf{D}\cdot\nabla C_s) &= q_{sn}(x_b, y_b, z_b, t) \\
\mathbf{n}\cdot(-\theta\mathbf{D}\cdot\nabla C_o) &= q_{on}(x_b, y_b, z_b, t) \\
\mathbf{n}\cdot(-\theta\mathbf{D}\cdot\nabla C_n) &= q_{nn}(x_b, y_b, z_b, t) \\
\mathbf{n}\cdot(-\theta\mathbf{D}\cdot\nabla C_p) &= q_{pn}(x_b, y_b, z_b, t) \qquad on \quad B_n \\
\mathbf{n}\cdot(-\theta\mathbf{D}\cdot\nabla C_1) &= q_{1n}(x_b, y_b, z_b, t) \\
\mathbf{n}\cdot(-\theta\mathbf{D}\cdot\nabla C_2) &= q_{2n}(x_b, y_b, z_b, t) \\
\mathbf{n}\cdot(-\theta\mathbf{D}\cdot\nabla C_3) &= q_{3n}(x_b, y_b, z_b, t)
\end{aligned}
\tag{2.21}
$$

where C_{si}, C_{oi}, C_{ni}, C_{pi}, C_{1i}, C_{2i}, and C_{3i}, are the initial concentrations of substrate, oxygen, nitrogen, nutrient, microbe #1, microbe #2, and microbe #3; and R is the region of interest; (x_b,y_b,z_b) is the spatial coordinate on the boundary; **n** is an outward unit vector normal to the boundary; C_{sd}, C_{od}, C_{nd}, C_{pd}, C_{1d}, C_{2d}, C_{3d}, and C_{sv}, C_{ov}, C_{nv}, C_{pv}, C_{1v}, C_{2v}, C_{3v}, are the prescribed concentrations of substrate, oxygen, nitrogen, nutrient, microbe #1, microbe #2, and microbe #3, on the Dirichlet boundary and the specified concentrations of water through the variable boundary, respectively; B_d, and B_v are the Dirichlet and variable boundaries, respectively; q_{sc}, q_{oc}, q_{nc}, q_{pc}, q_{1c}, q_{2c}, q_{3c} and q_{sn}, q_{on}, q_{nn}, q_{pn}, q_{1n}, q_{2n}, q_{3n}, are the prescribed total flux and gradient flux of substrate,

oxygen, nitrogen, nutrient, microbe #1, microbe #2, and microbe #3 through the Cauchy and Neumann boundaries B_c and B_n, respectively.

2.2 Numerical Approximation

Flow Equation

The pressure head can be approximated to Eq.(2.22) by the finite element method.

$$h \approx \sum_{j=1}^{N} h_j(t) N_j(x,z) \tag{2.22}$$

where N is the total number of nodes in the region and N_j and h_j are the basis function and the amplitude of h, respectively, at nodal point j. Substituting Eq.(2.22) into Eq.(2.1) and choosing Galerkin finite element method, the governing flow equation can be approximated to the following.

$$\left[\int_R N_i \frac{\rho}{\rho_w} F N_j dR\right]\frac{dh_j}{dt} + \left[\int_R (\nabla N_i)\cdot\mathbf{K}\cdot(\nabla N_j) dR\right] h_j =$$

$$\int_R N_i \frac{\rho^*}{\rho_w}(\text{or} - \frac{\rho}{\rho_w}) q dR - \int_R (\nabla N_i)\cdot\mathbf{K}\cdot(\frac{\rho}{\rho_w}\nabla z) dR + \int_B \mathbf{n}\cdot\mathbf{K}\cdot(\nabla h + \frac{\rho}{\rho_w}\nabla z) N_i dB, \tag{2.23}$$

$$\text{where } i = 1,2,...,N. \qquad F = \frac{d\theta}{dt}$$

Equation (2.23) written in matrix form is:

$$[M]\{\frac{dh}{dt}\} + [S]\{h\} = \{G\} + \{Q\} + \{B\} \tag{2.24}$$

where {dh/dt} and {h} are the column vectors containing the values of dh/dt and h, respectively, at all nodes; [M] is the mass matrix resulting from the storage term; [S] is stiffness matrix resulting from the action of conductivity; and {G}, {Q} and {B} are the load vectors from the gravity force, internal source/sink, and boundary conditions, respectively. The matrices, [M] and [S] are given by

$$M_{ij} = \sum_{e \in M_e} \int_{R_e} N_\alpha^e \frac{\rho}{\rho_w} F N_\beta^e dR \tag{2.25}$$

$$S_{ij} = \sum_{e \in M_e} \int_{R_e} \nabla\left(N_\alpha^e\right) \cdot \mathbf{K} \cdot \nabla\left(N_\beta^e\right) dR \tag{2.26}$$

where

R_e = the region of element e,

M_e = the set of elements that have a local side α-β coinciding with the global side i-j,

N_α^e = the α-th local basis function of element e.

Similarly, the load vectors {G}, {Q} and {B} are given by

$$G_i = -\sum_{e \in M_e} \int_{R_e} (\nabla N_\alpha^e) \cdot \mathbf{K} \cdot \frac{\rho}{\rho_w} \nabla z dR \tag{2.27}$$

$$B_i = -\sum_{e \in N_{se}} \int_{B_e} N_\alpha^e \cdot [-\mathbf{K} \cdot (\nabla h + \frac{\rho}{\rho_w} \nabla z)] dB \tag{2.28}$$

$$Q_i = \sum_{e \in M_e} \int_{R_e} N_\alpha^e \frac{\rho^*}{\rho_w} (\text{or} - \frac{\rho}{\rho_w}) q dR \tag{2.29}$$

where

B_e = the length of boundary segment e,

N_{se} = the set of boundary segments that have a local node α coinciding with the global node i.

The reduction of the partial differential equation Eq. (2.1) to the set of ordinary differential equations Eq. (2.24) simplifies the evaluation of integrals on the right hand side of Eqs. (2.25) through (2.29) for every element for boundary surface e. The major tasks that remain to be done are the specification of base and

weighting functions and the performance of integration to yield the element matrices. Linear hexahedral elements are demonstrated in the Appendix C of users' manual of 3DFEMFAT (Yeh et al., 1994).

The following steps demonstrate the incorporation of boundary conditions into a matrix equation by the finite element method.

For the Cauchy boundary condition given by Eq.(2.7), Eq.(2.7) is simply substituted into Eq.(2.28) to yield a boundary-element column vector $\{B_c^e\}$ for a Cauchy segment:

$$\{B_c^e\} = \{q_c^e\} \tag{2.30}$$

where $\{q_c^e\}$ is the Cauchy boundary flux vector given by

$$q_{c\alpha}^e = -\int_{B_e} N_\alpha^e \frac{\rho}{\rho_w} q_c dB \ , \qquad \alpha = 1 \text{ or } 2 \tag{2.31}$$

The Cauchy boundary flux vector represents the normal fluxes through the two nodal points of the segment B_e on B_c.

For the Neumann boundary condition given by Eq.(2.6), Eq.(2.6) is substituted into Eq.(2.28) to yield a boundary-element column vector $\{B_n^e\}$ for a Neumann segment:

$$\{B_n^e\} = \{q_n^e\} \tag{2.32}$$

where $\{q_{n\alpha}^e\}$ is the Neumann boundary flux vector given by:

$$q_{n\alpha}^e = \int_{B_e} \left(N_\alpha^e \mathbf{n} \cdot \mathbf{K} \cdot \frac{\rho}{\rho_w} \nabla z - N_\alpha^e q_n \right) dB \ ; \quad \alpha = 1 \text{ or } 2 \tag{2.33}$$

which is independent of pressure head.

The implementation of the variable-type boundary condition is more involved. During the iteration of boundary conditions on the variable boundary, one of Eqs.(2.8a) through (2.8e) is used at a node. If either Eq.(2.8b) or (2.8e) is used, it is substituted into Eq.(2.28) to yield a boundary element column vector $\{B_v^e\}$ for a variable boundary segment:

$$\{B_v^e\} = \{q_v^e\} \tag{2.34}$$

where $\{q_v^e\}$ is the variable boundary flux given by:

$$q_{v\alpha}^e = -\int_{B_e} N_\alpha^e \frac{\rho}{\rho_w} q_p dB, \quad \text{or} \quad q_{v\alpha} = -\int_{B_e} N_\alpha^e \frac{\rho}{\rho_w} q_e dB \; ; \quad \alpha = 1 \text{ or } 2 \tag{2.35}$$

Assembling over all Neumann, Cauchy, and variable boundary segments, one obtains the global boundary column vector {B} as:

$$\{B\} = \{q\} \tag{2.36}$$

in which

$$\{q\} = \sum_{e \in N_{ne}} \{q_n^e\} + \sum_{e \in N_{ce}} \{q_c^e\} + \sum_{e \in N_{ve}} \{q_v^e\} \tag{2.37}$$

where N_{ne}, N_{ce}, and N_{ve} are the number of Neumann boundary segments, Cauchy boundary segments, and variable boundary segments with flux conditions imposed on them, respectively. The boundary flux {B} given by Eqs.(2.36) and (2.37) should be added to the right hand side of Eq.(2.24).

At nodes where Dirichlet boundary conditions are applied, an identity equation is generated for each node and included in the matrices of Eq.(2.24). The Dirichlet nodes include the nodes on the Dirichlet boundary and the nodes on the variable boundary to which either Eq.(2.8a), (2.8c), or (2.8d) is applied.

Transport Equation

To simplify the notation, the subscript s, o, n, p, 1, 2, or 3 in Eqs. (2.9) to (2.15) will be dropped for the development of numerical algorithm in this section. Since the hybrid Lagrangian-Eulerian approach is used to simulate Eq. (2.9) to (2.15), it is written in the Lagrangian-Eulerian form as

$$\begin{aligned}(\theta + \rho_b K_d)\frac{DC}{Dt} = \nabla\cdot(\theta \mathbf{D}\cdot\nabla C) - \Lambda(\theta C + \rho_b K_d) + QC_{in} - \frac{\rho^*}{\rho}QC + \frac{\rho_w}{\rho}\mathbf{V}\cdot\nabla(\frac{\rho}{\rho_w})C \\ - f(C_1, C_2, C_3, C_s, C_o, C_n, C_p)C + g(C_1, C_2, C_3, C_s, C_o, C_n, C_p)C\end{aligned} \tag{2.38}$$

$$\mathbf{V}^{*} = \frac{\mathbf{V}}{\theta + \rho_b K_d} \tag{2.39}$$

where $f(C_1, C_2, C_3, C_s, C_o, C_n, C_p)$ is a microbial-chemical interaction function and $g(C_1, C_2, C_3, C_s, C_o, C_n, C_p)$ is a microbial growth function . Applying the Galerkin finite element method to Eq. (2.9) through Eq. (2.15), one obtains

$$[M]\{\frac{DC}{Dt}\} + \big([A] + [D] + [K] + [B]\big)\{C\} = \{Q\} + \{B\} \tag{2.40}$$

where {C} is a vector whose components are the concentrations at all nodes, {DC/Dt} is the time derivative of {C} with respect to time, [M] is the mass matrix associated with the time derivative term, [A] is the stiffness matrix associated with the velocity term which is only computed as steady-state is considered, [D] is the stiffness matrix associated with the dispersion term, [K] is the stiffness matrix associated with the decay term and microbial-chemical interaction, [B] is the stiffness matrix resulting from boundary conditions, {Q} is the load vector associated with all source/sink terms, and {B} is the load vector associated with boundary conditions. These matrices and vectors are given as follows.

$$M_{ij} = \sum_{e \in M_e} \int_{R_e} N_\alpha^e (\theta + \rho_b K_d) N_\beta^e dR \tag{2.41a}$$

$$A_{ij} = \sum_{e \in M_e} \int_{R_e} W_\alpha^e \mathbf{V} \cdot \nabla N_\beta^e dR \tag{2.41b}$$

$$D_{ij} = \sum_{e \in M_e} \int_{R_e} \nabla N_\alpha^e \cdot \mathbf{D} \cdot \nabla N_\beta^e dR \tag{2.41c}$$

$$K_{ij} = \sum_{e \in M_e} \int_{R_e} N_\alpha^e \left[\Lambda(\theta + \rho_b K_d) + f(C_1, C_2, C_3, C_s, C_o, C_n, C_p) + \frac{\rho^*}{\rho} q_{in} - \frac{\rho_w}{\rho} \mathbf{V} \cdot \nabla \frac{\rho}{\rho_w} \right] N_\beta^e dR \tag{2.41d}$$

$$B_{ij} = -\left[\sum_{B_e \in B_v^+} \int_{B_e} N_\alpha^e (\mathbf{n}\cdot\mathbf{V}) N_\beta^e dB + \sum_{B_e \in B_c} \int_{B_e} N_\alpha^e (\mathbf{n}\cdot\mathbf{V}) N_\beta^e dB\right] \tag{2.41e}$$

$$Q_i = \sum_{e \in M_e} \int_{R_e} N_\alpha^e q_{in} C_{in} dR + \sum_{e \in M_e} \int_{R_e} N_\alpha^e g(C_1, C_2, C_3, C_s, C_o, C_n, C_p) dR \tag{2.41f}$$

$$B_i = -\left[\sum_{B_e \in B_v^+} \int_{B_e} N_\alpha^e (\mathbf{n}\cdot\mathbf{V}) C_v dB + \sum_{B_e \in B_c} \int_{B_e} N_\alpha^e q_c dB + \sum_{B_e \in B_n} \int_{B_e} N_\alpha^e q_n dB\right] \tag{2.41g}$$

where B_v^+ is that part of variable boundary for which the flow is directed into the region, C is the concentration of the incoming fluid through the variable boundary segment B_v^+, and B_c, B_n are the Cauchy and Neumann boundary segments.

The numerical algorithm for solving this partial differential equation is a modified Lagrangian-Eulerian method with adapted zooming and peak capturing (LEZOOMPC). Before the LEZOOMPC algorithm is described, two terms need to be defined, namely smooth elements and rough elements, which shall be used throughout this document. A smooth element is defined as an element within which any physical quantity at all points can be interpolated with its node values to within error tolerance. A rough element is defined as an element within which there exists at least one point for which the physical quantity cannot be interpolated with its node values to within error tolerance. Basically, LEZOOMPC is a modified method of the Lagrangian-Euleran decoupling with zoomable (LEZOOM) hidden fine-mesh approach (Yeh, 1990) and exact peak capturing and oscillation-free scheme (EPCOF) (Yeh et al., 1992) to solve advection-dispersion transport equations. To compute the concentration C^{n+1} at time t_{n+1}, the Lagrangian concentration, C_i^*'s, must be determined first [It is noted that the Lagrangian concentrations C_i^*'s at all global nodes are exact if concentrations C^n at time t_n represent the exact solution through the region, not just at the nodes]. The diffusion transport problem is then solved over all the global nodes and activated forward-tracked nodes at time t_{n+1}

with the Galerkin finite element method, taking the Lagrangian concentrations C_i^* at all global nodes and activated forward-tracked nodes as the initial condition, to complete the computation.

Figure 2.1 shows the basic concept structure of solving transport of 3DFATMIC. It contains two main steps, namely the Lagrangian and Eulerian steps.

First, the concentrations at the last time step t^n, C^n's, are the known quantities for the computation of this time step. Second (GNTRAK module), one computes the Lagrangian concentration C_i^*'s at global nodes using the backward node tracking as

$$C_i^* = \sum_{j=1}^{N+N_n} C_j^n N_j(x_i^*, y_i^*, z_i^*), \quad i=1,2,.,N \tag{2.42}$$

in which

$$\begin{aligned} x_i^* &= x_i - \int_{t_n}^{t_{n+1}} V_x dt \\ y_i^* &= y_i - \int_{t_n}^{t_{n+1}} V_y dt \\ z_i^* &= z_i - \int_{t_n}^{t_{n+1}} V_z dt \qquad i=1,2,..,N \end{aligned} \tag{2.43}$$

where $N_j(x_i^*,y_i^*,z_i^*)$ is the base function associated with node (x_j,y_j,z_j) evaluated at (x_i^*,y_i^*,z_i^*); V_x, V_y, and V_z are the velocities along x-, y- , and z-directions, respectively.

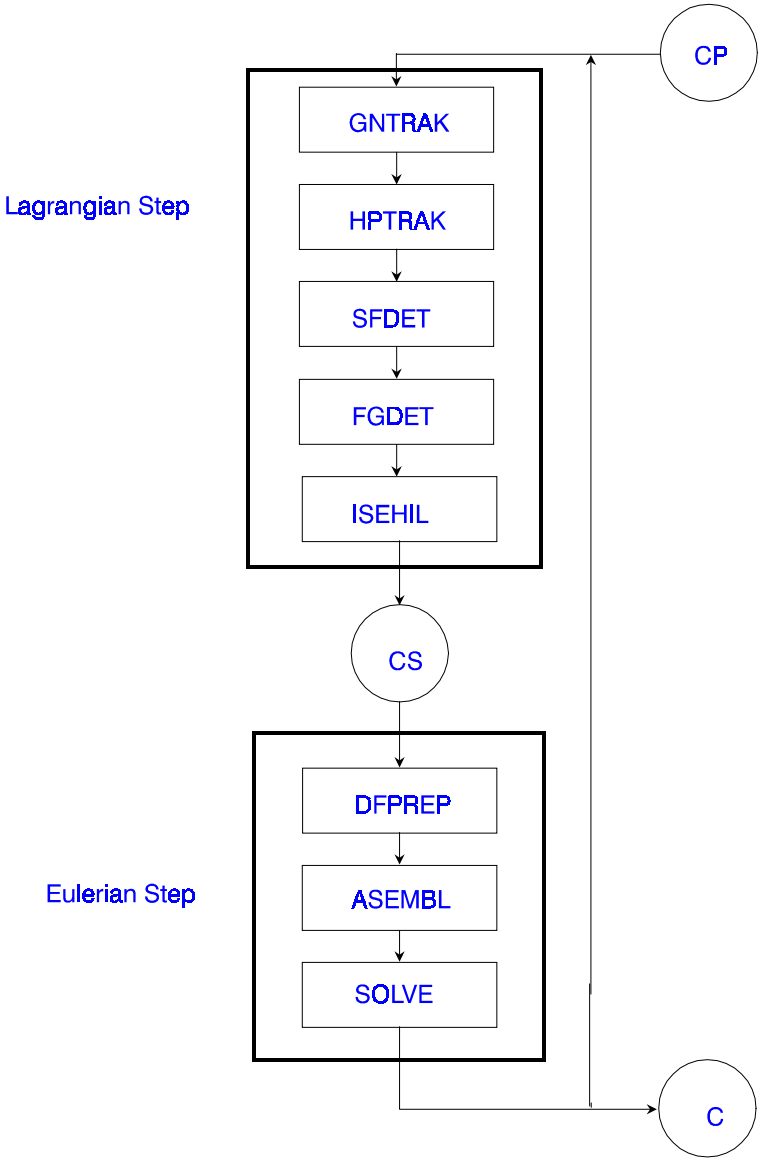


Figure 2.1 The basic structure for coding transport part of 3DFATMIC

Third (HPTRAK modules), all the activated fine grid nodes and the global nodes are forwardly tracked to obtain the Lagrangian concentration C_j^f by the following equations:

$$C_j^f = C\left(x_j^f, y_j^f, z_j^f, t_{n+1}\right) = C\left(x_j, y_j, z_j, t_n\right) = C_j^n \qquad j = 1,2,.....,N+N_n \qquad (2.44)$$

in which

$$x_j^f = x_j + \int_{t_n}^{t_{n+1}} V_x dt \quad , \quad y_j^f = y_j + \int_{t_n}^{t_{n+1}} V_y dt \quad , \quad z_j^f = z_j + \int_{t_n}^{t_{n+1}} V_z dt \tag{2.45}$$

It should be noted that C_j^{f}'s are exact if C_j^{n}'s are exact and Eq.(2.45) is integrated exactly.

Fourth (SFDET and FGDET modules), it is determined whether an element is a rough element in the SFDET module (Yeh et al., 1992) based on prescribed error tolerance. The criteria is shown in the following formula:

$$\begin{aligned} \left| \left(C_j^a - C_j^f \right) / C_j^f \right| &\le \epsilon_1 \\ \left| \left(C_j^a - C_j^f \right) / C_M^f \right| &\le \epsilon_2 \end{aligned} \tag{2.46}$$

where C_j^a is the approximate value determined from finite element interpolation, ϵ_1, ϵ_2 are two error tolerances and C_M^f is the maximum concentration of C_j^{f}s. FGDET module generates the regular fine-mesh points in every rough element determined in the SFDET module.

Fifth (ISEHIL module), if the element is a smooth element, all forward-tracked nodes for dispersion computation at the present time t_{n+1} and advection computation at the next time t_{n+2} are removed. Otherwise, the number of regular fine grids, which is determined by users, is imbedded into every rough element. The indices of subelements are stored in the ISE array. In addition to regular fine grids refinement, this module also captures all the highest and lowest concentrations within each subelement. This demonstrates the idea called adapted zooming and peak capturing. The above five steps form the Lagrangian computation of the advective transport.

The next three steps (DFPREP, ASEMBL, and SOLVE modules) are Eulerian steps to solve the dispersion matrix equation. The module DFPREP prepares all the needed information for assembling the subelemental matrices, which are zoomed in the Eulerian step. The inclusion of this module gets rid of the inaccuracy due to the dispersion calculation. In this module, the number of fine grids generated in each global element is determined by users and may be different from that in the module FGDET. If the element is a

smooth element, no fine grids are imbedded. If the element is a rough element, the element is zoomed and connected with the surrounding smooth elements. At the end of this module, the nodal connection information of each point has to be prepared to compose the matrix and solve the matrix equation.

The module ASEMBL is designed to yield the following element matrix equation

$$\{A^e\}\{C^e\} = \{R^e\} \tag{2.47}$$

which is based on Eqs.(2.9) to (2.15), where $[A^e]$ is the element coefficient matrix, $\{C^e\}$ is the unknown vector of the concentration, and $\{R^e\}$ is the element load vector. Element e can be a global element or a subelement generated in a rough region by DFPREP. Then, this module assembles all the element matrix equations to a global matrix equation with the slave point concept to take care of the interface between rough regions and smooth regions. The resulting matrix equation will be solved by a diffusion solver.

The module SOLVE solves the assembled global matrix equation by a block iterative solver, pointwise iteration, or preconditioned conjugate method. If the diffusion zoomed approach is activated in the Eulerian step, the block iteration method is changed to pointwise iteration solver forcefully.

At the very end of this time step, i.e., at t_{n+1}, the concentrations at all activated fine grid nodes generated in the Lagrangian step are obtained by finite element interpolations as follows:

$$C_k^{n+1} = C_k^f + \sum_{i=1}^{N} \left(C_i^{n+1} - C_i^*\right) N_i\left(x_k^f, y_k^f, z_k^f\right), \qquad k = 1,2,...,N_n+1 \tag{2.48}$$

2.3 Description of 3DFATMIC Subroutines

3DFATMIC consists of a MAIN program and 120 subroutines. The MAIN is utilized to specify the sizes of all arrays. The control and coordinate activity are performed by the subroutine HTMICH. Figure 2.2 shows the structure of the program. The functions of these subroutines are described below.

Program MAIN

The MAIN is used to specify the sizes of all arrays. The flow of data input for the model is also anchored by the MAIN. The subroutine RDATIO is called to read the geometric and material data. MAIN then calls subroutine PAGEN to generate pointer arrays; SURF to identify the boundary sides and compute the directional cosine. The source/sink data for flow and transport computations are read in by the subroutines FSSDAT and TSSDAT, respectively. The boundary conditions for flow and transport calculations are then read in by the subroutines FBCDAT and TBCDAT, respectively. Control is then passed to subroutine HTMICH to coordinate and perform flow and/or transport computations.

Subroutine RDATIO

The subroutine RDATIO is called by the program MAIN to read in the soil property functions and geometric data for the area of interest.

Subroutine FSSDAT

The subroutine FSSDAT is called by the program MAIN to read in the sources/sinks profiles, nodes, and/or elements for flow simulations. The source/sink type for each node/element is also assigned in this subroutine according to the data given by the users.

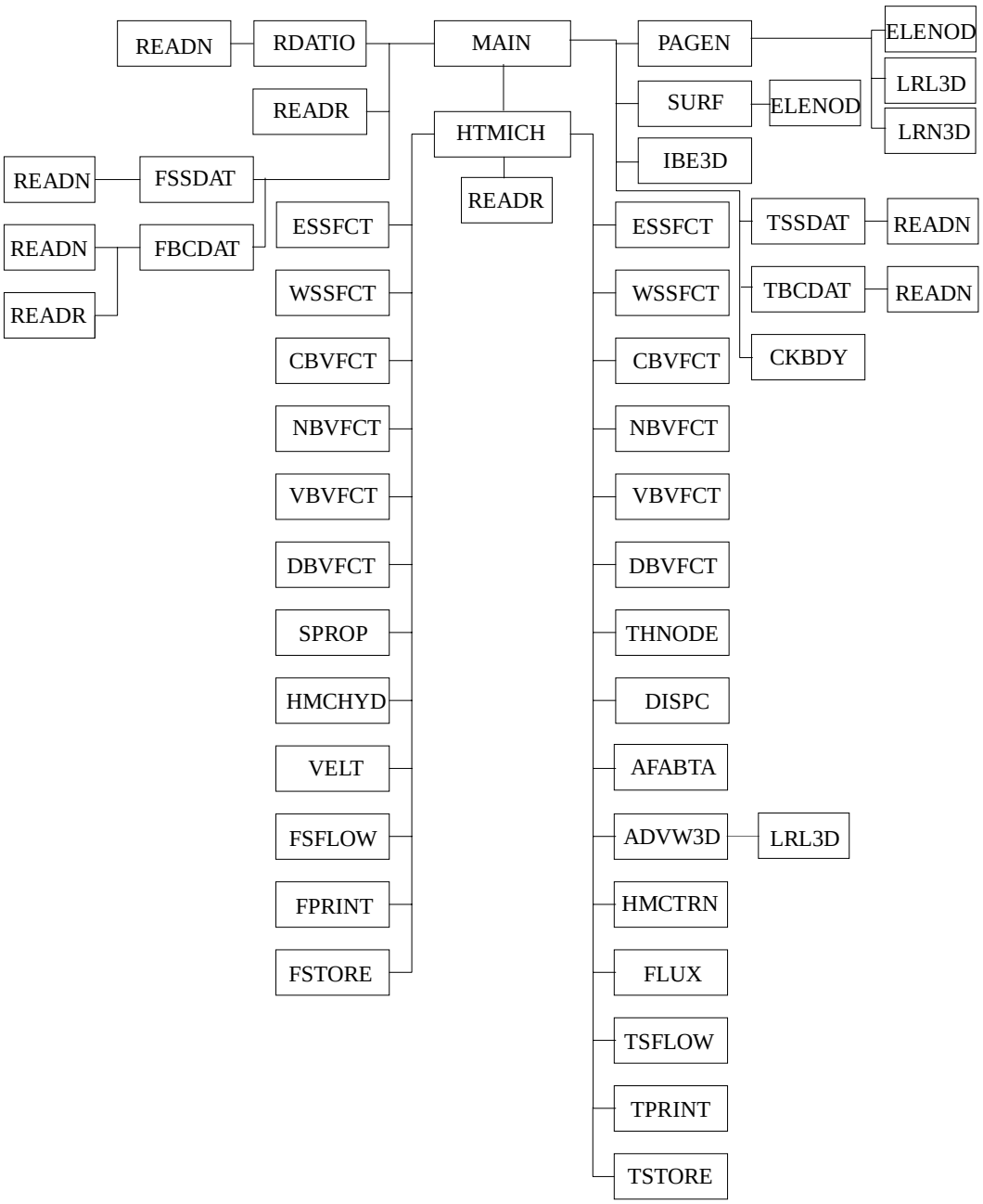


Figure 2.2 Program Structure of 3DFATMIC (MAIN)

Subroutine TSSDAT

The subroutine TSSDAT is called by the program MAIN to read in the sources/sinks profiles, nodes, and/or elements for transport simulations. The source/sink type for each node/element is also assigned in this subroutine according to the data given by the users.

Subroutine FBCDAT

The subroutine FBCDAT controls the input of boundary condition, in time and space, assigned to each boundary node/element for flow simulations. Users need to give the boundary profiles, to specify the global node/element numbers of the boundary, and to assign boundary profile type to each node/element.

Subroutine TBCDAT

The subroutine TBCDAT controls the input of boundary condition, in time and space, assigned to each boundary node/element for transport simulations. Users need to give the boundary profiles, to specify the global node/element numbers of the boundary, and to assign boundary profile type to each node/element.

Subroutine CKBDY

This subroutine checks all the boundary sides and generates the arrays, including NBDYB and IBDY, for later use in along boundary tracking on both the unspecified and the Neumann boundary sides. NBDYB(I) represents the accumulated number the unspecified/Neumann boundary sides connecting with the 1-st through the (I-1)-th global node. IBDY(I) indicates the global boundary side to which the I-th unspecified/Neumann boundary side relates.

Subroutine HTMICH

The subroutine HTMICH controls the entire sequence of operations, a function generally performed by the MAIN program. It is, however, preferable to keep a short MAIN and supplement it with several subroutines with variable storage allocation. This makes it possible to place most of the FORTRAN deck on a permanent file and to deal with a site-specific problem without making changes in array dimensions throughout all subroutines.

Depending on the combinations of the parameters KSSf, KSSt, NTI, and IMOD, the subroutine HTMICH will perform either the steady state flow and/or transport computations only, or the transient state flow and/or transport computations using the flow and/or transport steady-state solution as the initial conditions, or the transient flow and/or transport computation using user-supplied initial conditions.

HTMICH calls the subroutines ESSFCT, WSSFCT, CBVFCT, NBVFCT, VBVFCT, and DBVFCT to obtain sources/sinks and boundary values; subroutine SPROP to obtain the relative hydraulic conductivity, water capacity, and moisture content from the pressure head; subroutine VELT to compute Darcy's velocity; subroutine FSFLOW to calculate flux through all types of boundaries and water accumulated in the media; subroutine FPRINT to print out the results; and subroutine FSTORE to store the flow variables for plotting; subroutine HMCHYD to perform the flow computations; subroutine FLUX to compute material flux; subroutine AFABTA to obtain upstream weighting factor based on velocity and dispersivity; subroutine TSFLOW to calculate material flux through all types of boundaries and water accumulated in the media; subroutine TPRINT to print out the transport computation results; subroutine TSTORE to store the transport computation results for plotting; subroutine THNODE to compute the value of moisture content plus bulk density times distribution coefficient in the case of linear isotherm, or the moisture content in the case of nonlinear isotherm at all nodes; subroutine DISPC to compute the dispersion coefficients; and subroutine HMCTRN to perform the transport computations.

Subroutine READR

This subroutine is called by the MAIN as well as subroutines FBCDAT and HTMICH to automatically generate real numbers if required. Automatic generation of regular patterned data is built into the subroutine (see Appendix A).

Subroutine READN

This subroutine is also called by the subroutines RDATIO, FBCDAT, and TBCDAT to generate integers if required (see Appendix A).

Subroutine PAGEN

This subroutine is called by the controlling program MAIN to preprocess pointer arrays that are needed to store the global matrix in compressed form and to construct the subregional block matrices. The pointer arrays automatically generated in this subroutine include the global node connectivity (stencil) GNOJCN(J,N), regional node connectivity LNOJCN(J,I,K), total node number for each subregion NTNPLR(K), bandwidth indicator for each subregion LMAXDF(K), and partial fill-up for the mapping array between global node number and local subregion node number GNPLR(I,K) with I = NNPLR(K) + 1 to NTNPLR(K). Here GNOJCN(J,N) is the global node number of J-th node connected to the global node N; LNOJCN(J,I,K) is the local node number of the J-th node connected to the local node I in K-th subregion; NTNPLR(K) is the total number of nodes in the K-th subregion, including the interior nodes, the global boundary nodes, and intra-boundary nodes; LMAXDF(K) is the maximum difference between any two nodes of any element in K-th subregion; and GNPLR(I,K) is the global node number of I-th local-region node in the K-th subregion. These pointer arrays are generated based on the element connectivity IE(M,J), the number of node for each subregion NNPLR(K), and the mapping between global node and local-region node GNLR(I,K) with I = 1, NNPLR(K). Here IE(M,J) is the global node number of J-th node of element M; NNPLR(K) is the number of nodes in the K-th subregion including the interior nodes and the global boundary nodes but not the intraboundary nodes. If a preconditioned conjugate gradient solver is selected to solve linear matrix equations, this subroutine will rearrange LRN(J,N) such that LRN(1,N) = N.

Subroutine ELENOD

This subroutine determines the number of nodes, the number of faces, and the elemental shape index of element M by using the IE(M,5) and IE(M,7) information.

Subroutine LRL3D

This subroutine is called by subroutines PAGEN and ADVW3D. This subroutine generates the node-element connection pointer arrays NLRL, LRL, NLRLW, and LRLW used in particle tracking.

Subroutine LRN3D

This subroutine is called by subroutine PAGEN. This subroutine generates the node-node connection pointer arrays NLRN and LRN used in composing the linearized matrix equations.

Subroutine SURF

Subroutine SURF identifies the boundary sides, sequences the boundary nodes, and computes the directional cosine of the surface sides. The mappings from boundary nodes to global nodes are stored in NPBB(I) (where NPBB(I) is the global node number of the I-th boundary node). The boundary node numbers of the four nodes for each boundary side are stored in ISB(I,J) (where ISB(I,J) is the boundary node number of I-th node of J-th side, I = 1 to 4). There are six, five, or four sides for each hexahedral, triangular prism, or tetrahedral element, respectively. Which of these sides is the boundary side is determined automatically in the subroutine SURF and is stored in ISB(5,J). The global element number, to which the J-th boundary side belongs, is also preprocessed in the subroutine SURF and is stored in ISB(6,J). The directional cosines of the J-th boundary side are computed and stored in DCOSB(I,J) (where DCOSB(I,J) is the directional cosine of the J-th surface with I-th coordinate, I = 1 to 3). The information contained in NPBB, ISB, and DCOSB, along with the number of boundary nodes and the number of boundary sides, is returned to subroutine MAIN program for other users.

Subroutine IBE3D

The subroutine IBE3D is used to generate the index of boundary element stored in IBE array. If IBE(M) = 0, it means no boundary element side in the M-th element. If IBE(M)=12, the element side 1 and 2 are the boundary element sides of the M-th element globally.

Subroutine ESSFCT

This subroutine is called by the subroutine HTMICH to compute the elemental source strength. It uses the linear interpolation of the tabular data or it computes the value with analytical function. If the latter option is used, the user must supply the function into this subroutine.

Subroutine WSSFCT

This subroutine is called by the subroutine HTMICH to compute the well source strength. It uses the linear interpolation of the tabular data or it computes the value with analytical function. If the latter option is used, the user must supply the function into this subroutine.

Subroutine VBVFCT

This subroutine is called by the subroutine HTMICH to compute the variable boundary values. It uses the linear interpolation of the tabular data or it computes the value with analytical function. If the latter option is used, the user must supply the function into this subroutine.

Subroutine DBVFCT

This subroutine is called by the subroutine HTMICH to compute the Dirichlet boundary values. It uses the linear interpolation of the tabular data or it computes the value with analytical function. If the latter option is used, the user must supply the function into this subroutine.

Subroutine CBVFCT

This subroutine is called by the subroutine HTMICH to compute the Cauchy fluxes. It uses the linear interpolation of the tabular data or it computes the value with analytical function. If the latter option is used, the user must supply the function into this subroutine.

Subroutine NBVFCT

This subroutine is called by the subroutine HTMICH to compute the Neumann fluxes. It uses the linear interpolation of the tabular data or it computes the value with analytical function. If the latter option is used, the user must supply the function into this subroutine.

Subroutine FPRINT

This subroutine is used to line-print the flow variables. These include the fluxes through variable boundary surfaces, the pressure head, total head, moisture content, and Darcy's velocity components.

Subroutine FSTORE

This subroutine is used to store the flow variables on Logical Unit 11. It is intended to for plotting purposes. The information stored includes region geometry, subregion data, and hydrological variables such as pressure head, total head, moisture content, and Darcy's velocity components.

Subroutine TPRINT

This subroutine is used to line-print the simulation results of contaminant transport. These include the material flux components and the concentration at each global node.

Subroutine TSTORE

This subroutine is used to store the simulation results of contaminant transport on Logical Unit 12. It is intended for plotting purpose. The information stored includes region geometry, concentrations, and material flux components at all nodes for any desired time step.

Subroutine ADVW3D

This subroutine is called by HTMICH to generate all the working arrays including IBW, IEW, NLRLW, and LRLW, for 'in-element' tracking in the Lagrangian step computation used in the transient-state simulation. The more subelements generated for particle tracking, the more accurate result obtained. In this subroutine, the working arrays are for the following types of elements: (1) tetrahedral elements (if ISHAPE=4 or 0), (2) triangular prism elements (if ISHAPE=6 or 0), and (3) hexahedral elements (if ISHAPE=8 or 0).

Subroutine HMCHYD

HMCHYD calls subroutine SPROP to obtain the relative hydraulic conductivity, water capacity, and moisture content from the pressure head; subroutine VELT to compute Darcy's velocity; subroutine BCPREP to determine if a change of boundary conditions is required; subroutine FASEMB to assemble the element matrices over all elements; subroutine FBC to implement the boundary conditions; subroutine BLKITR, PISS, PPCG, or ILUCG to solve the matrix equations; subroutine FSFLOW to calculate flux through all types of boundaries and water accumulated in the media; subroutine FPRINT to print out the results; and subroutine

FSTORE to store the flow variables in binary format for plotting. Figure 2.3 shows the flow chart of this subroutine.

Subroutine SPROP

This subroutine calculates the values of moisture content, relative hydraulic conductivity, and the water capacity. This subroutine calls subroutine SPFUNC to calculate soil property function by either tabular input or analytical functions.

Subroutine BCPREP

This subroutine is called by HMCHYD to prepare the infiltration-seepage boundary conditions during a rainfall period or the seepage-evapotranspiration boundary conditions during non-rainfall periods. It decides the number of nodal points on the variable boundary to be considered as Dirichlet or Cauchy points. It computes the number of points that change boundary conditions from ponding depth (Dirichlet types) to infiltration (Cauchy types), or from infiltration to ponding depth, or from minimum pressure (Dirichlet types) to infiltration during rainfall periods. It also computes the number of points that change boundary conditions from potential evapotranspiration (Cauchy types) to minimum pressure, or from ponding depth to potential evapotranspiration, or from minimum pressure to potential evapotranspiration during non-rainfall periods. Upon completion, this subroutine returns the Darcy flux (DCYFLX), infiltration/potential evapotranspiration rate (FLX), the ponding depth nodal index (NPCON), the flux-type nodal index (NPFLX), the minimum pressure nodal index (NPMIN), and the number of nodal points (NCHG) that have changed boundary conditions.

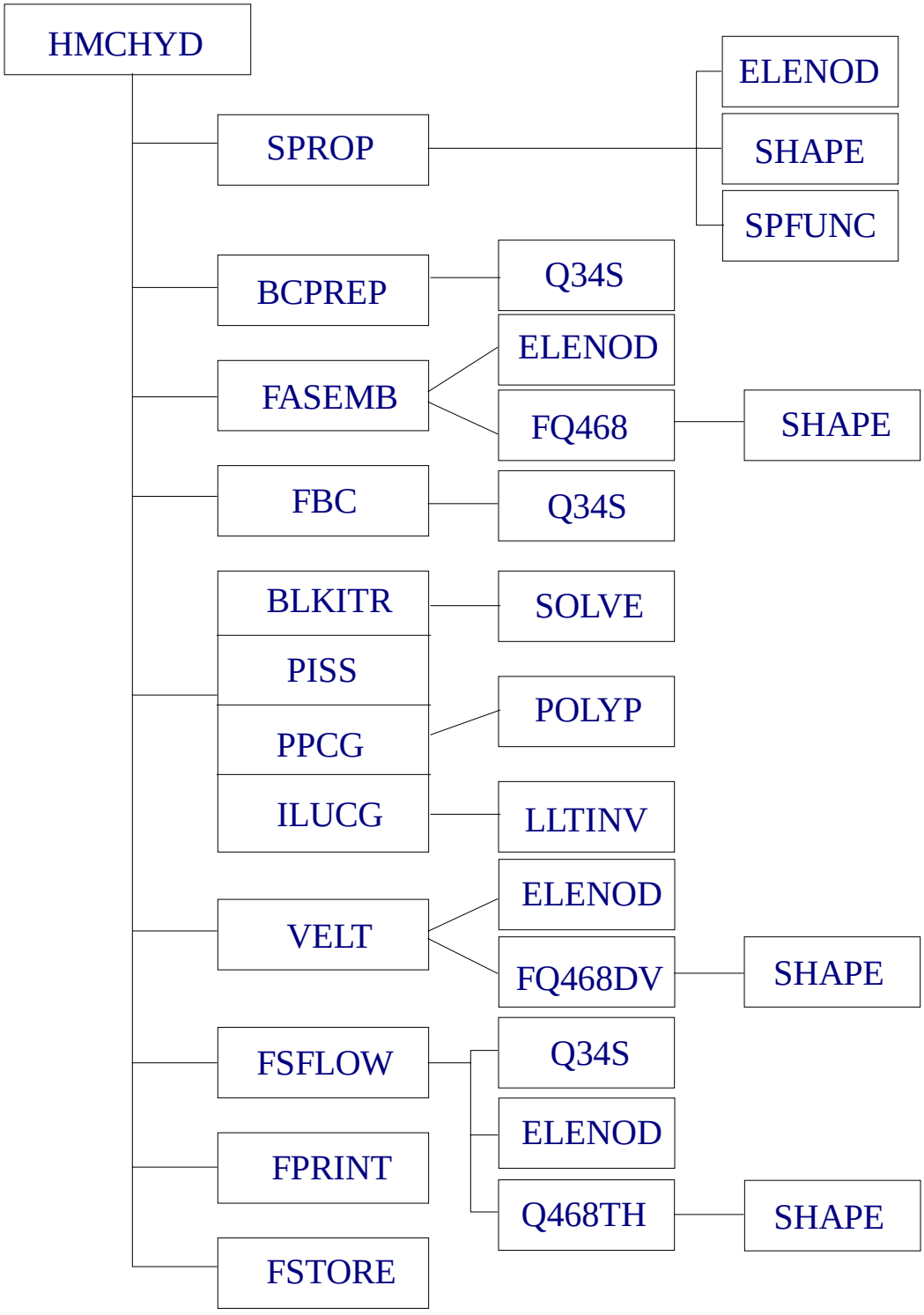


Figure 2.3 Program Structure of 3DFATMIC (Flow Part)

Subroutine SPFUNC

This subroutine calculates the soil property function by either tabular input or analytical functions. When analytical functions are used, the users must supply the functional form and modify this subroutine.

Subroutine FASEMB

This subroutine calls FQ468 to evaluate the element matrices. It then sums over all element matrices to form a global matrix equation governing the pressure head at all nodes.

Subroutine FQ468

This subroutine is called by the subroutine FASEMB to compute the element matrix given by

$$QA(I,J) = \int_{R_e} N_i^e \frac{\rho}{\rho_o} \frac{d\theta}{dh} N_j^e dR \ , \tag{2.49a}$$

$$QB(I,J) = \int_{R_e} (\nabla N_i^e) \cdot \mathbf{K_s} K_r \cdot (\nabla N_j^e) dR \ , \tag{2.49b}$$

Subroutine FQ468 also calculates the element load vector given by

$$RQ(I) = \int_{R_e} [- (\nabla N_i^e) \cdot \mathbf{K} \cdot \frac{\rho}{\rho_o} (\nabla z) + N_i^e \frac{\rho^*}{\rho_o} q] dR \ , \tag{2.49c}$$

where q is the source/sink.

Subroutine SHAPE

This subroutine is called by subroutines SPROP, FQ468, FQ468DV, Q468TH, TQ468DV,TQ468, and Q468R to evaluate the value of the base and weighting functions and their derivatives at a Gaussian point. The computation is straightforward.

Subroutine FBC

This subroutine incorporates Dirichlet, Cauchy, Neumann, and variable boundary conditions. For a Dirichlet boundary condition, an identity algebraic equation is generated for each Dirichlet nodal point. Any

other equation having this nodal variable is modified accordingly to simplify the computation. For a Cauchy surface, the integration of the surface source is obtained by calling the subroutine Q34S, and the result is added to the load vector. For a Neumann surface, the integrations of both the gradient and gravity fluxes are obtained by calling the subroutine Q34S. These fluxes are added to the load vector. The subroutine FBC also implements the variable boundary conditions. First, it checks all infiltration-evapotranspiration-seepage points, identifying any of them that are Dirichlet points. If there are Dirichlet points, the method of incorporating Dirichlet boundary conditions mentioned above is used. If a given point is not the Dirichlet point, the point is bypassed. Second, it checks all rainfall-evaporation-seepage points again to see if any of them is a Cauchy point. If it is a Cauchy point, then the computed flux by infiltration or potential evapotranspiration is added to the load vector. If a given point is not a Cauchy point, it is bypassed. Because the infiltration-evaporation-seepage points are either Dirichlet or Cauchy points, all points are taken care of in this manner.

Subroutine Q34S

This subroutine is called by the subroutines BCPREP, FBC and FSFLOW to compute the surface node flux of the type

$$RQ(I) = \int_{B_e} N_i^e \frac{\rho}{\rho_o} q dB \ , \tag{2.50}$$

where q is either the Cauchy flux, Neumann flux, or gravity flux.

Subroutine BLKITR

This subroutine is called by the subroutines HMCHYD and HMCTRN to solve the matrix equation with block iteration methods. For each subregion, a block matrix equation is constructed based on the global matrix equation and two pointer arrays GNPLR and LNOJCN (see subroutine PAGEN), and the resulting block matrix equation is solved with the direct band matrix solver by calling subroutine SOLVE. This is done for all subregions for each iteration until a convergent solution is obtained. This subroutine and the subroutine SOLVE, to be described in the next paragraph, are needed only when the block iteration option is used.

Subroutine SOLVE

This subroutine is called by the subroutine BLKITR to solve for the matrix equation of the type

$$[C]\{x\} = \{y\} \tag{2.51}$$

where [C] is the coefficient matrix and {x} and {y} are two vectors. {x} is the unknown to be solved, and {y} is the known load vector. The computer returns the solution {y} and stores it in {y}. The computation is a standard banded Gaussian direct elimination procedure.

Subroutine PISS

This subroutine is called by subroutine HMCHYD and HMCTRN, if necessary, to solve the linearized matrix equation with pointwise iteration solution strategies.

Subroutine PPCG

This subroutine is called by the subroutines HMCHYD and HMCTRN, if necessary, to solve the linearized matrix equation with the preconditioned conjugate gradient method using the polynomial as a preconditioner. It calls to POLYP to invert the preconditioner.

Subroutine POLYP

This subroutine is called by the subroutine PPCG to solve for a modified residual that will be used in the preconditioned conjugate gradient algorithm.

Subroutine ILUCG

This subroutine is called by the subroutines HMCHYD and HMCTRN, if necessary, to solve the linearized matrix equation with the preconditioned conjugate gradient method using the incomplete Cholesky decomposition as a preconditioner. It calls to LLTINV to invert the preconditioner.

Subroutine LLTINV

This subroutine is called by the subroutine ILUCG to solve for a modified residual that will be used in the preconditioned conjugate gradient algorithm.

Subroutine VELT

This subroutine calls FQ468DV to evaluate the element matrices and the derivatives of the total head. It then sums over all element matrices to form a matrix equation governing the velocity components at all nodal points. To save computational time, the matrix is diagonalized by lumping. The velocity components can thus be solved point by point. The computed velocity field is then returned to HTMICH or HMCHYD through the argument. This velocity field is also passed to subroutine BCPREP to evaluate the Darcy flux across the seepage-infiltration-evapotranspiration surfaces.

Subroutine FQ468DV

Subroutine FQ468DV is called by the subroutine VELT to compute the element matrices given by

$$QB(I,J) = \int_{B_e} N_i^e N_j^e dR \ , \tag{2.52}$$

where N_i^e and N_j^e are the basis functions for nodal point i and j of element e, respectively. Subroutine FQ468DV also evaluates the element load vector:

$$QRX(I) = -\int_{R_e} N_i^e \mathbf{i}\cdot\mathbf{K}\cdot\frac{\rho_o}{\rho}(\nabla N_j^e)h_j dR - \int_{R_e} N_i^e \mathbf{i}\cdot\mathbf{K}\cdot\nabla z dR \tag{2.53a}$$

$$QRY(I) = -\int_{R_e} N_i^e \mathbf{j}\cdot\mathbf{K}\cdot\frac{\rho_o}{\rho}(\nabla N_j^e)h_j dR - \int_{R_e} N_i^e \mathbf{j}\cdot\mathbf{K}\cdot\nabla z dR \tag{2.53b}$$

$$QRZ(I) = -\int_{R_e} N_i^e \mathbf{k}\cdot\mathbf{K}\cdot\frac{\rho_o}{\rho}(\nabla N_j^e)h_j dR - \int_{R_e} N_i^e \mathbf{k}\cdot\mathbf{K}\cdot\nabla z dR \tag{2.53c}$$

where

h_j = the referenced pressure head at nodal point j,
i = the unit vector along the x-coordinate,
j = the unit vector along the y-coordinate,
k = the unit vector along the z-coordinate,
K = the hydraulic conductivity tensor.

Subroutine FSFLOW

This subroutine is used to compute the fluxes through various types of boundaries and the increasing rate of water content in the region of interest. The function of FRATE(7) is to store the flux through the whole boundary enclosing the region of interest. It is given by

$$\text{FRATE}(7) = \int_B (V_x n_x + V_y n_y + V_z n_z) dB \ , \qquad (2.54)$$

where B is the global boundary of the region of interest; V_x, V_y, and V_z are Darcy's velocity components; and n_x, n_y, and n_z are the directional cosines of the outward unit vector normal to boundary B. FRATE(1) through FRATE(5) store the flux through Dirichlet boundary B_D, Cauchy boundary B_C, Neumann boundary B_N, the seepage/evapotranspiration boundary B_s, and infiltration boundary B_r, respectively, and are given by

$$\text{FRATE}(1) = \int_{B_d} (V_x n_x + V_y n_y + V_z n_z) dB \ , \qquad (2.55a)$$

$$\text{FRATE}(2) = \int_{B_c} (V_x n_x + V_y n_y + V_z n_z) dB \ , \qquad (2.55b)$$

$$\text{FRATE}(3) = \int_{B_n} (V_x n_x + V_y n_y + V_z n_z) dB \ , \qquad (2.55c)$$

$$\text{FRATE}(4) = \int_{B_s} (V_x n_x + V_y n_y + V_z n_z) dB \ , \qquad (2.55d)$$

$$\text{FRATE}(5) = \int_{B_R} (V_x n_x + V_y n_y + V_z n_z) dB \ , \qquad (2.55e)$$

FRATE(6), which is related to the numerical loss, is given by

$$\text{FRATE(6)} = \text{FRATE(7)} - \sum_{I=1}^{5} \text{FRATE(I)} \tag{2.56}$$

FRATE(8) and FRATE(9) are used to store the source/sink and increased rate of water within the media, respectively:

$$\text{FRATE(8)} = -\int_R \frac{\rho^*}{\rho} q dR \ , \tag{2.57}$$

and

$$\text{FRATE(9)} = \int_R \frac{\rho}{\rho_o} \frac{d\theta}{dh} \frac{\partial h}{\partial t} dR \ , \tag{2.58}$$

If there is no numerical error in the computation, the following equation should be satisfied:

$$\text{FRATE(9)} = -[\text{FRATE(7)} + \text{FRATE(8)}] \tag{2.59}$$

and FRATE(6) should be equal to zero. Equation (2.58) simply states that the negative rate of water going out from the region through the entire boundary and due to a source/sink is equal to the rate of water accumulated in the region.

Subroutine Q468TH

This subroutine is used to compute the contribution of the increasing rate of the water content from an element e

$$\text{QTHP} = \int_{R_e} \frac{\rho}{\rho_o} \frac{d\theta}{dh} \frac{\partial h}{\partial t} dR \ , \tag{2.60}$$

The computation of the above integration is straightforward.

Subroutine HMCTRN

The subroutine HMCTRN controls the entire sequence of transport computations. HMCTRN calls subroutine AFABTA to obtain upstream weighting factor based on velocity and dispersivity; subroutine

DISPC to calculate the dispersion coefficient associated with each Gaussian point in every element; subroutine THNODE to compute the value of moisture content plus bulk density times distribution coefficient in the case of linear isotherm, or the moisture content in the case of nonlinear isotherm at all nodes; subroutine GNTRAK to compute the Lagrangian concentrations at all global nodes, subroutine HPTRAK to perform forward particle tracking to obtain the Lagrangian concentrations at all activated forward nodes; subroutine ADVBC to implement boundary conditions in the Lagrangian step; subroutine ADVRX to calculate the Lagrangian concentrations with microbial-chemical involved; subroutine SFDET to determine sharp front elements; subroutine FGDET to imbed fine grids into every sharp front element; subroutine ISEHIL to prepare ISE array which stores the indices of subelements and to determine the activation of the points with the highest or lowest concentrations in each subelement; subroutine DFPREP to prepare the fine mesh nodes and elements for diffusion zooming; subroutine TASEMB to assemble the element matrices over all elements; subroutine TBC to implement the boundary conditions globally; subroutine TBC1 to apply intra-boundary conditions which implement the slave point concept to overcome the incompatibility; subroutine BLKITR, PISS, PPCG, or ILUCG to solve the resulting matrix equations; subroutine FLUX to compute material flux; subroutine TSFLOW to calculate flux through all types of boundaries and water accumulated in the media; subroutine TPRINT to print out the results; and subroutine TSTORE to store the results for plotting; Figure 2.4 shows the flow chart of this subroutine.

Subroutine THNODE

This subroutine is called by HMCTRN to compute the $(\theta + \rho_b dS/dC)$.

Subroutine AFABTA

This subroutine calculates the values of upstream weighting factors along 12 , 9, or 6 sides of all hexahedral, triangular prism, and tetrahedral elements, respectively.

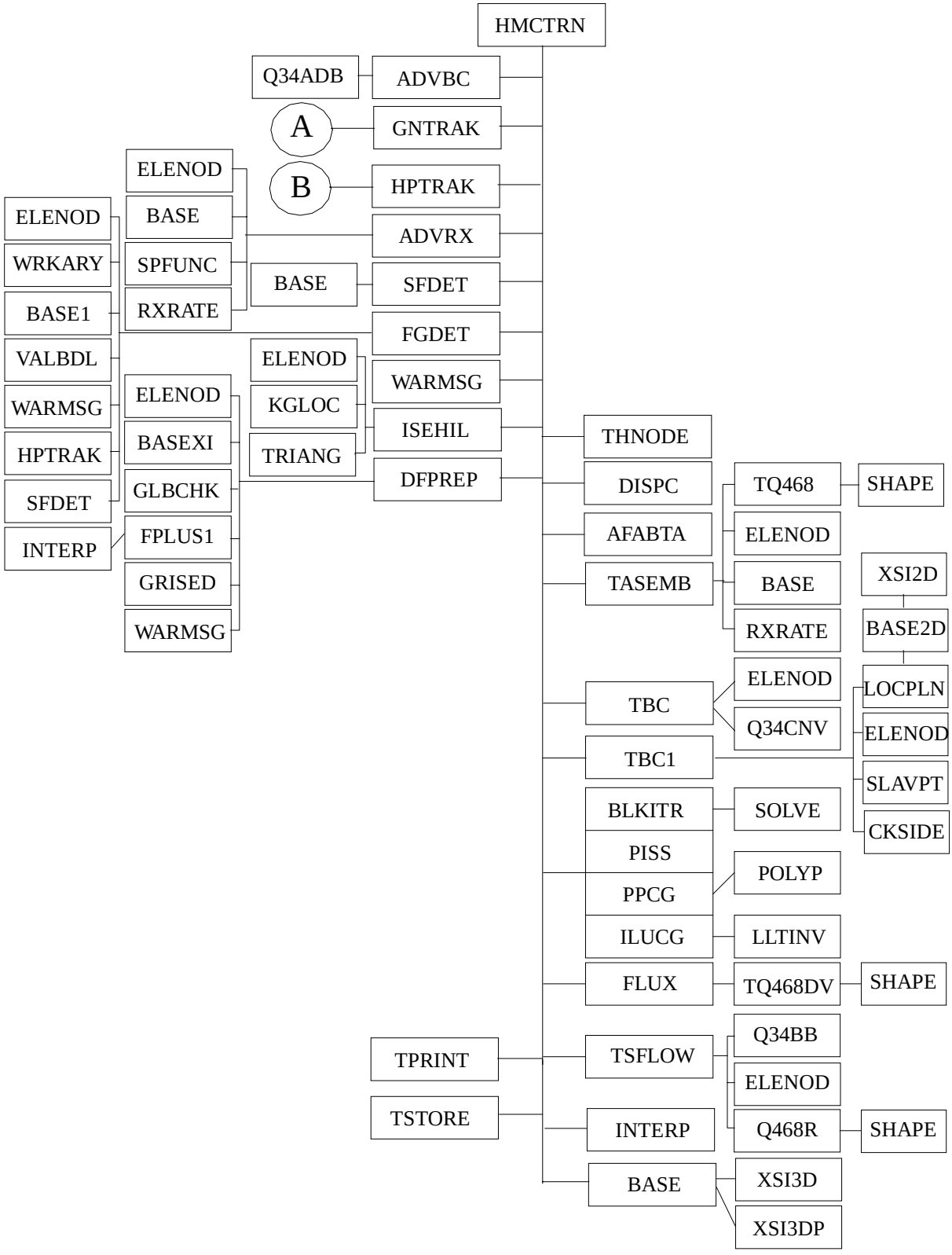


Figure 2.4 Program Structure of 3DFATMIC (Transport Part 1 of 3)

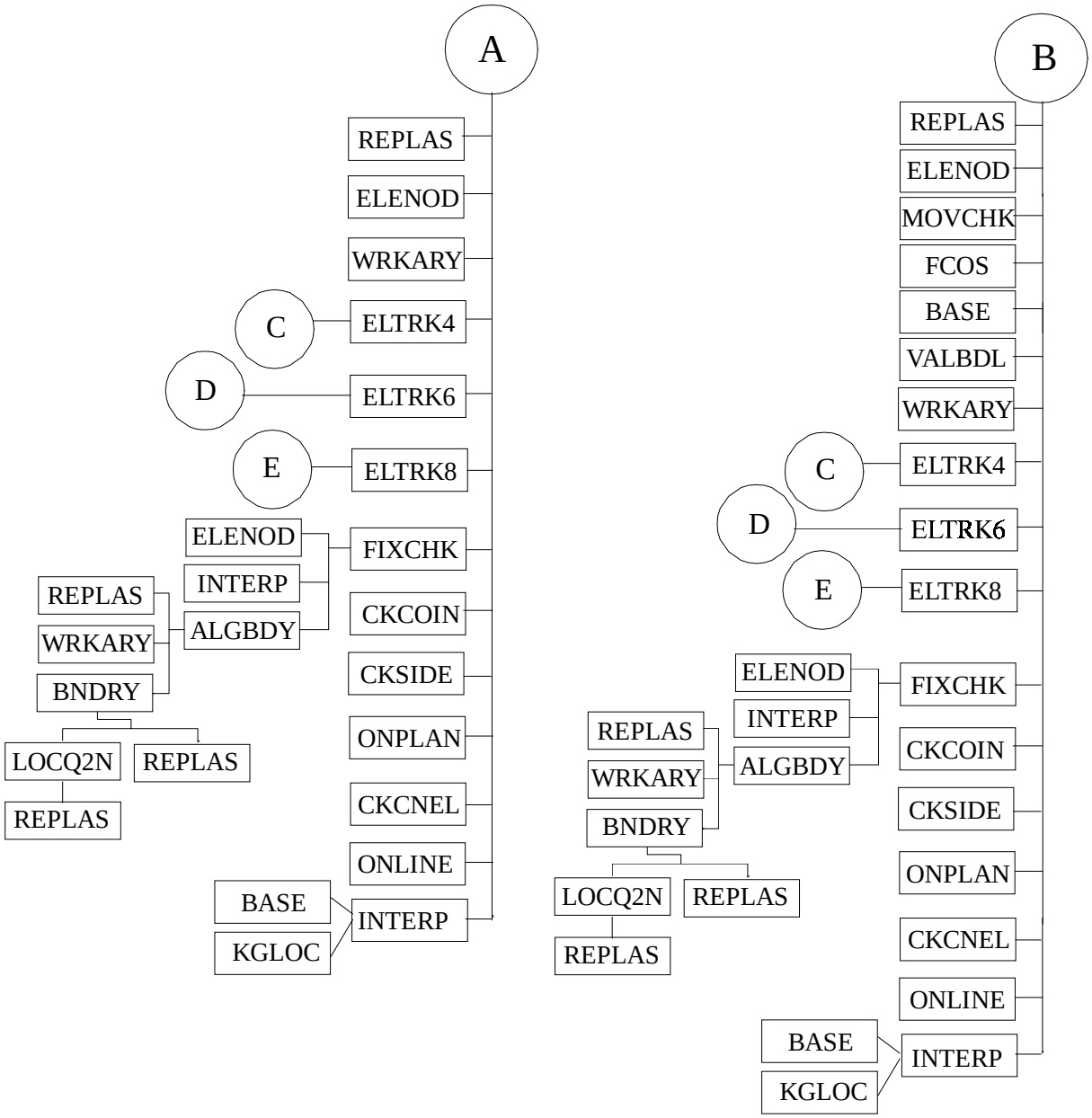


Figure 2.4 Program Structure of 3DFATMIC (Transport Part 2 of 3)

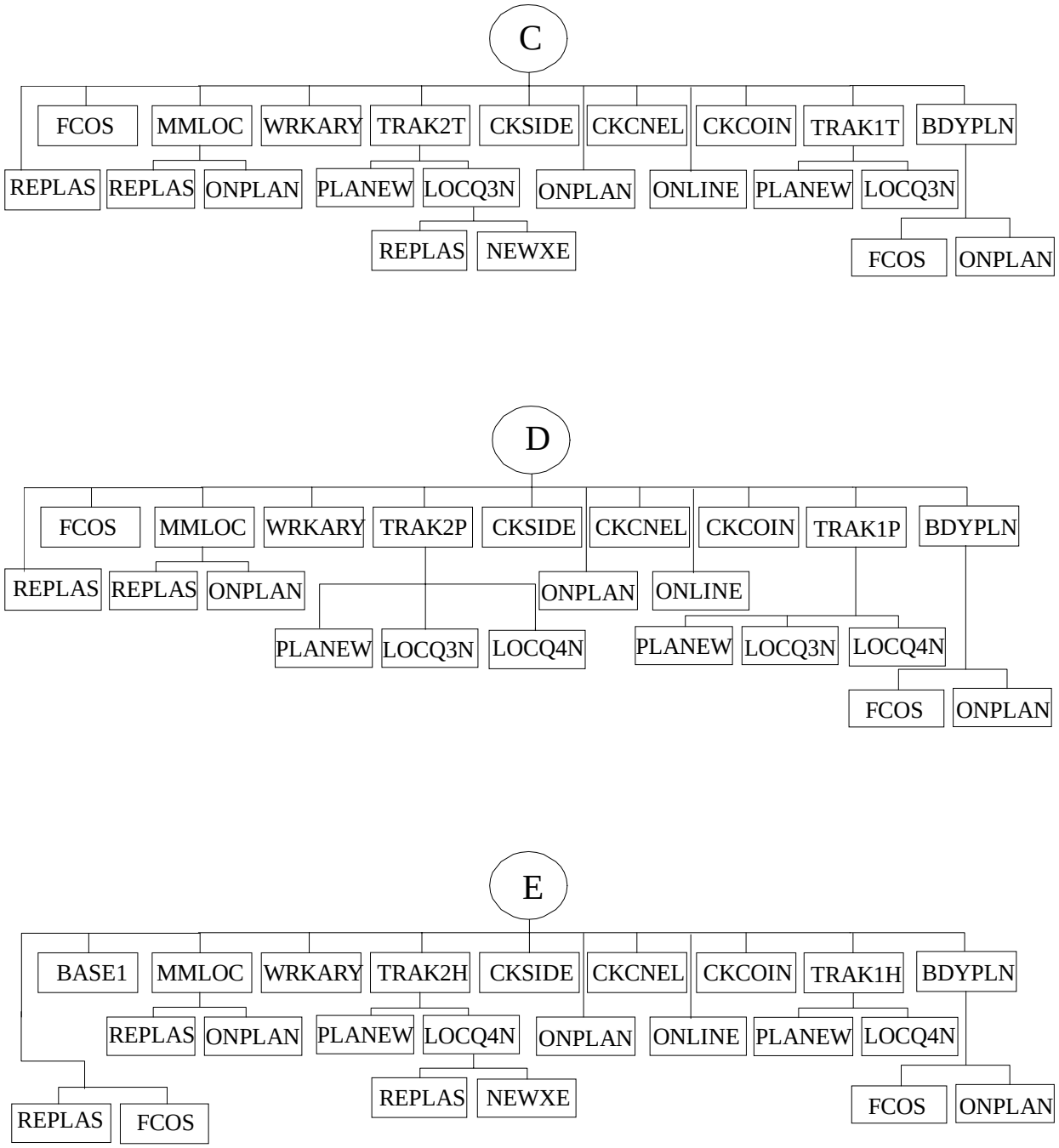


Figure 2.4 Program Structure of 3DFATMIC (Transport Part 3 of 3)

Subroutine DISPC

Subroutine DISPC calculates the dispersion coefficient associated with each Gaussian point of an element.

Subroutine TASEMB

This subroutine calls TQ468 to evaluate the element matrices. It then sums over all element matrices to form a global matrix equation governing the concentration distribution at all nodes.

Subroutine TQ468

This subroutine is called by the subroutine TASEMB to compute the element matrix given by

$$QA(I,J) = \int_{R_e} N_i^e \theta N_j^e dR \ , \tag{2.61a}$$

$$QAA(I,J) = \int_{R_e} N_j^e \rho_b \frac{dS}{dC} N_j^e dR \ , \tag{2.61b}$$

$$QB(I,J) = \int_{R_e} (\nabla N_i^e) \cdot \theta \mathbf{D} \cdot (\nabla N_j^e) dR \ , \tag{2.61c}$$

$$QV(I,J) = \int_{R_e} N_i^e \mathbf{V} \cdot (\nabla N_j^e) dR \ , \tag{2.61d}$$

$$QC(I,J) = \int_{R_e} N_i^e \left[\lambda(\theta + \rho_b \frac{dS}{dC}) + \frac{\rho^*}{\rho} q - \frac{\rho_o}{\rho} \mathbf{V} \cdot \nabla \left(\frac{\rho}{\rho_o} \right) \right] N_j^e dR \ , \tag{2.61e}$$

where dS/dC should be evaluated at C_w, the dissolved concentration at previous iteration. Subroutine TQ468 also calculates the element load vector given by:

$$QR(I) = \int_{R_e} N_i^e \left[-\lambda \rho_b \left(S_w - \frac{dS}{dC} C_w \right) + qC_{in} \right] dR \ , \qquad (2.61f)$$

where C_w and S_w are the dissolved and adsorbed concentrations at previous iteration, respectively.

Subroutine TBC

This subroutine incorporates Dirichlet, variable boundary, Cauchy, and Neumann boundary conditions. For a Dirichlet boundary condition, an identity algebraic equation is generated for each Dirichlet nodal point. Any other equation having this nodal variable is modified accordingly to simplify the computation. For a variable surface, the integration of the normal velocity times the incoming concentration is added to the load vector and the integration of normal velocity is added to the matrix. For the Cauchy boundaries, the integration of Cauchy flux is added to the load vector and the integration of normal velocity is added to the matrix. For the Neumann boundary, the integration of gradient flux is added to the load vector.

Subroutine Q34CNV

This subroutine is called by the subroutines TBC to compute the surface node flux of the type

$$RQ(I) = \int_{R_e} N_i^e q dB \ , \qquad (2.62)$$

where q is either the Cauchy flux, Neumann flux, or $\mathbf{n} \cdot \mathbf{V} C_v$. It also computes the boundary element matrices

$$BQ(I,J) = \int_{R} N_i^e \mathbf{V} N_j^e dR \qquad (2.63)$$

Subroutine TBC1

This subroutine is called whenever the total number of nodes for composing matrix is greater than the total number of global nodes, i.e., the diffusion zooming scheme is employed. The "slave point" concept takes care of the incompatibility for the intraboundary points between rough and smooth regions. This subroutine implements the concept so that the entries for the intraboundary points of the matrix equation can be modified. If there are diffusion fine grids falling on the global boundaries, the "slave point" concept also resolves the

problems of implementation of boundary conditions for these fine grids. Subroutine LOCPLN is called to obtain the basis functions of the intraboundary point in the intraboundary surface which may be a four point quadrilateral or three point triangular. Subroutine SLAVPT is called to implement the spirit of "slave point" concept. For simplicity, two point line segment is used for obtaining basis functions instead of surface after calling subroutine CKSIDE.

Subroutine SLAVPT

This subroutine implements the "slave point" concept on the intraboundary points between rough and smooth regions. This subroutine is called by subroutine TBC1 to modify the entries of the matrix equation related to these points.

Subroutine FLUX

This subroutine calls TQ468DV to evaluate the element matrices and the derivatives of concentrations. It then sums over all element matrices to form a matrix equation governing the flux components at all nodal points. To save computational time, the matrix is diagonalized by lumping. The flux components due to dispersion can thus be solved point by point. The flux due to the velocity is then added to the computed flux due to dispersion. The computed total flux field is then returned to HMCTRN through the argument.

Subroutine TQ468DV

Subroutine TQ468DV is called by the subroutine FLUX to compute the element matrices given by

$$QB(I,J) = \int_{R_e} N_i^e N_j^e dR \ , \tag{2.64}$$

where N_i^e and N_j^e are the basis functions for nodal point i and j of element e, respectively. Subroutine TQ468DV also evaluates the element load vector:

$$QRX(I) = -\int_{R_e} N_i^e \mathbf{i}\cdot\theta\mathbf{D}\cdot(\nabla N_j^e)C_j dR \ , \tag{2.65a}$$

$$QRY(I) = -\int_{R_e} N_i^e \mathbf{j}\cdot\theta\mathbf{D}\cdot(\nabla N_j^e)C_j dR \ , \tag{2.65b}$$

$$QRZ(I) = -\int_{R_e} N_i^e \mathbf{k}\cdot\theta\mathbf{D}\cdot(\nabla N_j^e)C_j dR \ , \tag{2.65c}$$

where C_j is the concentration at nodal point j, **i** is the unit vector along the x-direction, **j** is the unit vector along the y-coordinate, **k** is the unit vector along the z-coordinate, θ is the moisture content, and **D** is the dispersion coefficient tensor.

Subroutine TSFLOW

This subroutine is used to compute the flux rates through various types of boundaries and the increasing rate of material in the region of interest. FRATE(7) is to store the flux through the whole boundary

$$FRATE(7) = \int_B (F_x n_x + F_y n_y + F_z n_z) dB \ , \tag{2.66}$$

where B is the global boundary of the region of interest; F_x, F_y, and F_z are the flux components; and n_x, n_y, and n_z are the directional cosines of the outward unit vector normal to the boundary B. FRATE(1) stores the flux rates through Dirichlet boundary B_d. FRATE(2) and FRATE(3) store the flux rate through Cauchy and Neumann boundaries, respectively. FRATE(4) and FRATE(5) store incoming flux and outgoing flux rates, respectively, through the variable boundaries B_v^- and B_v^+, as given by

$$FRATE(1) = \int_{B_d} (F_x n_x + F_y n_y + F_z n_z) dB \ , \tag{2.67a}$$

$$FRATE(2) = \int_{B_c} (F_x n_x + F_y n_y + F_z n_z) dB \ , \tag{2.67b}$$

$$\text{FRATE}(3) = \int_{B_n} (F_x n_x + F_y n_y + F_z n_z)\, dB \ , \tag{2.67c}$$

$$\text{FRATE}(4) = \int_{B_{v^-}} (F_x n_x + F_y n_y + F_z n_z)\, dB \ , \tag{2.67d}$$

$$\text{FRATE}(5) = \int_{B_{v^+}} (F_x n_x + F_y n_y + F_z n_z)\, dB \ , \tag{2.67e}$$

where B_{v^-} and B_{v^+} are that part of variable boundary where the fluxes are directed into the region and out from the region, respectively. The integration of Eqs. (2.67a) through (2.67e) is carried out by the subroutine Q34BB.

FRATE(6) stores the flux rate through unspecified boundaries as

$$\text{FRATE}(6) = \text{FRATE}(7) - \sum_{I=1}^{5} \text{FRATE}(I) \tag{2.68}$$

FRATE(8) and FRATE(9), which store the accumulate rate in dissolved and adsorbed phases, respectively, are given by

$$\text{FRATE}(8) = \int_R \frac{\partial \theta C}{\partial t} dR \ , \tag{2.69}$$

$$\text{FRATE}(9) = \int_R \frac{\partial \rho_b S}{\partial t} dR \ , \tag{2.70}$$

FRATE(10) stores the rate loss due to decay and FRATE(11) through FRATE(13) are set to zero as given by

$$\text{FRATE}(10) = \int_R \lambda(\theta C + \rho_b S) dR \ , \tag{2.71}$$

$$\text{FRATE}(11)=\text{FRATE}(12)=\text{FRATE}(13)=0\ , \tag{2.72}$$

FRATE(14) is used to store the source/sink rate as

$$\text{FRATE}(14)=\int_R \text{QC}_{in}\frac{1+\text{sign}(\text{Q})}{2}+\text{QC}\frac{1-\text{sign}(\text{Q})}{2}\,\text{dR} \tag{2.73}$$

If there is no numerical error in the computation, the following equation should be satisfied:

$$\sum_{\text{I}=7}^{14}\text{FRATE}(\text{I})=0 \tag{2.74}$$

and FRATE(6) should be equal to zero.

Subroutine Q34BB

This subroutine is called by the subroutine TSFLOW to perform surface integration of the following type

$$\text{RRQ}(\text{I})=\int_{R_e} N_i^{\,e}\text{F}\,\text{dB}\ , \tag{2.75}$$

where F is the normal flux.

Subroutine Q468R

This subroutine is used to compute the contributions to FRATE(8), FRATE(9), FRATE(10), and FRATE(14):

$$\text{QRM}=\int_R \theta\text{C}\,\text{dR}\ , \tag{2.76a}$$

$$\text{QDM}=\int_R \text{S}\,\text{dR}\ , \tag{2.76b}$$

$$SOSM = \int_R \frac{QC_{in}(1 + sign(Q)) + QC(1 - sign(Q))}{2} dR \ , \qquad (2.76c)$$

The computation of the above integration is straightforward.

Subroutine ADVBC

This subroutine is called by HMCTRN to implement the boundary conditions. For Dirichlet boundary, the Lagrangian concentration is specified. For variable boundaries, if the flow is directed out of the region, the fictitious particle associated with the boundary node must come from the interior nodes. Hence the Lagrangian concentration for the boundary node has already computed from subroutine GNTRAK and the implementation for such a boundary segment is bypassed. For variable boundaries, if the flow is directed into the region, the concentration of incoming fluid is specified. An intermediate concentration C^{**} is calculated according to

$$C_i^{**} = \int_{B_v^-} N_i V_n C_{in} dB / \int_{B_v^-} N_i V_n dB \ , \qquad (2.77a)$$

where C_i^{**} is the concentration due to the boundary source at the boundary node i, V_n is the normal vertically integrated Darcy's velocity, and C_{in} is the concentration of incoming fluid.

Cauchy boundary conditions are normally applied to the boundary where flow is directed into the region, where the material flux of incoming fluid is specified. The intermediate concentration is thus calculated according to

$$C_i^{**} = \int_{B_c} N_i q_c dB / \int_{B_c} N_i V_n dB \ , \qquad (2.77b)$$

where C_i^{**} is the concentration due to Cauchy fluxes at the boundary node i, V_n is the normal Darcy's velocity, and q_c is the Cauchy flux of the incoming fluid.

The Lagrangian concentration is obtained by using the value C_i^{**} and C_i^n (the concentration at previous time step) as follows

$$C_i^* = \frac{\int_B N_i \theta N_j C_i^{**} dB + \int_B N_i \rho_b K_d N_j C_j^n dB}{\int_B N_i (\theta + \rho_b K_d) dB} \quad \text{for linear isotherm} \tag{2.78a}$$

$$C_i^* = C_i^{**} \quad \text{for nonlinear isotherm} \tag{2.78b}$$

Subroutine Q34ADB

This subroutine is used to perform surface integration of Eqs. (2.77a), (2.77b), and (2.78a) for Cauchy and variable boundary conditions. Each surface elemental matrix is returned to subroutine ADVBC to compose a global surface elemental matrix equation so that the Lagrangian concentrations of all the specified boundary points can be solved.

Subroutine GNTRAK

This subroutine is called by HMCTRN to control the process of backward particle tracking starting from global nodes. In the subroutine, each particle is tracked one element by one element until either the tracking time is completely consumed or the particle encounters a specified boundary side. During the particle tracking, this subroutine calls (1) subroutine ELTRK4 to track a particle in a tetrahedral element, (2) subroutine ELTRK6 to track a particle in a triangular prism element, and (3) subroutine ELTRK8 to track a particle in a hexahedral element. When the particle can not be tracked by normally elemental tracking, it calls subroutine FIXCHK to check if it hits specified or unspecified boundaries. In order to make the particle tracking complete and remedy the given velocity field error on the unspecified boundaries, subroutine FIXCHK calls subroutine ALGBDY to continue tracking particles along the unspecified/Neumann boundaries. At the end of backward particle tracking, the concentrations are obtained by interpolation executed in subroutine INTERP.

Subroutine HPTRAK

This subroutine is called by HMCTRN to compute the locations and concentrations of all forward-tracked find-mesh nodes. Basically, the algorithm of this subroutine is the same as that of subroutine GNTRAK.

Subroutine ADVRX

This subroutine solves the following seven nonlinear simultaneous ordinary differential equations

$$\left(\theta+\rho_b K_{ds}\right)\frac{DC_s}{Dt} = -\left[\left(\theta+\rho_b K_{d1}\right)C_1\right]\left\{\frac{\mu_o^{(1)}}{Y_o^{(1)}}\left[\frac{C_s}{K_{so}^{(1)}+C_s}\right]\left[\frac{C_o}{K_o^{(1)}+C_o}\right]\left[\frac{C_p}{K_{po}^{(1)}+C_p}\right]\right\}$$

$$-\left[\left(\theta+\rho_b K_{d2}\right)C_2\right]\left\{\frac{\mu_n^{(2)}}{Y_n^{(2)}}\left[\frac{C_s}{K_{sn}^{(2)}+C_s}\right]\left[\frac{C_n}{K_n^{(2)}+C_n}\right]\left[\frac{C_p}{K_{pn}^{(2)}+C_p}\right]\right\} \qquad (2.79a)$$

$$-\left[\left(\theta+\rho_b K_{d3}\right)C_3\right]\left\{\begin{array}{l}\dfrac{\mu_o^{(3)}}{Y_o^{(3)}}\left[\dfrac{C_s}{K_{so}^{(3)}+C_s}\right]\left[\dfrac{C_o}{K_o^{(3)}+C_o}\right]\left[\dfrac{C_p}{K_{po}^{(3)}+C_p}\right] \\ +\dfrac{\mu_n^{(3)}}{Y_n^{(3)}}\left[\dfrac{C_s}{K_{sn}^{(3)}+C_s}\right]\left[\dfrac{C_n}{K_n^{(3)}+C_n}\right]\left[\dfrac{C_p}{K_{pn}^{(3)}+C_p}\right]I\left(C_o\right)\end{array}\right\}$$

$$\left(\theta+\rho_b K_{do}\right)\frac{DC_o}{Dt} =$$

$$-\left[\left(\theta+\rho_b K_{d1}\right)C_1\right]\left\{\gamma_o^{(1)}\mu_o^{(1)}\left[\frac{C_s}{K_{so}^{(1)}+C_s}\right]\left[\frac{C_o}{K_o^{(1)}+C_o}\right]\left[\frac{C_p}{K_{po}^{(1)}+C_p}\right]+\alpha_o^{(1)}\lambda_o^{(1)}\left[\frac{C_o}{\Gamma_o^{(1)}+C_o}\right]\right\} \qquad (2.79b)$$

$$-\left[\left(\theta+\rho_b K_{d3}\right)C_3\right]\left\{\gamma_o^{(3)}\mu_o^{(3)}\left[\frac{C_s}{K_{so}^{(3)}+C_s}\right]\left[\frac{C_o}{K_o^{(3)}+C_o}\right]\left[\frac{C_p}{K_{po}^{(3)}+C_p}\right]+\alpha_o^{(3)}\lambda_o^{(3)}\left[\frac{C_o}{\Gamma_o^{(3)}+C_o}\right]\right\}$$

$$\left(\theta + \rho_b K_{dn}\right)\frac{DC_n}{Dt} =$$

$$-\left[\left(\theta + \rho_b K_{d2}\right)C_2\right]\left\{\gamma_n^{(2)}\mu_n^{(2)}\left[\frac{C_s}{K_{sn}^{(2)} + C_s}\right]\left[\frac{C_n}{K_n^{(2)} + C_n}\right]\left[\frac{C_p}{K_{pn}^{(2)} + C_p}\right] + \alpha_n^{(2)}\lambda_n^{(2)}\left[\frac{C_n}{\Gamma_n^{(2)} + C_n}\right]\right\} \qquad (2.79c)$$

$$-\left[\left(\theta + \rho_b K_{d3}\right)C_3\right]\left\{\gamma_n^{(3)}\mu_n^{(3)}\left[\frac{C_s}{K_{sn}^{(3)} + C_s}\right]\left[\frac{C_n}{K_n^{(3)} + C_n}\right]\left[\frac{C_p}{K_{pn}^{(3)} + C_p}\right] + \alpha_n^{(3)}\lambda_n^{(3)}\left[\frac{C_n}{\Gamma_n^{(3)} + C_n}\right]\right\}$$

$$\left(\theta + \rho_b K_{dp}\right)\frac{DC_p}{Dt} = -\left[\left(\theta + \rho_b K_{d1}\right)C_1\right]\left\{\epsilon_o^{(1)}\frac{\mu_o^{(1)}}{Y_o^{(1)}}\left[\frac{C_s}{K_{so}^{(1)} + C_s}\right]\left[\frac{C_o}{K_o^{(1)} + C_o}\right]\left[\frac{C_p}{K_{po}^{(1)} + C_p}\right]\right\}$$

$$-\left[\left(\theta + \rho_b K_{d2}\right)C_2\right]\left\{\epsilon_n^{(2)}\frac{\mu_n^{(2)}}{Y_n^{(2)}}\left[\frac{C_s}{K_{sn}^{(2)} + C_s}\right]\left[\frac{C_n}{K_n^{(2)} + C_n}\right]\left[\frac{C_p}{K_{pn}^{(2)} + C_p}\right]\right\} \qquad (2.79d)$$

$$-\left[\left(\theta + \rho_b K_{d3}\right)C_3\right]\left\{\begin{array}{l}\epsilon_o^{(3)}\frac{\mu_o^{(3)}}{Y_o^{(3)}}\left[\frac{C_s}{K_{so}^{(3)} + C_s}\right]\left[\frac{C_o}{K_o^{(3)} + C_o}\right]\left[\frac{C_p}{K_{po}^{(3)} + C_p}\right] \\ + \epsilon_n^{(3)}\frac{\mu_n^{(3)}}{Y_n^{(3)}}\left[\frac{C_s}{K_{sn}^{(3)} + C_s}\right]\left[\frac{C_n}{K_n^{(3)} + C_n}\right]\left[\frac{C_p}{K_{pn}^{(3)} + C_p}\right]I\left(C_o\right)\end{array}\right\}$$

$$\left(\theta + \rho_b K_{d1}\right)\frac{DC_1}{Dt} = \left(\theta + \rho_b K_{d1}\right)C_1\left\{\mu_o^{(1)}\left[\frac{C_s}{K_{so}^{(1)} + C_s}\right]\left[\frac{C_o}{K_o^{(1)} + C_o}\right]\left[\frac{C_p}{K_{po}^{(1)} + C_p}\right] - \lambda_o^{(1)}\right\} \qquad (2.79e)$$

$$\left(\theta + \rho_b K_{d2}\right)\frac{DC_2}{Dt} = \left(\theta + \rho_b K_{d2}\right)C_2\left\{\mu_n^{(2)}\left[\frac{C_s}{K_{sn}^{(2)} + C_s}\right]\left[\frac{C_n}{K_n^{(2)} + C_n}\right]\left[\frac{C_p}{K_{pn}^{(2)} + C_p}\right] - \lambda_n^{(2)}\right\} \qquad (2.79f)$$

$$\left(\theta + \rho_b K_{d3}\right)\frac{DC_3}{Dt} = \left(\theta + \rho_b K_{d3}\right)C_3\{\mu_o^{(3)}\left[\frac{C_s}{K_{so}^{(3)} + C_s}\right]\left[\frac{C_o}{K_o^{(3)} + C_o}\right]\left[\frac{C_p}{K_{po}^{(3)} + C_p}\right] - \lambda_o^{(3)}$$

$$+ \mu_n^{(3)}\left[\frac{C_s}{K_{sn}^{(3)} + C_s}\right]\left[\frac{C_n}{K_n^{(3)} + C_n}\right]\left[\frac{C_p}{K_{pn}^{(3)} + C_p}\right]I(C_o) - \lambda_n^{(3)}I(C_o)\} \quad (2.79g)$$

This subroutine is called right after the Lagrangian concentrations have been obtained.

Subroutine RXRATE

This subroutine is called by subroutine ADVRX, and TASEMB at steady state simulations. Basically, the subroutine calculates the removal rate of substrate which is represented as the terms within the braces on the right hand side of Eqs. (2.79a) to (2.79g). The values of each bracket within the braces are returned to the calling subroutines for each component.

Subroutine SFDET

This subroutine determines if an element is a rough element based on the prescribed error tolerance criteria shown in Eq.(2.46). If the M-th element is a rough element, the array IE(M,11) is activated to M.

Subroutine FGDET

This subroutine generates regular fine grids prescribed by users within each rough element based on the information of IE(M,11) resulted from subroutine SFDET. It calls subroutine HPTRAK to obtain the Lagrangian concentrations of each activated fine grid.

Subroutine ISEHIL

This subroutine removes all the forward-tracked nodes in smooth elements and stores the indices of subelements into ISE array. In addition to regular fine grids refinement, subroutine ISEHIL also captures all the highest and lowest concentrations within each subelement. The located subelements of the high-low points

are determined by subroutine KGLOC. Once these high-low points are activated, subroutine TRIANG is called to tetrangulate this subelement and the indices of each tetrahedral are also stored in the ISE array.

Subroutine TRIANG

This subroutine is called by ISEHIL for tetrangulating the subelement including the points with peak/valley values. The indices of new created tetrahedrals are also stored in the ISE array.

Subroutine DFPREP

This subroutine prepares all the needed information for assembling the fine grid elemental matrices. It calls subroutines GLBCHK to check those points on the elemental boundary connecting to the outermost layer of rough region, which is smooth after the determination of subroutine SFDET bout rough in the Eulerian step; FPLUS1 to imbed diffusion fine grid points prescribed by users and calculate the associated concentrations; GRISED to prepare element indices for each subelement in the Eulerian step for composing the matrix equation and to store the arrays for the intra-boundary points between rough and smooth regions to overcome the incompatibility by implementing the "slave point" concept.

Subroutine BASEXI

This subroutine is called by subroutine DFPREP to calculate the coordinates of imbedded grids according to the passed global coordinates, the associated local coordinate, and computed base functions in the element.

Subroutine GLBCHK

This subroutine is called by subroutine DFPREP to check those generated fine grid points located on the elemental boundary sides of each global element to see if the fine grids coincide with global nodes, locate on the global boundaries, or intraboundaries between rough and smooth regions. The concentrations are interpolated by calling subroutine INTERP for all generated fine grids.

Subroutine FPLUS1

This subroutine is called by subroutine DFPREP to calculate concentrations of the generated fine grids which are not located on the elemental boundary sides of the element.

Subroutine GRISED

This subroutine is called by subroutine DFPREP to generate ISED array which stores the indices of each fine mesh for the Eulerian step. The information associated with the intraboundary points, which includes the global nodes composing this intraboundary surface and nodal connection data locally, is also prepared in this subroutine.

Subroutine REPLAS

This subroutine replaces the last six arguments with the first six arguments orderly.

Subroutine WRKARY

This subroutine prepares six working arrays for later usage.

Subroutine WARMSG

The arguments passed to this subroutine are N, MAXN, SUBNAM, VARNAM, and NO. The stop statement is activated whenever N is greater than MAXN, and a message is written in the output file to indicate which variable is overflow in subroutine SUBNAM.

Subroutine VALBDL

This subroutine calculates three interpolated values by the passed working arrays and basis functions.

Subroutine MOVCHK

This subroutine determines the concentrations and travel time of a fixed particle.

Subroutine ELTRK4

This subroutine counts the particle tracking in a tetrahedral element. In the subroutine, the subelement in which the starting point locates is dug out first. Starting from that subelement, the particle is tracked one subelement by one subelement until either the tracking time is completely consumed or the particle encounters a boundary side of the element being considered. During the particle tracking, this subroutine calls (1)

subroutine TRAK1T to track a particle in the considered subelement if that particle is right standing on a node of the subelement, and (2) subroutine TRAK2T to track a particle if that particle is not on any nodes of the subelement. In the particle tracking process, the average velocity approach is used if IJUDGE=1; the single velocity approach is used if IJUDGE=2.

Subroutine ELTRK6

This subroutine counts the particle tracking in a triangular prism element. In the subroutine, the subelement in which the starting point locates is dug out first. Starting from that subelement, the particle is tracked one subelement by one subelement until either the tracking time is completely consumed or the particle encounters a boundary side of the element being considered. During the particle tracking, this subroutine calls (1) subroutine TRAK1P to track a particle in the considered subelement if that particle is right standing on a node of the subelement, and (2) subroutine TRAK2P to track a particle if that particle is not on any nodes of the subelement. In the particle tracking process, the average velocity approach is used if IJUDGE=1; the single velocity approach is used if IJUDGE=2.

Subroutine ELTRK8

This subroutine counts the particle tracking in a hexahedral element. In the subroutine, the subelement in which the starting point locates is dug out first. Starting from that subelement, the particle is tracked one subelement by one subelement until either the tracking time is completely consumed or the particle encounters a boundary side of the element being considered. During the particle tracking, this subroutine calls (1) subroutine TRAK1H to track a particle in the considered subelement if that particle is right standing on a node of the subelement, and (2) subroutine TRAK2H to track a particle if that particle is not on any nodes of the subelement. In the particle tracking process, the average velocity approach is used if IJUDGE=1; the single velocity approach is used if IJUDGE=2.

Subroutine FIXCHK

This is a control panel to check the ongoing process when a particle hits the boundary of the region of interest. The backward tracked concentrations are obtained by interpolation if the boundary is specified including Dirichlet, Cauchy, and variable types. Otherwise, the particle tracking continues along the unspecified boundary till either the specified boundary is encountered or tracking time is consumed.

Function FCOS

This function computes the inner product of the normal vector of a given plane with a specified vector whose starting point stands on the plane. The result helps to determine where the endpoint of the specified vector is located.

Subroutine MMLOC

This subroutine is called by ELTRK4, ELTRK6, and ELTRK8 to locate the particle associated with a specific subelement for subsequent elemental tracking. If this particle coincides with the nodes of a subelement, ICODE=0 is returned. In addition, the information of the particle location with respect to each surface of this element is also registered.

Subroutine BDYPLN

This subroutine locates the four global nodal numbers for returning to GNTRAK when the particle hits a boundary of the working element. In addition, it calls subroutine ONPLAN to adjust the coordinate so that these five points are really on the same plane.

Subroutine TRAK1T

This subroutine computes the particle tracking in a specified tetrahedral subelement when the starting point coincides with a node of the subelement. This subroutine calls subroutine PLANEW to determine (1) whether the particle would move into the subelement or not, and (2) which side (a triangular side) of the subelement the particle would head onto if the particle does move into the subelement. After determining which side the particle is going to move onto, this subroutine calls subroutine LOCQ3N to compute the exact

location of the target point on the side. For accuracy, using the average velocity of both the starting point and the target point to locate the target point is firstly considered in the subroutine. However, if this average velocity approach is not able to deal with very complex velocity fields, the single velocity of the starting point is used to determine the location of the target point.

Subroutine TRAK2T

This subroutine computes the particle tracking in a specified tetrahedral subelement when the starting point does not coincide with a node of the subelement. This subroutine calls subroutine PLANEW to determine (1) whether the particle would move into the subelement or not, and (2) which side (a triangular side) of the subelement the particle would head onto if the particle does move into the subelement. After determining which side the particle is going to move onto, this subroutine calls subroutine LOCQ3N to compute the exact location of the target point on the side. For accuracy, using the average velocity of both the starting point and the target point to locate the target point is first considered in the subroutine. However, if this average velocity approach is not able to deal with very complex velocity fields, the single velocity of the starting point is used to determine the location of the target point.

Subroutine CKCNEL

This subroutine checks the elements connecting to a specific side plane.

Subroutine CKCOIN

This subroutine checks if a specific point coincides with a global node.

Subroutine ONPLAN

This subroutine adjusts the particle coordinates to be on the same plane with the element side.

Subroutine CKSIDE

This subroutine checks if a specific point is on a side line of a side plane.

Subroutine ONLINE

This subroutine adjusts the particle coordinates to be on the same line with the other two points.

Subroutine PLANEW

This subroutine determine which one of the two sides, separated by a specified plane, the particle would move onto. All the computations are made according to the average velocity approach and the single velocity approach, as the index parameter IJUDGE is 1 and 2, respectively.

Subroutine LOCQ3N

This subroutine locates the target point of a particle tracking in a specified element, which is either a tetrahedral or a triangular prism element. All the computations are made according to either the average velocity approach or the single velocity approach as the index parameter IJUDGE is 1 and 2, respectively. The Newton-Raphson method is used to solve a set of two simultaneous nonlinear algebraic equations such that the natural coordinates of the target point on the pre-determined element side (a triangular side) can be determined. With these natural coordinates, the location of the target point can be easily determined based on both the velocity of the source point and the geometrical relationship between the source point and the pre-determined element side. This subroutine also calls subroutine NEWXE to compute the new guess of this pair of natural coordinates.

Subroutine NEWXE

This subroutine is called by subroutines LOCQ3N and LOCQ4N for taking a new guess of local coordinates within the iteration loop built with Newton-Ralphson scheme.

Subroutine BASE2D

This subroutine is called by LOCPLN to compute the base function values associated with a specified point based on the given two-dimensional global coordinates. For the cases of quadrilateral elements, it calls XSI2D to calculate the local coordinates, and computes base functions with these determined local coordinates. For the cases of triangular elements, the base functions can be analytically determined based on the given global coordinates.

Subroutine XSI2D

This subroutine is called by BASE2D to compute the local coordinate of a quadrilateral element given the global coordinate within that element.

Subroutine TRAK1P

This subroutine computes the particle tracking in a specified triangular prism subelement when the starting point coincides with a node of the subelement. This subroutine calls subroutine PLANEW to determine (1) whether the particle would move into the subelement or not, and (2) which side (either a quadrilateral or a triangular side) of the subelement the particle would head onto if the particle does move into the subelement. After determining which side the particle is going to move onto, this subroutine calls subroutine LOCQ4N (if the side is a quadrilateral one) or subroutine LOCQ3N (if the side is a triangular one) to compute the exact location of the target point on the side. For accuracy, using the average velocity of both the starting point and the target point to locate the target point is first considered in the subroutine. However, if this average velocity approach is not able to deal with very complex velocity fields, the single velocity of the starting point is used to determine the location of the target point.

Subroutine TRAK2P

This subroutine computes the particle tracking in a specified triangular prism subelement when the starting point does not coincide with a node of the subelement. This subroutine calls subroutine PLANEW to determine (1) whether the particle would move into the subelement or not, and (2) which side (either a quadrilateral or a triangular side) of the subelement the particle would head onto if the particle does move into the subelement. After determining which side the particle is going to move onto, this subroutine calls subroutine LOCQ4N (if the side is a quadrilateral one) or subroutine LOCQ3N (if the side is a triangular one) to compute the exact location of the target point on the side. For accuracy, using the average velocity of both the starting point and the target point to locate the target point is first considered in the subroutine. However,

if this average velocity approach is not able to deal with very complex velocity fields, the single velocity of the starting point is used to determine the location of the target point.

Subroutine LOCQ4N

This subroutine locates the target point of a particle tracking in a specified element, which is either a hexahedral or a triangular prism element. All the computations are made according to the average velocity approach and the single velocity approach, as the index parameter IJUDGE is 1 and 2, respectively. When the average velocity approach is considered, the Newton-Ralphson method is used to solve a set of two simultaneous nonlinear algebraic equations such that the local coordinates of the target point on the pre-determined element side (a quadrilateral side) can be determined. With these local coordinates, the location of the target point can be easily determined based on both the velocity of the source point and the geometrical relationship between the source point and the pre-determined element side. This subroutine also calls subroutine NEWXE to compute the new guess of this pair of natural coordinates.

Subroutine BASE1

This subroutine is called by ELTRK8 to compute the base functions for hexahedral elements.

Subroutine TRAK1H

This subroutine computes the particle tracking in a specified hexahedral subelement when the starting point coincides with a node of the subelement. This subroutine calls subroutine PLANEW to determine (1) whether the particle would move into the subelement or not, and (2) which side (a quadrilateral side) of the subelement the particle would head onto if the particle does move into the subelement. After determining which side the particle is going to move onto, this subroutine calls subroutine LOCQ4N to compute the exact location of the target point on the side. For accuracy, using the average velocity of both the starting point and the target point to locate the target point is first considered in the subroutine. However, if this average velocity approach is not able to deal with very complex velocity fields, the single velocity of the starting point is used to determine the location of the target point.

Subroutine TRAK2H

This subroutine computes the particle tracking in a specified hexahedral subelement when the starting point does not coincide with a node of the subelement. This subroutine calls subroutine PLANEW to determine (1) whether the particle would move into the subelement or not, and (2) which side (a quadrilateral side) of the subelement the particle would head onto if the particle does move into the subelement. After determining which side the particle is going to move onto, this subroutine calls subroutine LOCQ4N to compute the exact location of the target point on the side. For accuracy, using the average velocity of both the starting point and the target point to locate the target point is first considered in the subroutine. However, if this average velocity approach is not able to deal with very complex velocity fields, the single velocity of the starting point is used to determine the location of the target point.

Subroutine ALGBDY

This subroutine is called by FIXCHK to control the process of backward particle tracking along the unspecified boundaries. In the subroutine, the particle tracking is executed one boundary side by one boundary side based on the nodal velocity component along the side being considered. The tracking will not be stopped until either the tracking time is completely consumed or the particle encounters a specified boundary side. This subroutine calls BNDRY to track a particle along a predetermined boundary side. For accuracy, using the average velocity of both the source point and the target point to locate the target point is first considered in the subroutine. However, if this average velocity approach is not able to deal with very complex velocity fields, the single velocity of the source point is used to determine the location of the target point.

Subroutine BNDRY

This subroutine is called by ALGBDY to locate the target point of a particle tracking along a specified boundary side. All the computations are made according to the average velocity approach and the single velocity approach, when the index parameter IJUDGE is 1 and 2, respectively. For both approaches, the location of the target point can be determined by calling subroutine LOCQ2N. However, when the velocity

field is very complex, there might be no solution with the average approach. Thus, IJUDGE is originally set to 1 and is changed to 2 if the average approach fails. This control is executed in ALGBDY.

Subroutine LOCQ2N

This subroutine locates the target point of a particle tracking on a line segment in a specified element. All the computations are made according to the average velocity approach and the single velocity approach, as the index parameter IJUDGE is 1 and 2, respectively. When the average velocity approach is considered, the Newton-Raphson method is used to solve nonlinear algebraic equations such that the local coordinates of the target point on the pre-determined element segment can be determined. With these local coordinates, the location of the target point can be easily determined based on both the velocity of the source point and the geometrical relationship between the source point and the pre-determined element side.

Subroutine INTERP

This subroutine computes the contaminant concentrations by interpolation with the basis functions calculated by subroutine BASE. Prior to preforming the interpolation, this subroutine may call subroutine KGLOC to locate the subelement on which the point falls if the global element is a rough element. This subroutine can also get the interpolated concentrations for a multi-component system.

Subroutine KGLOC

This subroutine is called by subroutine INTERP to obtain the subelement on which the point falls if the global element is a rough element. This subroutine also calls subroutine ONPLAN to guarantee the point is exactly on the plane if it has been checked to be on the plane within a very small distance.

Subroutine BASE

This subroutine calculates basis functions and the derivatives of basis functions for a specific point. The element shape can be either hexahedral, triangular prism, or tetrahedral. It also calls subroutine XSI3D and XSI3DP for transferring the global coordinate to local coordinate in a hexahedral element and triangular prism element, respectively.

Subroutine XSI3DP

This subroutine computes the local coordinate (in the vertical direction) and the natural coordinate (in the horizontal direction) of a triangular prism element given the global coordinates for both the specified and element nodes.

Subroutine XSI3D

This subroutine computes the local coordinates of a hexahedral element given the global coordinates for both the specified point and element nodes.

3. ADAPTATION OF 3DFATMIC TO SITE SPECIFIC APPLICATIONS

The following describes how one should apply the 3DFATMIC code for site-specific applications and how the data file should be prepared.

3.1 Parameters Specifications

For each site-specific problem, the users only need to specify the size of the problem by assigning 74 maximum control-integers with PARAMETER statement in the MAIN program. The list and definitions of the maximum control-integers required for both flow and transport simulations are given below:

Maximum Control-Integers for the Spatial Domain

MAXNPK = maximum no. of nodes,
MAXELK = maximum no. of elements,
MXBESK = maximum no. of boundary-element surfaces,
MXBNPK = maximum no. of boundary nodal points,
MXJBDK = maximum no. of nodes connected to any node,
MXKBDK = maximum no. of elements connected to any node,
MXTUBK = maximum no. of accumulated unspecified boundary sides which connected to each global node (used for transport part with the Lagrangian approach),
MXADNK = maximum no. of points used to solve matrix equation for transport part;

Maximum Control-Integers for the Time Domain

MXNTIK = maximum no. of time steps,
MXDTCK = maximum no. of times to reset the time step size;

Maximum Control-Integers for Subregions

LTMXNK = maximum no. of total nodal points in any subregion, including interior nodes, global boundary nodes, and intraboundary nodes. LTMXNK = 1 if the block iteration is not used.
LMXNPK = maximum no. of nodal points in any subregion, including interior nodes and global boundary nodes. LMXNPK = 1 if the block iteration is not used.
LMXBWK = maximum no. of the bandwidth in any subregion. LMXBWK = 1 if the block iteration is not used.
MXRGNK = maximum no. of subregions. MXRGNK = 1 if the block iteration is not used.

Maximum Control-Integers for Material and Soil Properties

MXMATK = maximum no. of material types,
MXSPMK = maximum no. of soil parameters per material to describe soil characteristic curves,
MXMPMK = maximum no. of material properties per material;

The maximum control-integers for flow simulations and their definitions are given as the following:

Maximum Control-Integers for Source/sinks, flow

MXSELh = maximum no. of source elements,
MXSPRh = maximum no. of source profiles,
MXSDPh = maximum no. of data points on each element source/sink profile,
MXWNPh = maximum no. of well nodal points,
MXWPRh = maximum no. of well source/sink profiles,
MXWDPh = maximum no. of data points on each well source/sink profile;

Maximum Control-Integers for Cauchy Boundary Conditions, flow

MXCNPh = maximum no. of Cauchy nodal points,
MXCESh = maximum no. of Cauchy element surfaces,
MXCPRh = maximum no. of Cauchy-flux profiles,
MXCDPh = maximum no. of data points on each Cauchy-flux profile;

Maximum Control-Integers for Neumann Boundary Conditions, flow

MXNNPh = maximum no. of Neumann nodal points,
MXNESh = maximum no. of Neumann element surfaces,
MXNPRh = maximum no. of Neumann-flux profiles,
MXNDPh = maximum no. of data points on each Neumann-flux profile;

Maximum Control-Integers for Rainfall-Seepage Boundary Conditions, flow

MXVNPh = maximum no. of variable nodal points,
MXVESh = maximum no. of variable element surfaces,
MXVPRh = maximum no. of rainfall profiles,
MXVDPh = maximum no. of data point on each rainfall profile;

Maximum Control-Integers for Dirichlet Boundary Conditions, flow

MXDNPh = maximum no. of Dirichlet nodal points,
MXDPRh = maximum no. of Dirichlet total head profiles,

MXDDPh = maximum no. of data points on each Dirichlet profile;

The maximum control-integers for transport simulations and their definitions are given as the following:

Maximum Control-Integers for Source/sinks, transport

MXSELc = maximum no. of source elements,
MXSPRc = maximum no. of source profiles,
MXSDPc = maximum no. of data points on each element source/sink profile,
MXWNPc = maximum no. of well nodal points,
MXWPRc = maximum no. of well source/sink profiles,
MXWDPc = maximum no. of data points on each well source/sink profile;

Maximum Control-Integers for Cauchy Boundary Conditions, transport

MXCNPc = maximum no. of Cauchy nodal points,
MXCESc = maximum no. of Cauchy element surfaces,
MXCPRc = maximum no. of Cauchy-flux profiles,
MXCDPc = maximum no. of data points on each Cauchy-flux profile;

Maximum Control-Integers for Neumann Boundary Conditions, transport

MXNNPc = maximum no. of Neumann nodal points,
MXNESc = maximum no. of Neumann element surfaces,
MXNPRc = maximum no. of Neumann-flux profiles,
MXNDPc = maximum no. of data points on each Neumann-flux profile;

Maximum Control-Integers for Flowin-Flowout Boundary Conditions, transport

MXVNPc = maximum no. of variable nodal points,
MXVESc = maximum no. of variable element surfaces,
MXVPRc = maximum no. of rainfall profiles,
MXVDPc = maximum no. of data point on each rainfall profile;

Maximum Control-Integers for Dirichlet Boundary Conditions, transport

MXDNPc = maximum no. of Dirichlet nodal points,
MXDPRc = maximum no. of Dirichlet total head profiles,
MXDDPc = maximum no. of data points on each Dirichlet profile;

Control-Integers for Number of Components in the system

MXNCCK = maximum no. of components in this system,

Maximum Control-Integers for Refined System

MXKGLDK = maximum no. of subelements in the Eulerian step;
MXLSVK = maximum no. of subelement sides located on the intra-boundaries between extended rough and smooth regions;
MXMSVK = maximum no. of global element sides located on the intra-boundaries between extended rough and smooth regions;
MXNDBK = maximum no. of diffusion fine nodal-points located on the global boundary;
MXNEPK = maximum no. of all forward tracked nodal points in the region of interest when the exact peak capture and oscillation free (EPCOF) numerical scheme is used. When EPCOF is not used, set MXNEPK = 1;
MXEPWK = maximum no. of forward tracked nodal points in any rough element when the exact peak capture and oscillation free (EPCOF) numerical scheme is used. When EPCOF is not used, set MXEPWK = 1;

MXNPWK = maximum no. of fine nodal-points in any global element for particle tracking;
MXELWK = maximum no. of subelements in any global element for particle tracking;
MXNPWS = maximum no. of fine nodal-points in any global element which surrounds point sources/sinks for obtaining more accurate Lagrangian concentrations with injection/extraction wells in the region of interest;
MXELWS = maximum no. of subelements in any global element which surrounds point sources/sinks for obtaining more accurate Lagrangian concentrations with injection/extraction wells in the region of interest.
MXNPFGK = maximum no. of forward tracked nodal points over the region of interest or maximum no. of fine nodal points plus peak/valley nodal points;
MXKGLK = maximum no. of subelements in the Lagrangian step;

For flow simulations only, to demonstrate how to specify the above maximum control-integers with PARAMETER statement in the MAIN, an example is given in the following.

Assume that a region of interest is discretized by 30 x 20 x 10 nodes and 29 x 19 x 9 hexahedral elements. In other words, the region is discretized with 30 nodes along the longitudinal or x-direction, 20 nodes along the lateral or y-direction, and 10 nodes along the vertical or z-direction. Since we have a total of 30 x 20 x 10 = 6,000 nodes, the maximum number of nodes is MAXNPK = 6000. The total number of elements is 29 x 19 x 9 = 4,959, i.e, MAXELK = 4959. For this simple discretization problem, the maximum connecting number of nodes to any of the 6,000 nodes in the region of interest is 27, i.e., MXJBDK = 27, and

the maximum connecting number of elements to any of the 6,000 nodes is 8, i.e. MXKBDK = 8. There will be 29 x 19 = 551 element surfaces each on the bottom and top faces of the region, 29 x 9 = 261 element-surfaces each on the front and back faces of the region, and 19 x 9 = 171 element-surfaces each on the left and right faces of the region. Thus, there will be a total of 1966 element-surfaces, i.e., MXBESK = 1966. Similarly, we can compute the surface-boundary nodes to be 1968, i.e., MXBNPK = 1968. Because no transport simulation is involved in this problem, MXADNK = MAXNPK = 6000.

In order to specify maximum control-integers related to subregion data, one has to know how the region of interest is subdivided into subregions. Assume that the region of interest is subdivided into 20 subregions, each subregion has 30 x 10 nodes. It is seen, in fact, a vertical slice is taken as a subregion. For this subregionalization, one has MXRGNK = 20. Each subregion has 30 x 10 = 300 nodes, resulting LMXNPK = 300. It is also seen that there will be 600 intraboundary nodes, 300 nodes each on the two neighboring slices of a subregion. Thus, one has LTMXNK = 900. For each subregion, the maximum bandwidth can be computed as LMXBWK = 23 if the nodes are labelled along the z-directions consecutively.

Assume that there will be a maximum of 11 elements that have the distributed sources/sinks (i.e., MXSELh = 11) and a maximum of 10 nodal points that can be considered as well sources/sinks (i.e., MXWNPh = 10). Also assume that there will be three different distributed source/sink profiles and five distinct point source/sink profiles. Then one will have MXSPRh = 3 and MXWPRh = 5. Further assume that four data points are needed to describe the distributed source/sink profiles as a function of time and that 8 data points are required to describe point source/sink profiles (i.e., MXSDPh = 4 and MXWDPh = 8).

To specify maximum control-integers for boundary conditions, it is assumed that the top face is a variable boundary (i.e., on the air-soil interface, either ponding, infiltration, or evapotranspiration may take place). On the left face, fluxes from the adjacent aquifer are known. On the right face, the total head is assumed known. On the bottom face, natural drainage is assumed to occur (i.e., the gradient of the pressure head can be assumed zero).

There are 20 x 10 = 200 nodes on the left face and 19 x 9 = 171 element surfaces; thus MXCNPh = 200 and MXCESh = 171. It is further assumed that there are two different fluxes going into the region through the left face and that each flux can be described by four data points as a function of time (i.e., MXCPRh = 2, and MXCDPh = 4). On the bottom surface, there are 30 x 20 = 600 nodes and 29 x 19 = 551 surface elements. Since the gradient of pressure head on the bottom surface is zero, there is only one Neumann flux profile, and two data points, one at zero time and the other at infinite time, are sufficient to describe the constant value of zero. Hence, one has MXNNPh = 600, MXNESh = 551, MXNPRh = 1, and MXNDPh = 2. On the top face, there will be 30 x 20 = 600 nodes and 29 x 19 = 551 surface elements. Assume that there are three different rainfall intensities that might fall on the air-soil interface, and that each rainfall intensity is a function of time and can be described by 24 data points. With these descriptions, one has MXVNPh = 600, MXVESh = 551, MXVPRh = 3, and MXVDPh = 24. On the right face, there are 20 x 10 = 200 nodes. Assume that there are twenty different values of the total head, one each on a vertical line of the right face. It is further assumed that each of these twenty total head can be described by 8 data points as function of time. One then has MXDNPh = 200, MXDPRh = 20, and MXDDPh = 8.

In this example, one has six material properties (six saturated hydraulic conductivity components) per material. Assume that the whole region of interest is made of three different kinds of materials. The characteristic curves of each material are assumed to be described by four parameters. One then has MXMATK = 3, MXMPMK = 6, and MXSPMK = 4. Assume that a 500-time-step simulation will be made and reinitiation of the change on the time-step size will be made for 20 times during the simulation, then one has MXNTIK = 500 and MXDTCK = 20. The other PARAMETER settings for transport part can be set to be 1.

From the above discussion, the following PARAMETER statements can be used to specify the maximum control-integers in the MAIN for the problem at hand:

```
      PARAMETER(MAXNPK=6000,MAXELK=4959,MXBNPK=1968,MXBESK=1966,
     >    MXTUBK=1,MXADNK=MAXNPK+0)
```

```
PARAMETER(MXJBDK=27,MXKBDK=8,MXNTIK=500,MXDTCK=20)
PARAMETER(LTMXNK=900,LMXNPK=300,LMXBWK=23,MXRGNK=20)
PARAMETER(MXMATK=4,MXSPMK=6,MXMPMK=6)

PARAMETER(MXSELh=11,MXSPRh=3,MXSDPh=4,MXWNPh=10,MXWPRh=5,MXWDPh=8)
PARAMETER(MXCNPh=200,MXCESh=171,MXCPRh=2,MXCDPh=4)
PARAMETER(MXNNPh=600,MXNESh=551,MXNPRh=1,MXNDPh=2)
PARAMETER(MXVNPh=600,MXVESh=551,MXVPRh=3,MXVDPh=24)
PARAMETER(MXDNPh=200,MXDPRh=20,MXDDPh=8)

PARAMETER(MXSELc=1,MXSPRc=1,MXSDPc=1,MXWNPc=1,MXWPRc=1,MXWDPc=1)
PARAMETER(MXCNPc=1,MXCESc=1,MXCPRc=1,MXCDPc=1)
PARAMETER(MXNNPc=1,MXNESc=1,MXNPRc=1,MXNDPc=1)
PARAMETER(MXVNPc=1,MXVESc=1,MXVPRc=1,MXVDPc=1)
PARAMETER(MXDNPc=1,MXDPRc=1,MXDDPc=1)

PARAMETER(MXNCCK=1)

PARAMETER(MXLSVK=1,MXMSVK=1,MXKGLDK=1,MXNDBK=1)
PARAMETER(MXNEPK=1,MXEPWK=1)
PARAMETER(MXNPWK=1,MXELWK=1,MXNPWS=1,MXELWS=1)
PARAMETER(MXNPFGK=1,MXKGLK=1)
```

In the following, for transport simulations only, it is demonstrated how to specify the maximum control-integers with PARAMETER statements in the MAIN with an example.

Assume that a region of interest is discretized by 30 x 20 x 10 nodes and 29 x 19 x 9 hexahedral elements. In other words, the region is discretized with 30 nodes along the longitudinal or x-direction, 20 nodes along the lateral or y-direction, and 10 nodes along the vertical or z-direction. In order to make sure that every element surface is on the same plane, the region of interest is re-discretized to triangular prism elements. Therefore, four triangular prisms are generated in each hexahedral element. As a matter of fact, 5,510 more nodes are installed and there are 19,836 elements in total. Since one has a total of 6,000+5,510 = 11,510 nodes, the maximum number of nodes is MAXNPK = 11,510. The total number of elements is 29 x 19 x 9 x 4 = 19,836, i.e, MAXELK = 19,836. For this simple discretization problem, the maximum connecting number of nodes to any of the 11,510 nodes in the region of interest is 15, i.e., MXJBDK = 15. The maximum number of elements connecting to any node is 8, thus MXKBDK = 8. There will be 29 x 19 x 4 = 2,204

element surfaces each on the bottom and top faces of the region, 29 x 9 = 261 element-surfaces each on the front and back faces of the region, and 19 x 9 = 171 element-surfaces each on the left and right faces of the region. Thus, there will be a total of 5,272 element-surfaces; i.e., MXBESK = 5,272. Similarly, one can compute the surface-boundary nodes to be 1968, i.e., MXBNPK = 3,302. Because this simulation selects the Lagrangian approach, MXTUBK value needs to be specified. For sake of safety one can assume that the maximum number of accumulated unspecified boundary element sides is equal to 4 times of the maximum number of boundary nodes; i.e. MXTUBK = 4 x MXBNPK = 13,208. According to the description of boundary conditions below, the front and back surfaces are not specified. Therefore, the total number of nodes with unspecified boundary conditions is 30×10×2 = 600. The maximum number of elements connected to each point on these two surfaces is 4. Actually, MXTUBK = 2,400 which saves a lot of storage in comparison to setting MXTUBK = 13,208. Assume that the number of imbedded diffusion fine grids in each rough element is NXD = 2, NYD =3, and NZD = 2. Then there are 2×2×2 = 8 fine grids imbedded in a triangular prism element. It is further assumed that 25 rough elements at the most existing through the whole simulation; i.e., MXADNK = 11,510 + 8 ×25 = 11,710.

In order to specify maximum control-integers related to subregion data, one has to know how the region of interest is subdivided into subregions. Assume one has subdivided the region of interest into 39 subregions. Twenty of them have 30 x 10 nodes, the other 19 subregions have 29 x 10 nodes each. It is seen, in fact, one has taken a vertical slice as a subregion. For this subregionalization, we have MXRGNK = 39. Each subregion has 300 or 290 nodes, resulting LMXNPK = 300. It is also seen that there will be 600 intraboundary nodes, 300 nodes each on the two neighboring slices of a subregion. Thus, one has LTMXNK = 890. For each subregion, the maximum bandwidth can be computed as LMXBWK = 23 if the nodes are labelled along the z-direction consecutively.

Assume that there will be a maximum of 11 elements that have the distributed sources/sinks (i.e., MXSELc = 11) and a maximum of 10 nodal points that can be considered as well sources/sinks (i.e.,

MXWNPc = 10). Also assume that there will be three different distributed source/sink profiles and five distinct point source/sink profiles. Then one will have MXSPRc = 3 and MXWPRc = 5. It is further assumed that four data points are needed to describe the distributed source/sink profiles as a function of time and that 8 data points are required to describe point source/sink profiles (i.e., MXSDPc = 4 and MXWDPc = 8).

To specify maximum control-integers for boundary conditions, assume that the top and right faces are variable boundaries. On the left face, fluxes from the adjacent aquifer are known. On the bottom face, the natural gradient is zero. The other faces are unspecified.

There are 20 x 10 = 200 nodes on the left face and 19 x 9 = 171 element surfaces; thus MXCNPc = 200 and MXCESc = 171. It is further assumed that there are two different fluxes going into the region through the left face and that each flux can be described by four data points as a function of time (i.e., MXCPRc = 2, and MXCDPc = 4). On the bottom surface, there are 30 x 20 + 29 x 19 = 1,151 nodes and 29 x 19 x 4 = 2,204 surface elements. Since the gradient of concentration on the bottom surface is zero, there is only one Neumann flux profile, and two data points, one at zero time and the other at infinite time, are sufficient to describe the constant value of zero. Hence, one has MXNNPc = 1,151, MXNESc = 2,204, MXNPRc = 1, and MXNDPc = 2. On the top face, there will be 30 x 20 + 29 x 19 = 1,151 nodes and 29 x 19 x 4 = 2,204 surface elements. The discretization on the right surface is the same as that on the left. Assume that there are three different mass intensities that might fall on the top and right faces, and that each concentration profile is a function of time and can be described by 24 data points. With these descriptions, one has MXVNPc = 1,351, MXVESc = 2,375, MXVPRc = 3, and MXVDPc = 24.

In this example, one has eight material properties per material. Assume that the whole region of interest is made of three different kinds of materials. One then has MXMATK = 3, and MXMPMK = 6. If one assumes that he will make a 500-time-step simulation and he will reinitiate the change on the time step size for 20 times during our simulation, then he has MXNTIK = 500 and MXDTCK = 20.

There are seven components, say microbe #1, microbe #2, microbe #3, substrate, oxygen, nitrate, and nutrient, involved in this system; i.e., MXNCCK = 7.

Assume that there are 25 rough elements and all of them are disconnected. It is further assumed that each element will be refined by 2 x 2 X 2 = 8 subelements in the Eulerian step to solve the diffusion problem. The maximum number of subelements for assembling in the diffusion step is MXKGLDK = 25 x 8 = 200. Since each rough triangular prism has 5 sides, the number of global element sides located on the intra-boundaries between rough and smooth regions is MXMSVK = 25 x 5 = 125. Each global element side is refined by 4 subelement sides, hence MXLSVK = 125 x 4 = 500. Assume that 5 out of the 25 rough elements have at least one side as the global boundary. It is further assumed that Rough Element 1 has two sides coinciding with the global boundary: one side has three global nodes and the other side has four global nodes. The 3-node side has 3 fine nodes and the 4-node side has 5 fine nodes. Thus, Rough Element 1 has 8 fine nodes on the global boundary. Also assume that Rough Elements 2 through 5 each has its 3-node side coinciding with the global boundary. For these 4 rough elements, one has 4 x 3 = 12 fine nodes on the global boundary. Hence, the number of diffusion fine nodal points on the global boundary is MXNDBK = 8 + 12 = 20.

The numerical schemes for solving transport equations are LEZOOMPC plus keeping EPCOF points in the Lagrangian step. For practical problems, EPCOF points will not be kept; thus, MXNEPK = 1, MXEPWK = 1. In the Lagrangian step, each element is assumed to be refined by 8 subelements (NXA = 2, NYA = 2, and NZA = 2) for accurate tracking. With this assumption, one has MXNPWK = (2+1) x (2+2) x (2+1)/2 = 18, MXELWK = (NXA x NYA x NZA) = 4. For each element connected to the sources/sinks, assume to it is refined with 3 x 3 x 2 elements for accurate computation of Lagrangian concentrations to yield MXNPWS = (3+1) x (3+2) x (2+1)/2 = 30 and MXELWS = 3 x 3 x 2 = 18.

The specification of MXNPFGK and MXKGLK is much more involved. These two control integers depend on many things: (1) how all the nodal points (including global nodes and fine nodal points) at the

beginning of a time-step simulation are forwardly tracked, (2) how many elements are rough at the end of the time-step computation, (3) how each rough element is refined, and (4) how many peak/valley points are kept. A detailed discussion on how to specify these two integers is given in Appendix C. For the time being, assume that MXNPFGK = 20000, MXKGLK = 10000,

From the above discussion, the following PARAMETER statements can be used to specify the maximum control-integers in the MAIN for the problem at hand:

```
      PARAMETER(MAXNPK=11510,MAXELK=19836,MXBNPK=3302,MXBESK=5272,
     >    MXTUBK=2400,MXADNK=MAXNPK + 200)
      PARAMETER(MXJBDK=15,MXKBDK=8,MXNTIK=500,MXDTCK=20)
      PARAMETER(LTMXNK=890,LMXNPK=300,LMXBWK=23,MXRGNK=39)
      PARAMETER(MXMATK=3,MXSPMK=6,MXMPMK=6)

      PARAMETER(MXSELh=1,MXSPRh=1,MXSDPh=1,MXWNPh=1,MXWPRh=1,MXWDPh=1)
      PARAMETER(MXCNPh=1,MXCESh=1,MXCPRh=1,MXCDPh=1)
      PARAMETER(MXNNPh=1,MXNESh=1,MXNPRh=1,MXNDPh=1)
      PARAMETER(MXVNPh=1,MXVESh=1,MXVPRh=1,MXVDPh=1)
      PARAMETER(MXDNPh=1,MXDPRh=1,MXDDPh=1)

      PARAMETER(MXSELc=11,MXSPRc=3,MXSDPc=4,MXWNPc=10,MXWPRc=5,MXWDPc=8)
      PARAMETER(MXCNPc=200,MXCESc=171,MXCPRc=2,MXCDPc=4)
      PARAMETER(MXNNPc=1151,MXNESc=2204,MXNPRc=1,MXNDPc=2)
      PARAMETER(MXVNPc=1351,MXVESc=2375,MXVPRc=3,MXVDPc=24)
      PARAMETER(MXDNPc=1,MXDPRc=1,MXDDPc=1)

      PARAMETER(MXNCCK=7)

      PARAMETER(MXLSVK=500,MXMSVK=125,MXKGLDK=200,MXNDBK=20)
      PARAMETER(MXNEPK=1,MXEPWK=1)
      PARAMETER(MXNPWK=18,MXELWK=8,MXNPWS=30,MXELWS=18)
      PARAMETER(MXNPFGK=20000,MXKGLK=10000)
```

3.2 Soil Property Function Specifications

Analytical functions are used to describe the relationships of water content, water capacity, and relative hydraulic conductivity with pressure head. Therefore, the user must supply three functions to compute the water content, water capacity, and relative hydraulic conductivity based on the current value of pressure head.

The parameters needed to specify the functional form are read and stored in SPP. One example is shown in the subroutine SPFUNC in the source code. In this example, the water content, water capacity, and relative hydraulic conductivity are given by (van Genuchten 1980):

$$\theta = \theta_r + \frac{\theta_s - \theta_r}{[1+(\alpha h)^n]^m} \tag{3.1}$$

$$\frac{d\theta}{dh} = \alpha(n-1)[1-f(\theta)]^m[f(\theta)](\theta_s - \theta_r) \tag{3.2}$$

$$K_r = [(\theta-\theta_r)/(\theta_s-\theta_r)]^{\frac{1}{2}}\{1-[1-f(\theta)]^m\}^2 \tag{3.3}$$

in which

$$f(\theta) = [\theta-\theta_r]/[\theta_s-\theta_r]^{1/m} \tag{3.4}$$

and

$$m = 1 - \frac{1}{n} \tag{3.5}$$

To further demonstrate how one should modify the subroutine SPFUNC in Appendix A to accommodate the material property functions that are different from those given by Eqs. (3.1) through (3.5), assume that the following Fermi types of functions are used to represent the unsaturated hydraulic properties (Yeh, 1987):

$$\theta = \theta_r + (\theta_s-\theta_r)/\{1+\exp[-\alpha(h-h_\theta)]\} \tag{3.6}$$

$$d\theta/dh = \alpha(\theta_s-\theta_r)\exp[-\alpha(h-h_\theta)]/\{1+\exp[-\alpha(h-h_\theta)]\}^2 \ , \tag{3.7}$$

and

$$\log_{10}(K_r) = \epsilon/\{1+\exp[-\beta(h-h_k)]\} - \epsilon \ , \tag{3.8}$$

where θ_s, θ_r, α, and h_θ are the parameters for computing the water content and water capacity; and β, ϵ, and h_k are the parameters for computing the relative hydraulic conductivity. The source code must be changed, for this example, to the following form for computing the moisture content and water capacity

```
      WCR=SPP(1,MTYP,1)
      WCS=SPP(2,MTYP,1)
      ALPHA=SPP(3,MTYP,1)
      HTHETA=SPP(4,MTYP,1)
      EPS=SPP(1,MTYP,2)
      BETA=SPP(2,MTYP,2)
      HSUBK=SPP(3,MTYP,2)
C
C ------- SATURATED CONDITION
C
      IF(HNP.LE.0.0) THEN
        TH=WCS
         IF(ISP .EQ. 1) GOTO 900
        DTH=0.0D0
        USKFCT=1.0D0
C
      ELSE
C
C ------ UNSATURATED CASE
C
       EXPAH=DEXP(-ALPHA*(HNP-HTHETA))
       TH=WCR+(WCS-WCR)/(1.0D0+EXPAH)
       DTH=ALPHA*(WCS-WCR)*EXPAH/(1.0D0+EXPAH)**2
       AKRLOG=EPS/(1.0D0+DEXP(-BETA*(HNP-HSUBK))) - EPS
       USKFCT=10.0D0**AKRLOG
      ENDIF
```

3.3 Input and Output Devices

Five logical units are needed to execute 3DFATMIC. Units 15 and 16 are standard card input and line printer devices, respectively. Unit 11 must be specified to store the flow simulation results, which can be used for plotting purposes. Unit 12 must be specified to store the transport simulation results, which can be used for plotting purposes. Unit 13 is used to store the boundary arrays for later uses, if these arrays are computed for the present job. Unit 14 is used to store pointer arrays for later uses, if these arrays are generated for the

present job. For large problems, experience has indicated that it would take too much time to process the boundary arrays and to generate pointer arrays. Hence, it is advisable that for multi-job executions, these boundary and pointer arrays should be computed only once and written on units 13 and 14, respectively. Once they are stored on units 13 and 14, the IGEOM described in Appendix A should be properly identified for the new job so they can be read via units 13 and 14, respectively. Finally, Unit 21 is used to print any variable for debugging purpose.

4. SAMPLE PROBLEMS

To verify 3DFATMIC, eight illustrative examples are used. Examples one, two, and three, originally designed for 3DFEMWATER (Yeh, 1993a), are the flow only problems. Examples four and five, originally designed for 3DLEWASTE (Yeh, 1993b), are the transport only problems. Example six is a two-dimensional biodegradation problem which is used to verify the flow and transport coupling loop and show the effects of biodegradation. Examples seven and eight illustrate the behavior of dissolved organic and oxygen plumes undergoing natural biodegradation in a uniform flow field.

4.1 Example 1: One-Dimensional Column Flow Problem

This example is selected to represent the simulation of a one-dimensional flow problem with 3DFATMIC. The column is 200 cm long and 50 by 50 cm in crosssection (Figure 5). The column is assumed to contain the soil with a saturated hydraulic conductivity of 10 cm/d, a porosity of 0.45 and a field capacity of 0.1. The unsaturated characteristic hydraulic properties of the soil in the column are given as

$$\theta = \theta_s - (\theta_s - \theta_r)\frac{h - h_a}{h_b - h_a} \tag{4.1}$$

and

$$K_r = \frac{\theta - \theta_r}{\theta_s - \theta_r} \tag{4.2}$$

where h_b and h_a are the parameters used to compute the water content and the relative hydraulic conductivity, respectively.

The initial conditions assumed are a pressure head of -90 cm imposed on the top surface of the column, 0 cm on the bottom surface of the column, and -97 cm elsewhere. The boundary conditions are given as: no flux is imposed on the left, front, right, and back surfaces of the column; pressure head is held at 0 cm on the bottom surface; and variable condition is used on the top surface of the column with a ponding

depth of zero, minimum pressure of -90 cm, and a rainfall of 5 cm/d for the first ten days and a potential evaporation of 5 cm/d for the second 10 days.

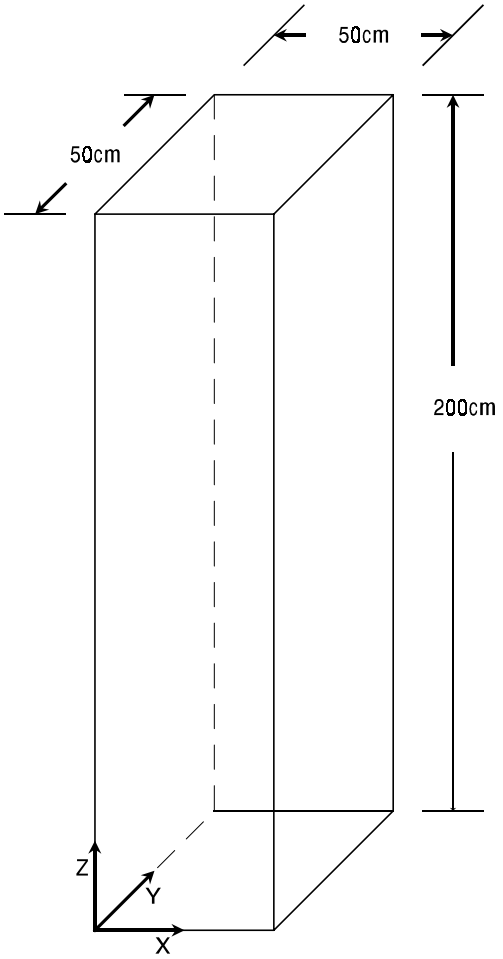


Figure 4.1 Problem definition and sketch for Example 1.

The region of interest, that is, the whole column, will be discretized with 1 x 1 x 40 = 40 elements with element size = 50 x 50 x 5 cm, resulting in 2 x 2 x 41 = 164 node points (Figure 6). For 3DFATMIC simulation, each of the four vertical lines will be considered a subregion. Thus, a total of four subregions, each with 41 node points, is used for the subregional block iteration simulation.

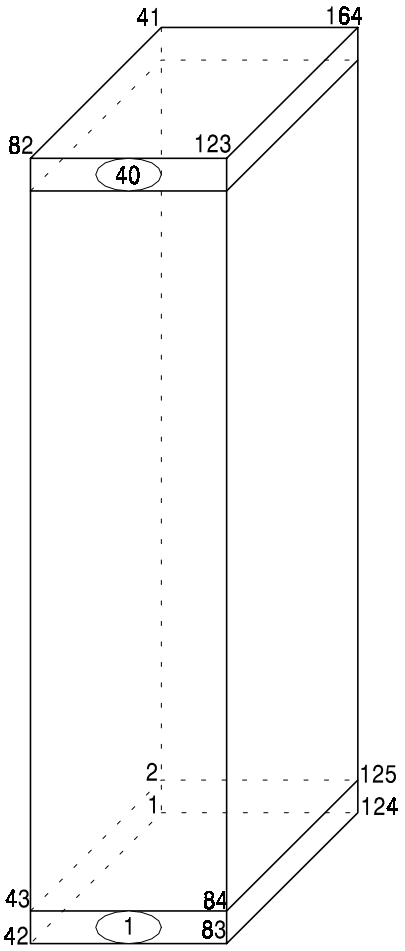


Figure 4.2 Finite element discretization for Example 1.

A variable time step size is used. The initial time step size is 0.05 days, and each subsequent time step size is increased by 0.2 times with a maximum time step size not greater than 1.0 d. Because there is an abrupt change in the flux value from 5 cm/d (infiltration) to -5 cm/d (evaporation) imposed on the top surface at day 10, the time step size is automatically reset to 0.05 d on the tenth day. A 20-day simulation will be made with 3DFATMIC. With the time step size described above, 44 time steps are needed.

The pressure head tolerance is $2 \cdot 10^{-2}$ cm for nonlinear iteration and is $1 \cdot 10^{-2}$ cm for block iteration. The relaxation factors for both the nonlinear iteration and block iteration are set equal to 0.5.

To execute the problem, the maximum control-integers in the main program should be specified as follows

```
C----- For Example 1 through Example 5
C
      PARAMETER(MAXNPK=2079,MAXELK=1600,MXBNPK=999,MXBESK=999,
      >                MXTUBK=3008,MXADNK=maxnpk+0)
       PARAMETER(MXJBDK=35,MXKBDK=8,MXNTIK=100,MXDTCK=4)
      PARAMETER(LTMXNK=693,LMXNPK=231,LMXBWK=49,MXRGNK=9)
      PARAMETER(MXMATK=8,MXSPMK=5,MXMPMK=9)

C-------- 2.  For flow source/sink, boundary conditions, and materials

      PARAMETER(MXSELh=1,MXSPRh=1,MXSDPh=1,MXWNPh=4,MXWPRh=2,MXWDPh=3)
      PARAMETER(MXCNPh=110,MXCESh=90,MXCPRh=1,MXCDPh=2)
      PARAMETER(MXNNPh=1,MXNESh=1,MXNPRh=1,MXNDPh=1)
      PARAMETER(MXVNPh=198,MXVESh=170,MXVPRh=2,MXVDPh=4)
      PARAMETER(MXDNPh=165,MXDPRh=11,MXDDPh=2)

C--------- 3.  For transport source/sink, boundary conditions, and materials
C
      PARAMETER(MXSELc=1,MXSPRc=1,MXSDPc=1,MXWNPc=4,MXWPRc=2,MXWDPc=5)
      PARAMETER(MXCNPc=55,MXCESc=40,MXCPRc=2,MXCDPc=4)
      PARAMETER(MXNNPc=11,MXNESc=4,MXNPRc=1,MXNDPc=2)
      PARAMETER(MXVNPc=638,MXVESc=560,MXVPRc=1,MXVDPc=2)
      PARAMETER(MXDNPc=70,MXDPRc=6,MXDDPc=2)
C
      PARAMETER(MXNCCK=2)
C
      PARAMETER(MXLSVK=500,MXMSVK=500,MXKGLDK=2000,MXNDBK=2000)
      PARAMETER(MXNEPK=20,MXEPWK=20)
      PARAMETER(MXNPWK=99,MXELWK=27, mxnpws=1331,mxelws=1000)
      PARAMETER(MXNPFGK=2900,MXKGLK=2800)
C
```

To reflect the soil property function given by Eqs. (4.1) and (4.2), one has to modify the subroutine SPFUNC. A segment of the code in the subroutine SPFUNC must be modified as follows:

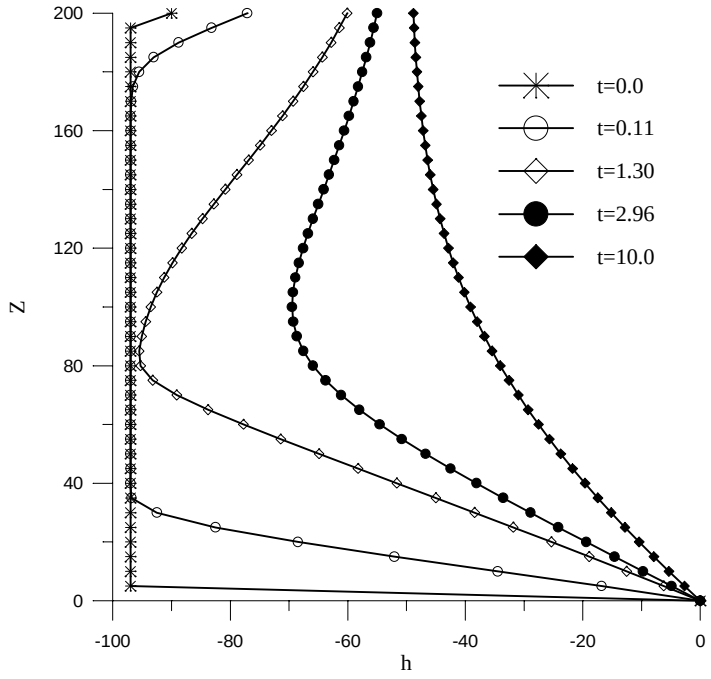
```
    WCR=SPP(1,MTYP,1)
    WCS=SPP(2,MTYP,1)
    HAA=SPP(3,MTYP,1)
    HAB=SPP(4,MTYP,1)
C
C ------- SATURATED CONDITION
C
    IF(HNP.LE.0) THEN
     TH=WCS
```

```
      IF(ISP .EQ. 1) GOTO 900
      DTH=0.0D0
      USKFCT=1.0D0
    ELSE
C
C ------- UNSATURATED CASE
C
      TH=WCS-(WCS-WCR)*(-HNP-HAA)/(HAB-HAA)
      IF(ISP.EQ.1) GOTO 900
      USKFCT=(TH-WCR)/(WCS-WCR)
      DTH=-(WCS-WCR)/(HAB-HAA)
    ENDIF
C
```

Figure 5 depicts the pressure profiles along the z-axis at various times.

4.2 Input and output for Example 1

With the above descriptions, the input data can be prepared according to the instructions given Appendix A. The input parameters are shown in Table 4.1 and the input data file content is given in Table 4.2. To save space, the output is available in electronic form.



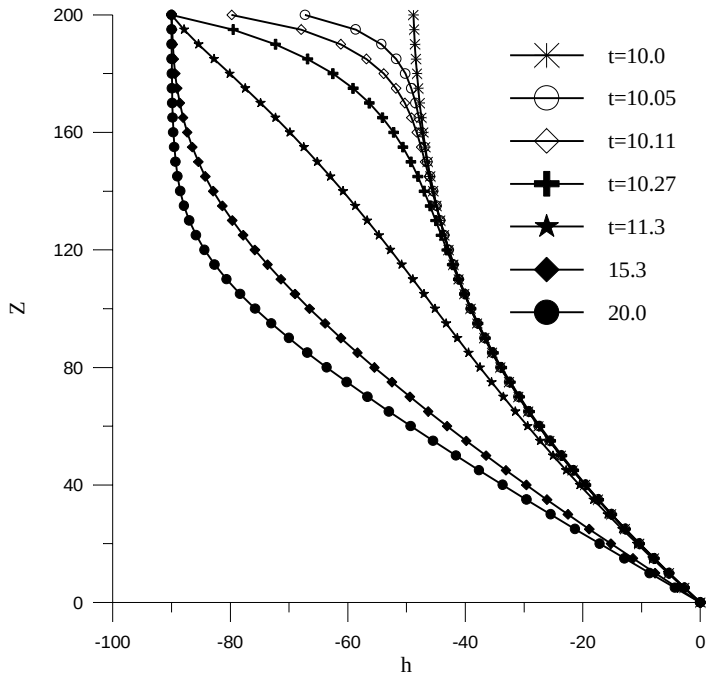


Figure 4.3 Pressure head profiles at various times.

Table 4.1 The list of input parameters for Example 1

Parameters	Notation in the data input guide	Value	Unit	Data set
number of points	NNP	164	Dimensionless	7. A.
Δx	XAD	50	cm	7. B.
Δy	YAD	50	cm	7. B.
Δz	ZAD	5	cm	7. B.
$K_{s,zz}$	PROPf(1,3)	10	cm/day	5. B.
θ_r	SPP(1,1,1)	0.15	dimensionless	6. B.
θ_s	SPP(2,1,1)	0.45	dimensionless	6. B.
h_a	SPP(3,1,1)	0	cm	6. B.
h_b	SPP(4,1,1)	-100	cm	6. B.
no. of subregion	NREGN	4	dimensionless	8. A.
no. of points in a subregion	NODES	41	dimensionless	8. B.
initial time step size	DELT	0.05	day	4. B.
time step size increment	CHNG	0.2	dimensionless	4. B.
maximum time step size	DELMAX	1	day	4. B.
no. of times to reset time step size	NDTCHG	1	dimensionless	4. A.
time to reset time step size	TDTCH(1)	10	day	5. E.
Total simulation time	TMAX	22	day	4. B.
no. of time steps	NTI	44	dimensionless	4. A.
tolerance for nonlinear iteration	TOLBf	2×10^{-2}	cm	3. A.
relaxation factor for nonlinear iteration	OMEf	0.5	dimensionless	2. C.
ρ_w	RHO	1.0	g/cm^3	5.B. & 6.A.
μ_w	VISC	9483.26	g/cm/day	5.B. & 6.A.
g	GRAV	7.32×10^{12}	cm/day^2	6.A.

Table 4.2 Input Data Set for Example 1

```
    1 One-Dimensional Column Flow Problem; L=CM, T=DAY, M=G
========= data set 2: option parameters
  10  0  1  0
 100  0.5d0  1.0d-4
 1  1  0  0  0  0  0  0 0 1
 1  1.0  0.5d0  0.5d0  0.0d0
 2  0  1  1  1
 1.0d0 0.5d0 1.0d0 1.0d0
========= data set 3: iteration parameters
 50 20 100 2.0d-2 2.0d-2
  1 100 1.0d-3  1.0d-4
========= data set 4: time control parameters
 44   2
 0.05d0    0.20d0    1.0d0    22.0d0
33303030003000300300003330303000300030030003
00000000000000000000000000000000000000000000
    1.0D01  2.0000D1
========= DATA SET 5:  MATERIAL PROPERTIES
  1 7 0 1
  0.0D0   0.0D0  10.0D0   0.0D0   0.0D0   0.0D0  1.0d0
  0.0d0
  1.0d0
========= DATA SET 6:  soil properties
    0    4    0    1.0d0    1.0d0   1.0d0
   0.150D0   0.450D0    0.00D0    -1.0D2   THPROP
   0.000D0   0.000D0    0.00D0     0.0D0   AKPROP
C ******* DATA SET 7:  NODE COORDINATES
  164
    1   40    1    0.0D0    50.0D0     0.0D0     0.0D0     0.0D0     5.0D0
   42   40    1    0.0D0     0.0D0     0.0D0     0.0D0     0.0D0     5.0D0
   83   40    1    50.0D0     0.0D0     0.0D0     0.0D0     0.0D0     5.0D0
  124   40    1    50.0D0    50.0D0     0.0D0     0.0D0     0.0D0     5.0D0
    0    0    0    0.0     0.0       0.0       0.0       0.0       0.0
C ******* DATA SET 8:  SUBREGIONAL DATA
    4
    1    3    1   41    0
    0    0    0    0    0        END OF NNPLR(K)
    1   40    1    1    1
    0    0    0    0    0        END OF GNLR(I,1)
    1   40    1   42    1
    0    0    0    0    0        END OF GNLR(I,2)
    1   40    1   83    1
    0    0    0    0    0        END OF GNLR(I,3)
    1   40    1  124    1
    0    0    0    0    0        END OF GNLR(I,4)
C ******* DATA SET 9:  ELEMENT INCIDENCES
   40
    1   39    1   42   83  124    1   43   84  125    2    1
    0    0    0    0    0    0    0    0    0   0    0   0   END OF IE
C ******* data set10: material correction
    0
C ******* DATA SET 11:  INITIAL CONDITIONS
    1    3   41          0.0D0     0.0D0     0.0D0
    2   38    1         -9.70D1     0.0D0     0.0D0
   43   38    1         -9.70D1     0.0D0     0.0D0
   84   38    1         -9.70D1     0.0D0     0.0D0
  125   38    1         -9.70D1     0.0D0     0.0D0
   41    3   41         -9.00D1     0.0D0     0.0D0
    0    0    0          0.0       0.0       0.0        END OF IC, flow
========= data set 12: element(distributed) source/sink, flow
```

```
    0 0 0 0
========= data set 13: point(well) source/sink, flow
    0 0 0 0
========= data set 16: rainfall/evaporation-seepage boundary conditions
    1  4  1  4  0
     0.0D0  5.0D0    10.0D0 5.0D0  10.001D0  -5.0D0    1.0D38 -5.0D0
    1    0    0    1    0
    0    0    0    0    0         END OF IRTYP
    1    0    0   82  123  164   41    0    0    0    0
    0    0    0    0    0    0    0    0    0    0    0 END OF ISV(J,I) J=1,4
    1    3    1   41   41
    0    0    0    0    0                          END OF NPVB
    1    3    1          0.0D0     0.0D0       0.0
    0    0    0          0.0       0.0         0.0   END OF HCON
    1    3    1        -90.0D0     0.0D0       0.0
    0    0    0          0.0       0.0         0.0   END OF HMIN
C ******* DATA SET 17:  DIRICHLET BOUNDARY CONDITIONS, flow
    4  1  2  0
     0.0D0     0.0D0    1.0D38     0.0D0
    1   3  1   1  41
    0   0  0   0  0
    1    3    1    1    0
    0    0    0    0    0                      END OF IDTYP
========= data set 18: cauchy boundary conditions, flow
    0 0 0 0 0
========= data set 19: neumann boundary conditions, flow
    0 0 0 0 0
    0                  END OF JOB
----------------------------------------0000
```

4.3 Example 2: Two-dimensional Flow Drainage Problem

This example is selected to represent the simulation of a two-dimensional flow problem with 3DFATMIC. The region of interest is bounded on the left and right by parallel drains fully penetrating the medium, on the bottom by an impervious aquifuge, and on the top by an air-soil interface (Figure 6). The distance between the two drains is 20 m apart (Figure 6).

The medium is assumed to have a saturated hydraulic conductivity of 0.01 m/d, a porosity of 0.25, and a field capacity of 0.05. The unsaturated characteristic hydraulic properties of the medium are given as

$$\theta = \theta_r + (\theta_s - \theta_r)\frac{A}{A + |h - h_a|^B} \tag{4.3}$$

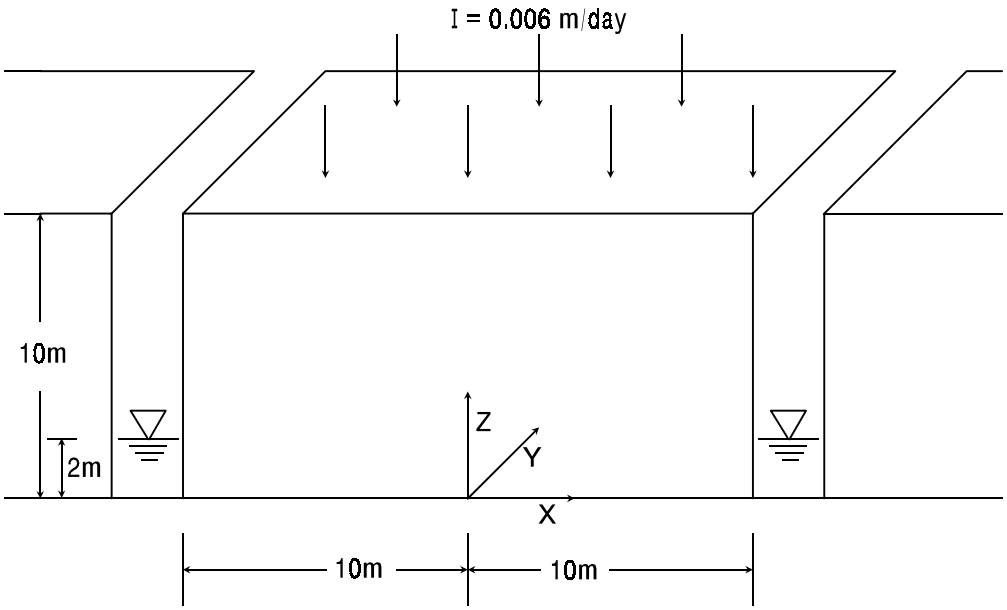


Figure 4.4 Problem definition and sketch for Example 2.

and

$$K_r = \left[\frac{\theta - \theta_r}{\theta_s - \theta_r}\right]^n \tag{4.4}$$

where h_a, A, and B are the parameters used to compute the water content and n is the parameter to compute the relative hydraulic conductivity.

Because of the symmetry, the region for numerical simulation will be taken as $0 < x < 10$ m and $0 < z < 10$ m, and 10 m wide along the y-direction will be assumed. The boundary conditions are given as: no flux is imposed on the left ($x = 0$), front ($y = 0$), back ($y = 10$), and bottom ($z = 0$) sides of the region; pressure head is assumed to vary from zero at the water surface ($z = 2$) to 2 m at the bottom ($z = 0$) on the right side ($x = 10$); and variable conditions are used elsewhere. Ponding depth is assumed to be zero meter on the whole variable boundary. Fluxes on the top side of the variable boundary are assumed equal to 0.006 m/d and on the right side above the water surface are equal to zero. A steady state solution will be sought. A pre-initial condition

is set, h = 10-z.

The region of interest is discretized with 10 x 1 x 10 = 100 elements with element size = 1 x 10 x 1 cm, resulting in 11 x 2 x 11 = 242 node points (Figure 7). For 3DFATMIC simulation, each of the two vertical planes will be considered a subregion. Thus, the total of two subregions, each with 121 node points, is used for the subregional block iteration simulation.

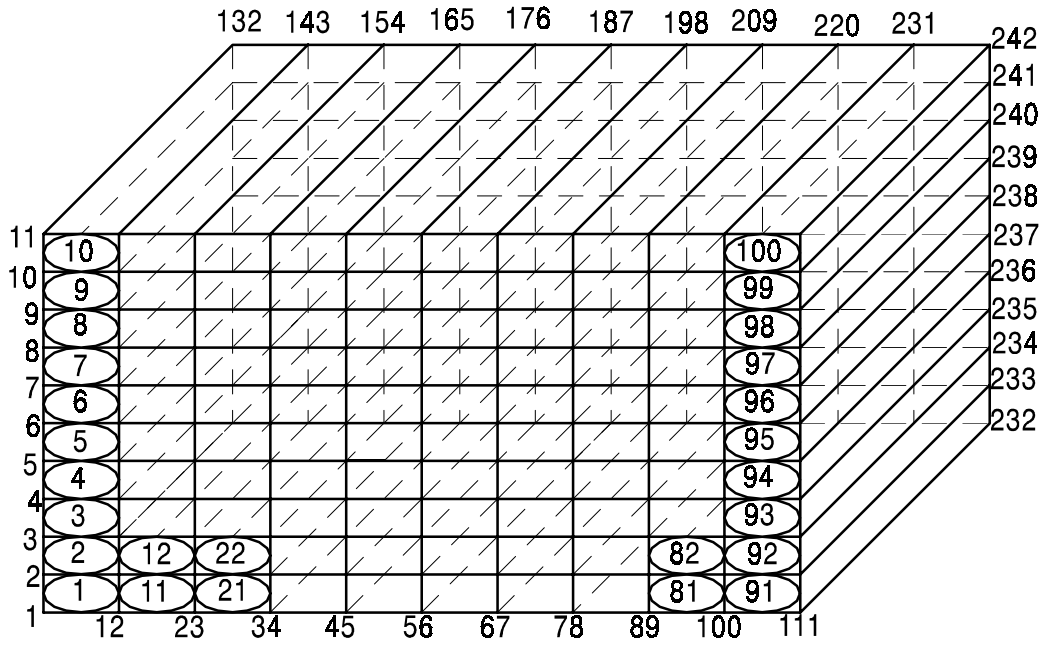


Figure 4.5 Finite element discretization for Example 2.

The pressure head tolerance is $2 \cdot 10^{-3}$ m for nonlinear iteration and is 10^{-3} m for block iteration. The relaxation factors for both the nonlinear iteration and block iteration are set equal to 0.5.

To execute the problem, the maximum control-integers in the MAIN should be specified as follows

```
C----- For Example 1 through Example 5
c
      PARAMETER(MAXNPK=2079,MAXELK=1600,MXBNPK=999,MXBESK=999,
     >          MXTUBK=3008,MXADNK=maxnpk+0)
```

```
      PARAMETER(MXJBDK=35,MXKBDK=8,MXNTIK=100,MXDTCK=4)
      PARAMETER(LTMXNK=693,LMXNPK=231,LMXBWK=49,MXRGNK=9)
      PARAMETER(MXMATK=8,MXSPMK=5,MXMPMK=9)

C-------- 2.  For flow source/sink, boundary conditions, and materials

      PARAMETER(MXSELh=1,MXSPRh=1,MXSDPh=1,MXWNPh=4,MXWPRh=2,MXWDPh=3)
      PARAMETER(MXCNPh=110,MXCESh=90,MXCPRh=1,MXCDPh=2)
      PARAMETER(MXNNPh=1,MXNESh=1,MXNPRh=1,MXNDPh=1)
      PARAMETER(MXVNPh=198,MXVESh=170,MXVPRh=2,MXVDPh=4)
      PARAMETER(MXDNPh=165,MXDPRh=11,MXDDPh=2)

C -------- 3.  For transport source/sink, boundary conditions, and materials
C
      PARAMETER(MXSELc=1,MXSPRc=1,MXSDPc=1,MXWNPc=4,MXWPRc=2,MXWDPc=5)
      PARAMETER(MXCNPc=55,MXCESc=40,MXCPRc=2,MXCDPc=4)
      PARAMETER(MXNNPc=11,MXNESc=4,MXNPRc=1,MXNDPc=2)
      PARAMETER(MXVNPc=638,MXVESc=560,MXVPRc=1,MXVDPc=2)
      PARAMETER(MXDNPc=70,MXDPRc=6,MXDDPc=2)
C
      PARAMETER(MXNCCK=2)
C
      PARAMETER(MXLSVK=500,MXMSVK=500,MXKGLDK=2000,MXNDBK=2000)
      PARAMETER(MXNEPK=20,MXEPWK=20)
      PARAMETER(MXNPWK=99,MXELWK=27, mxnpws=1331,mxelws=1000)
      PARAMETER(MXNPFGK=2900,MXKGLK=2800)
C
```

To reflect the soil property function given by Eqs. (4.3) and (4.4), one has to modify the subroutine SPFUNC given the source code.

```
    wcr=spp(1,mtyp,1)
    wcs=spp(2,mtyp,1)
    haa=spp(3,mtyp,1)
    thaa=spp(4,mtyp,1)
    thbb=spp(5,mtyp,1)
    power=spp(1,mtyp,2)
C
C ------- SATURATED CONDITION
C
    IF(HNP.LE.0) THEN
      TH=WCS
      IF(ISP .EQ. 1) GOTO 900
      DTH=0.0D0
      USKFCT=1.0D0
```

```
C
C ------- UNSATURATED CASE
C
      ELSE
            th=wcr+(wcs-wcr)*thaa/(thaa+(DABS(-hnp-haa))**thbb)
            IF(ISP.EQ.1) GOTO 900
            dnom=thaa+(DABS(-hnp-haa))**thbb
            dth=(wcs-wcr)*thaa*(DABS(-hnp-thaa))**(thbb-1.0d0)/dnom**2
            USKFCT=((th-wcr)/(wcs-wcr))**power
       ENDIF
C
```

Figure 8 and Figure 9 depict the pressure distribution and the velocity field, respectively, from the 3DFATMIC simulation.

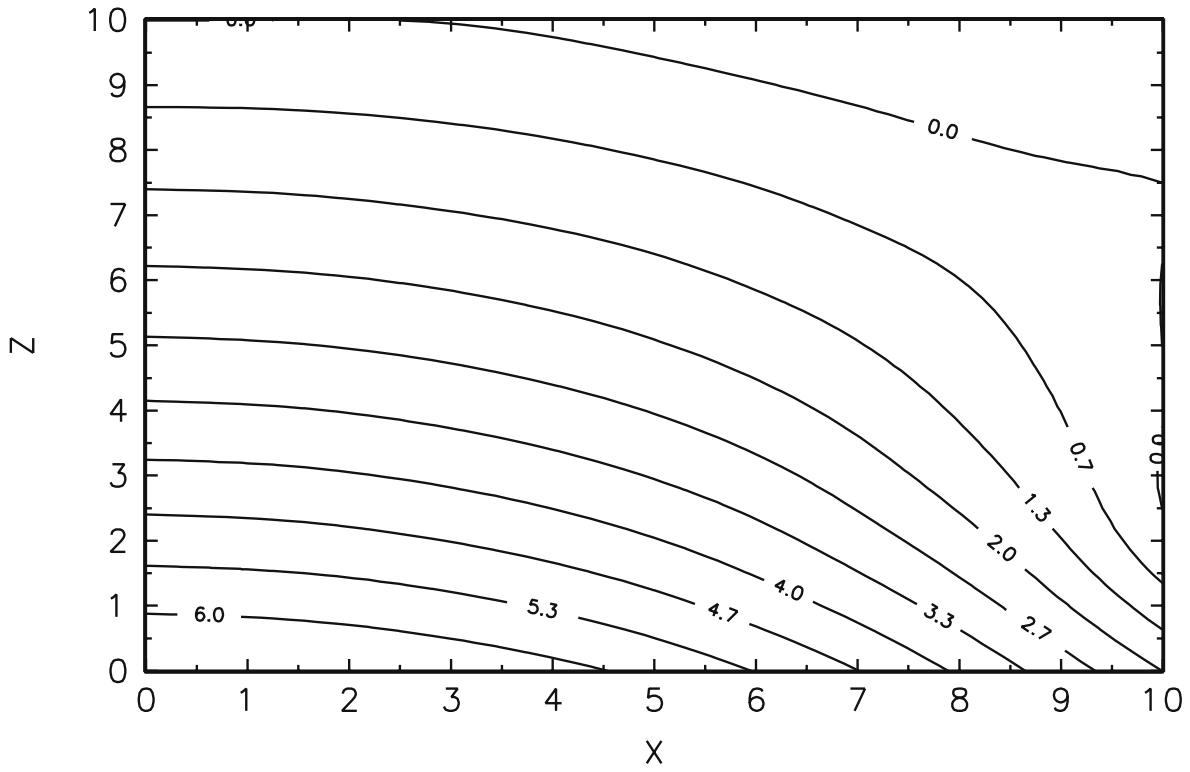


Figure 4.6 Pressure head distribution for Example 2.

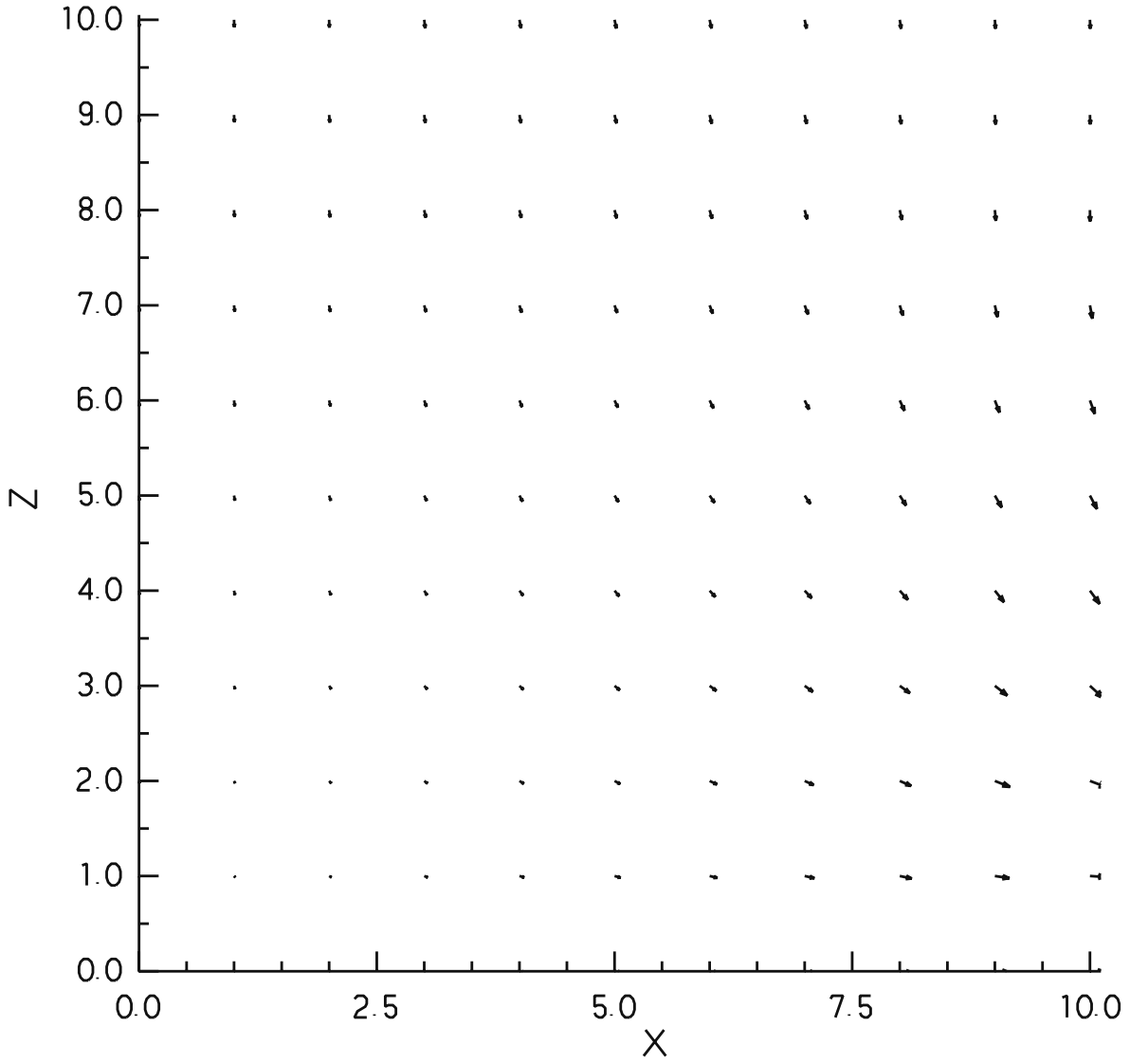


Figure 4.7 The velocity field for Example 2.

4.4 Input and Output for Example 2

With the above descriptions, the input data can be prepared according to the instructions in Appendix A. The input parameters are listed in Table 4.3 and the input data file content are given in Table 4.4. To save space, the output is available in electronic form.

Table 4.3 The list of input parameters for Example 2

Parameters	Notation in the data input guide	Value	Unit	Data set
number of points	NNP	242	Dimensionless	7. A.
$\triangle x$	XAD	1	m	7. B.
$\triangle y$	YAD	10	m	7. B.
$\triangle z$	ZAD	1	m	7. B.
$K_{s,xx}$	PROPf(1,1)	0.01	m/day	5. B.
$K_{s,zz}$	PROPf(1,3)	0.01	m/day	5. B.
θ_r	SPP(1,1,1)	0.05	dimensionless	6. B.
θ_s	SPP(2,1,1)	0.25	dimensionless	6. B.
h_a	SPP(3,1,1)	0	m	6. B.
A	SPP(4,1,1)	10	dimensionless	6. B.
B	SPP(5,1,1)	4	dimensionless	6. B.
n	SPP(1,1,2)	4	dimensionless	6. B.
no. of subregion	NREGN	2	dimensionless	8. A.
no. of points in each subregion	NODES	121	dimensionless	8. B.
steady-state simulation	KSSf	0	dimensionless	2. C.
no. of times to reset time step size	NDTCHG	0	dimensionless	4. A.
no. of time steps	NTI	0	dimensionless	4. A.
tolerance for nonlinear iteration	TOLAf	2×10^{-3}	m	3. A.
relaxation factor for nonlinear iteration	OMEf	0.5	dimensionless	2. C.
ρ_w	RHO	1.0×10^{3}	Kg/m^3	5.B., 6.A.
μ_w	VISC	948.3264	Kg/m/day	5.B. , 6.A.
g	GRAV	7.316×10^{10}	m/day^2	6.A.

Table 4.4 Input Data Set for Example 2

```
    2 Two-dimensional Drainage Flow Problem; L=M, T=DAY, M=KG
===== DATA SET 2: OPTION PARAMETERS
  10  0  1  0
 1  0.5D0 1.0D-4     NITRFT OMEFTF OMEFTT
 0  0 0  0  0 0 0 0 0 1 KSSF KSST ILUMP IMID IPNTSF IPNTST miconf nstrf nstrt
 1  1.0  0.5d0  0.5d0  0.0d0  KGRAV WF OMEF OMIF
 1 0  1  1  1                KVIT IWET IOPTIM ksorp lgran
 1.0d0 0.5d0 1.0d0 1.0d0      WT WVT OMET OMIT
===== DATA SET 3: ITERATION PARAMETERS
 50 20 100 2.0d-3 2.0d-3      NITERF NCYLF NPITRF TOLAF TOLBF
  1 100 1.0d-3  1.0d-4        NITERT NPITRT TOLAT TOLBT
===== DATA SET 4: TIME CONTROL PARAMETERS
 0    0                      NTI NDTCHG
 0.05d0  0.20d0 0.05d0  22.0d0   DELT CHNG DELMAX TMAX
55                             KPR0 KPR(1..NTI)
00                             KDSK0 KDSK(1..NTI)
 0.0
===== DATA SET 5: MATERIAL PROPERTIES
1  7  0  1                     NMAT NMPPM
0.01D0  0.0D0  0.01D0   0.0D0  0.0D0  0.0D0      1.0d0
PROPF
0.0
RHOMU
 1.0d0
===== DATA SET 6: SOIL PROPERTIES
0    5    0    1.0d0  7.316D10  1.1232d4        KSP NSPPM KCP GRAV
   0.050D0   0.250D0    0.00D0    10.0D0    4.0D0    THPROP
   4.000D0   0.000D0    0.00D0     0.0D0    0.0D0    AKPROP
===== DATA SET 7: NODE COORDINATES
  242   NNP
    1 10 11    0.0D0   0.0D0   0.0D0   1.0D0   0.0D0   0.0D0
    2 10 11    0.0D0   0.0D0   1.0D0   1.0D0   0.0D0   0.0D0
    3 10 11    0.0D0   0.0D0   2.0D0   1.0D0   0.0D0   0.0D0
    4 10 11    0.0D0   0.0D0   3.0D0   1.0D0   0.0D0   0.0D0
    5 10 11    0.0D0   0.0D0   4.0D0   1.0D0   0.0D0   0.0D0
    6 10 11    0.0D0   0.0D0   5.0D0   1.0D0   0.0D0   0.0D0
    7 10 11    0.0D0   0.0D0   6.0D0   1.0D0   0.0D0   0.0D0
    8 10 11    0.0D0   0.0D0   7.0D0   1.0D0   0.0D0   0.0D0
    9 10 11    0.0D0   0.0D0   8.0D0   1.0D0   0.0D0   0.0D0
   10 10 11    0.0D0   0.0D0   9.0D0   1.0D0   0.0D0   0.0D0
   11 10 11    0.0D0   0.0D0  10.0D0   1.0D0   0.0D0   0.0D0
  122 10 11    0.0D0  10.0D0   0.0D0   1.0D0   0.0D0   0.0D0
  123 10 11    0.0D0  10.0D0   1.0D0   1.0D0   0.0D0   0.0D0
  124 10 11    0.0D0  10.0D0   2.0D0   1.0D0   0.0D0   0.0D0
  125 10 11    0.0D0  10.0D0   3.0D0   1.0D0   0.0D0   0.0D0
  126 10 11    0.0D0  10.0D0   4.0D0   1.0D0   0.0D0   0.0D0
  127 10 11    0.0D0  10.0D0   5.0D0   1.0D0   0.0D0   0.0D0
  128 10 11    0.0D0  10.0D0   6.0D0   1.0D0   0.0D0   0.0D0
  129 10 11    0.0D0  10.0D0   7.0D0   1.0D0   0.0D0   0.0D0
  130 10 11    0.0D0  10.0D0   8.0D0   1.0D0   0.0D0   0.0D0
  131 10 11    0.0D0  10.0D0   9.0D0   1.0D0   0.0D0   0.0D0
  132 10 11    0.0D0  10.0D0  10.0D0   1.0D0   0.0D0   0.0D0
    0  0  0  0.0   0.0   0.0   0.0   0.0  0.0    END OF COORDINATES
===== DATA SET 8: SUBREGIONAL DATA
    2
    1    1    1  121    0
    0    0    0    0    0         END OF NNPLR(K)
    1  120    1    1    1
```

```
    0    0    0    0    0         END OF GNLR(I,1)
    1  120    1  122    1
    0    0    0    0    0         END OF GNLR(I,2)
===== DATA SET 9 : ELEMENT INCIDENCES
  100        NEL
    1    9    1    1   12  133  122    2   13  134  123    1
   11    9    1   12   23  144  133   13   24  145  134    1
   21    9    1   23   34  155  144   24   35  156  145    1
   31    9    1   34   45  166  155   35   46  167  156    1
   41    9    1   45   56  177  166   46   57  178  167    1
   51    9    1   56   67  188  177   57   68  189  178    1
   61    9    1   67   78  199  188   68   79  200  189    1
   71    9    1   78   89  210  199   79   90  211  200    1
   81    9    1   89  100  221  210   90  101  222  211    1
   91    9    1  100  111  232  221  101  112  233  222    1
    0    0    0    0    0    0    0    0    0    0    0    0 END OF IE
===== DATA SET 10: MATERIAL CORRECTION
    0    NCM
===== DATA SET 11: INITIAL CONDITIONS
    1   10   11          10.0D0     0.0D0     0.0D0
    2   10   11           9.0D0     0.0D0     0.0D0
    3   10   11           8.0D0     0.0D0     0.0D0
    4   10   11           7.0D0     0.0D0     0.0D0
    5   10   11           6.0D0     0.0D0     0.0D0
    6   10   11           5.0D0     0.0D0     0.0D0
    7   10   11           4.0D0     0.0D0     0.0D0
    8   10   11           3.0D0     0.0D0     0.0D0
    9   10   11           2.0D0     0.0D0     0.0D0
   10   10   11           1.0D0     0.0D0     0.0D0
   11   10   11           0.0D0     0.0D0     0.0D0
  122   10   11          10.0D0     0.0D0     0.0D0
  123   10   11           9.0D0     0.0D0     0.0D0
  124   10   11           8.0D0     0.0D0     0.0D0
  125   10   11           7.0D0     0.0D0     0.0D0
  126   10   11           6.0D0     0.0D0     0.0D0
  127   10   11           5.0D0     0.0D0     0.0D0
  128   10   11           4.0D0     0.0D0     0.0D0
  129   10   11           3.0D0     0.0D0     0.0D0
  130   10   11           2.0D0     0.0D0     0.0D0
  131   10   11           1.0D0     0.0D0     0.0D0
  132   10   11           0.0D0     0.0D0     0.0D0
    0    0    0           0.0D0     0.0D0     0.0D0  END OF IC FOR FLOW
===== DATA SET 12: ELEMENT(DISTRIBUTED) SOURCE/SINK OF FLOW
    0  0  0  0            NSELF NSPRF NSDPF KSAIF
===== DATA SET 13: POINT(WELL) SOURCE/SINK OF FLOW
    0  0  0  0            NWNPF NWPRF NWDPF KWAIF
===== DATA SET 16: RAINFALL/EVAPORATION-SEEPAGE BOUNDARY CONDITIONS OF FLOW
   18 38  2  2  0         NVESF NVNPF NRPRF NRDPF KRAIF
     0.0D0    6.0D-3    1.0D38    6.0D-3     TQVBFF QVBFF
     0.0D0    0.0D00    1.0D38    0.0D00     TQVBFF QVBFF
    1    9    1    1    0
   11    7    1    2    0
    0    0    0    0    0                 END OF IVTYPF
    1    9    1   11   22  143  132   11   11   11   11
   11    7    1  120  241  242  121   -1   -1   -1   -1
    0  0  0  0  0  0  0  0  0  0  0 END OF ISVF(J,I) J=1,4
    1   10    1   11   11
   12    7    1  120   -1
   20   10    1  132   11
   31    7    1  241   -1
    0    0    0    0    0         END OF NPVBF
    1   37    1          0.0D0     0.0D0     0.0D0
```

```
    0    0    0     0.0       0.0         0.0    END OF HCON
    1   37    1        -90.0D2     0.0D0     0.0D0
    0    0    0     0.0       0.0         0.0    END OF HMIN
===== DATA SET 17:  DIRICHLET BOUNDARY CONDITIONS OF FLOW
    6  1  2  0                      NDNPF NDPRF NDDPF KDAIF
     0.0D0     2.0D0    1.0D38     2.0D0    THDBFF HDBFF
    1   2   1   111   1
    4   2   1   232   1
    0   0   0    0     0
    1    5    1    1    0
    0    0    0    0    0                   END OF IDTYPF
===== DATA SET 18: CAUCHY BOUNDARY CONDITIONS OF FLOW
    0  0  0  0  0                     NCESF NCNPF NCPRF NCDPF KCAIF
===== DATA SET 19: NEUMANN BOUNDARY CONDITIONS, FLOW
    0  0  0  0  0                     NNESF NNNPF NNPRF NNDPF KNAIF
    0           ====== END OF JOB ======
```

4.5 Example 3: Three-Dimensional Pumping Flow Problem

This example is selected to represent the simulation of a three-dimensional problem with 3DFATMIC. The problem involves the steady state flow to a pumping well. The region of interest is bounded on the left and right by hydraulically connected rivers; on the front, back, and bottom by impervious aquifuges; and on the top by an air-soil interface (Figure 10.1). A pumping well is located at (x,y) = (540,400) (102). Initially, the water table is assumed to be horizontal and is 60 m above the bottom of the aquifer. The water level at the well is then lowered to a height of 30 m. This height is held until a steady state condition is reached. The medium in the region is assumed to be anisotropic and have saturated hydraulic conductivity components K_{xx} = 5 m/d, K_{yy} = 0.5 m/d, and K_{zz} = 2 m/d. The porosity of the medium is 0.25 and the field capacity is 0.0125. The unsaturated characteristic hydraulic properties of the medium are given as

$$\theta = \theta_r + \frac{\theta_s - \theta_r}{1 + (\alpha |h_a - h|)^{\beta}} \tag{4.5}$$

and

$$K_r = \left[\frac{\theta - \theta_r}{\theta_s - \theta_r} \right]^2 \tag{4.6}$$

where h_a, α, and β are the parameters used to compute the water content and the relative hydraulic conductivity.

Because of the symmetry, the region for numerical simulation will be taken as $0 < x < 1000$ m, $0 < y < 400$ m, and $0 < z < 72$ m. The boundary conditions are given as: pressure head is assumed hydrostatic on two vertical planes located at $x = 0$ and $0 < z < 60$, and $x = 1000$ and $0 < z < 60$, respectively; no flux is imposed on all other boundaries of the flow regime. A steady state solution will be sought. A pre-initial condition is set as $h = 60 - z$.

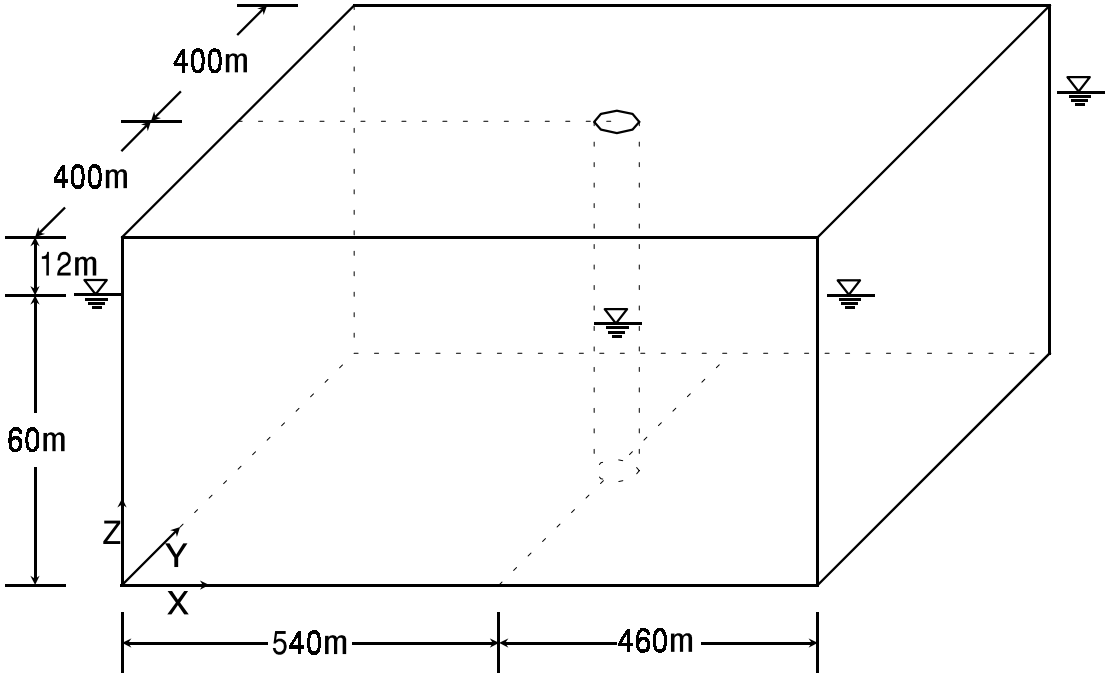


Figure 4.8 Problem definition and sketch for Example 3.

The region of interest is discretized with 20 x 8 x 10 = 1600 elements resulting in 21 x 9 x 11 = 2079 node points (Figure 10.2). The nodes are located at x = 0, 70, 120, 160, 200, 275, 350, 400, 450, 500, 540, 570, 600, 650, 700, 750, 800, 850, 900, 950, and 1000 in the x-direction, and at z = 0, 15, 30, 35, 40, 45, 50, 55, 60, 66, and 72 m in the z-direction as reported by Huyakorn et al. (1986). In the y-direction, nodes are spaced evenly at $\Delta y = 50$ m. For 3DFATMIC simulation, the matrix solver, incomplete Cholesky preconditioned conjugate gradient method, is selected to solve the assembled global matrix equation.

The pressure head tolerance is 10^{-2} m for nonlinear iteration and is $5 \cdot 10^{-3}$ m for matrix solver. The relaxation factors for nonlinear iteration is set equal to 1.0.

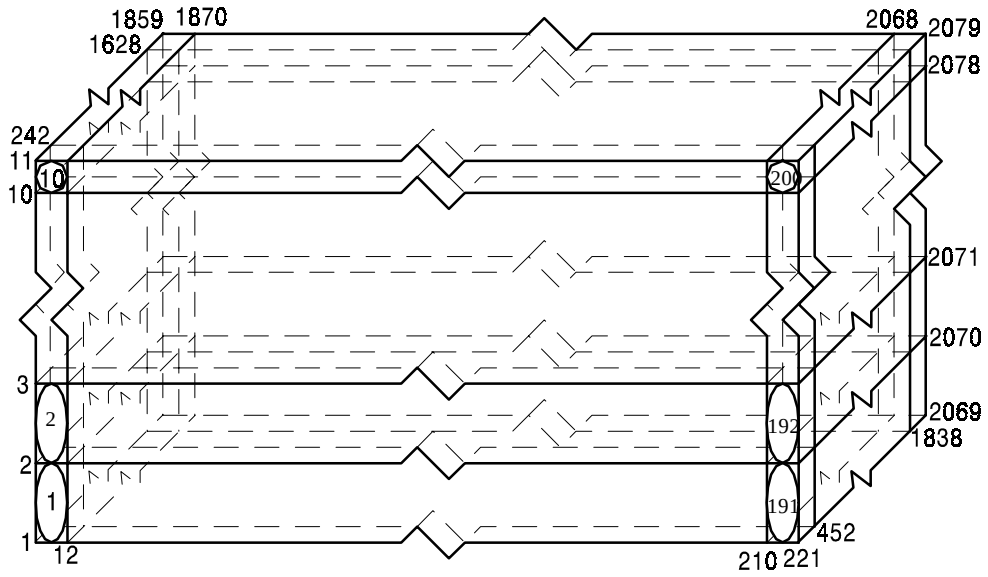


Figure 4.9 Finite element discretization for Example 3.

To execute the problem, the maximum control-integers in the MAIN should be specified as

```
C----- For Example 1 through Example 5
c
      PARAMETER(MAXNPK=2079,MAXELK=1600,MXBNPK=999,MXBESK=999,
      >                MXTUBK=3008,MXADNK=maxnpk+0)
      PARAMETER(MXJBDK=35,MXKBDK=8,MXNTIK=100,MXDTCK=4)
      PARAMETER(LTMXNK=693,LMXNPK=231,LMXBWK=49,MXRGNK=9)
      PARAMETER(MXMATK=8,MXSPMK=5,MXMPMK=9)

C-------- 2.  For flow source/sink, boundary conditions, and materials

      PARAMETER(MXSELh=1,MXSPRh=1,MXSDPh=1,MXWNPh=4,MXWPRh=2,MXWDPh=3)
      PARAMETER(MXCNPh=110,MXCESh=90,MXCPRh=1,MXCDPh=2)
      PARAMETER(MXNNPh=1,MXNESh=1,MXNPRh=1,MXNDPh=1)
      PARAMETER(MXVNPh=198,MXVESh=170,MXVPRh=2,MXVDPh=4)
      PARAMETER(MXDNPh=165,MXDPRh=11,MXDDPh=2)
```

```
C -------- 3.  For transport source/sink, boundary conditions, and materials
C
      PARAMETER(MXSELc=1,MXSPRc=1,MXSDPc=1,MXWNPc=4,MXWPRc=2,MXWDPc=5)
      PARAMETER(MXCNPc=55,MXCESc=40,MXCPRc=2,MXCDPc=4)
      PARAMETER(MXNNPc=11,MXNESc=4,MXNPRc=1,MXNDPc=2)
      PARAMETER(MXVNPc=638,MXVESc=560,MXVPRc=1,MXVDPc=2)
      PARAMETER(MXDNPc=70,MXDPRc=6,MXDDPc=2)
C
      PARAMETER(MXNCCK=2)
C
      PARAMETER(MXLSVK=500,MXMSVK=500,MXKGLDK=2000,MXNDBK=2000)
      PARAMETER(MXNEPK=20,MXEPWK=20)
      PARAMETER(MXNPWK=99,MXELWK=27, mxnpws=1331,mxelws=1000)
      PARAMETER(MXNPFGK=2900,MXKGLK=2800)
C
```

To reflect the soil property function given by Eqs. (4.5) and (4.6), one has to modify the subroutine SPFUNC in the source code as follows.

```
      WCR=SPP(1,MTYP,1)
      WCS=SPP(2,MTYP,1)
      HAA=SPP(3,MTYP,1)
      ALPHA=SPP(4,MTYP,1)
      BETA=SPP(5,MTYP,1)
C
C ------- SATURATED CONDITION
C
      IF(HNP.LE.0.0) THEN
        TH=WCS
        IF(ISP .EQ. 1) GOTO 900
        DTH=0.0D0
        USKFCT=1.0D0
     ELSE
C
C ------- UNSATURATED CASE
C
      TH=WCR+(WCS-WCR)/(1.0D0+(ALPHA*DABS(-HNP-HAA))**BETA)
      IF(ISP.EQ.1) GOTO 900
      USKFCT=((TH-WCR)/(WCS-WCR))**2
      DNOM=1.0D0+(ALPHA*DABS(-HNP-HAA))**BETA
      DTH=(WCS-WCR)*(ALPHA*DABS(-HNP-HAA))**(BETA-1.0D0)/DNOM**2
     ENDIF
```

Figure 4.10 and Figure 4.11 depict the pressure distribution and the velocity field in 3-D perspective

view (top figure) and along the x-z crosssection through the well (bottom figure) as simulated by 3DFATMIC.

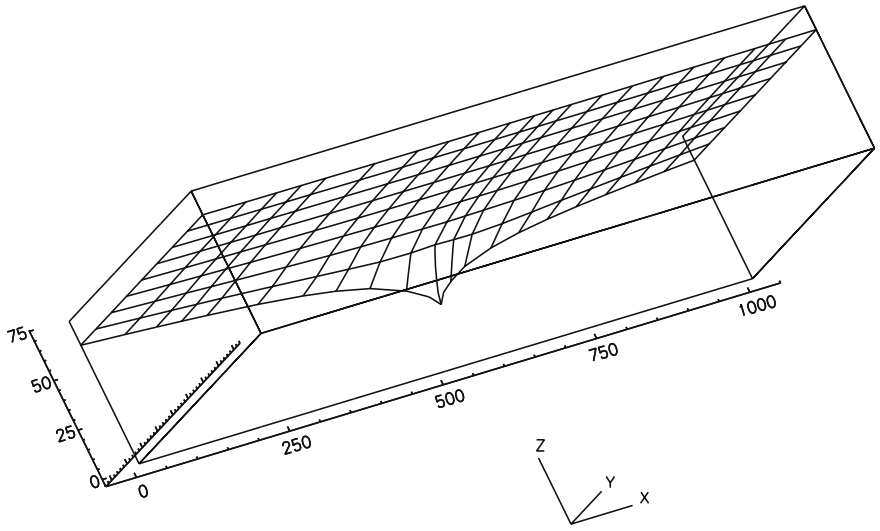


Figure 4.10a Water table for problem No. 3.

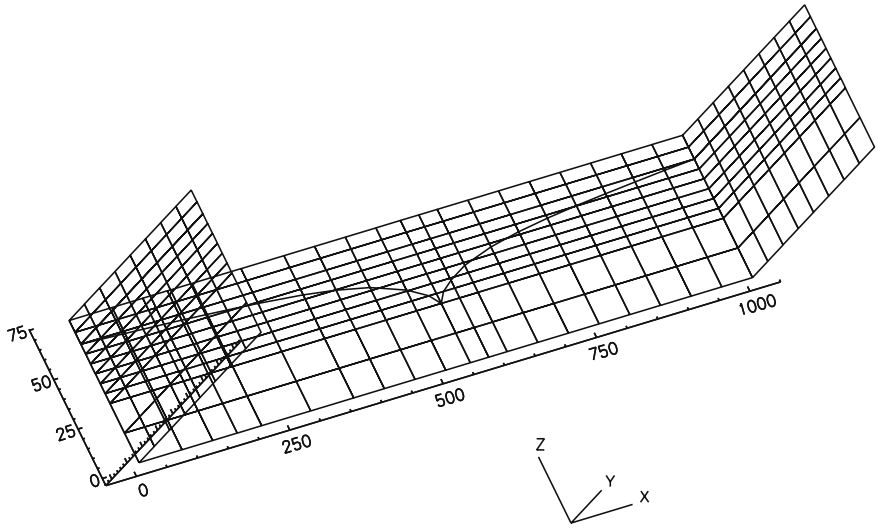


Figure 4.10b Water table on the x-z crosssection through the pumping well for Problem 3.

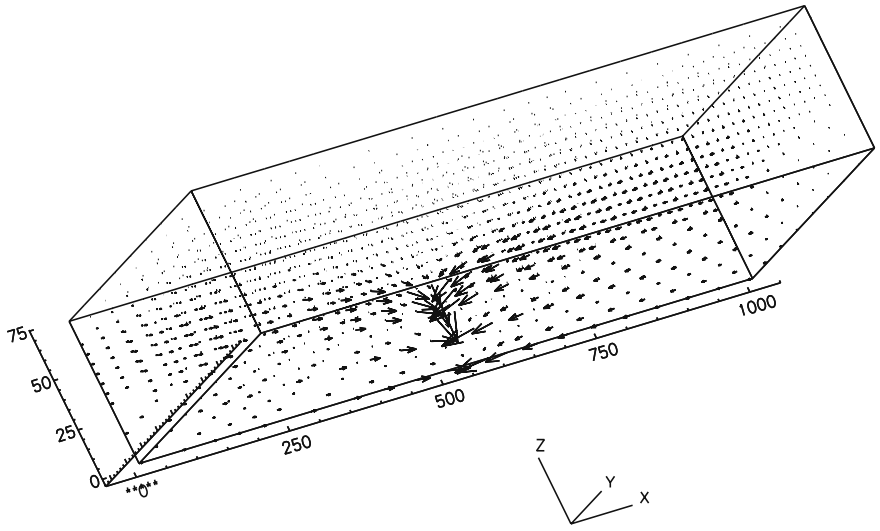


Figure 4.11a Velocity distribution throughout the domain for Problem 3.

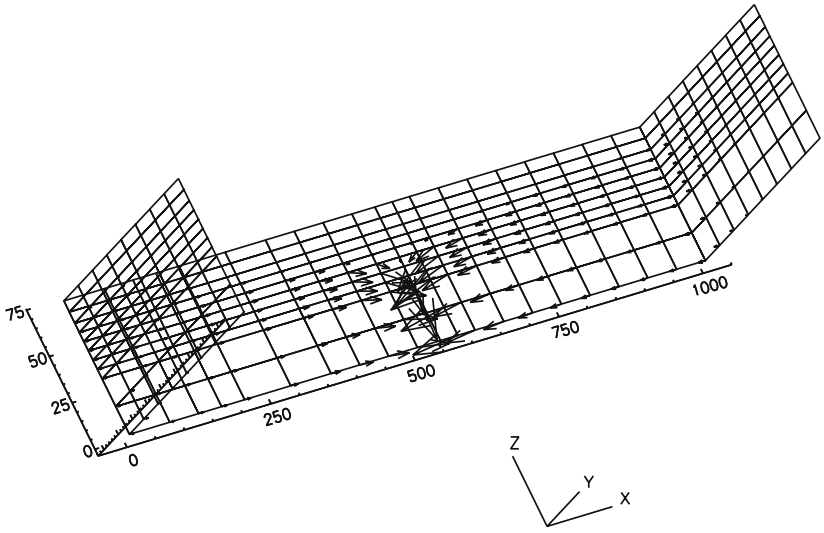


Figure 4.11b Velocity distribution on the x-z crosssection through the well for Problem 3.

4.6 Input and Output for Example 3

With the above descriptions, the input data can be prepared according to the instructions in Appendix A. The input parameters are listed in Table 4.5 and the data input file content is given in Table 4.6. To save space, the output isavailable in electronic form.

Table 4.5 The list of input parameters for Example 3.

Parameters	Notation in the data input guide	Value	Unit	Data set
number of points	NNP	2079	Dimensionless	7. A.
no.of elements	NEL	1600	dimensionless	9. A.
$K_{s,xx}$	PROPf(1,1)	5	m/day	5. B.
$K_{s,yy}$	PROPf(1,2)	0.5	m/day	5. B.
$K_{s,zz}$	PROPf(1,3)	2	m/day	5. B.
θ_r	SPP(1,1,1)	0.0125	dimensionless	6. B.
θ_s	SPP(2,1,1)	0.25	dimensionless	6. B.
h_a	SPP(3,1,1)	0	m	6. B.
α	SPP(4,1,1)	0.5	dimensionless	6. B.
β	SPP(5,1,1)	2	dimensionless	6. B.
ICP solver	IPNTSf	3	dimensionless	2. B.
steady-state simulation	KSSf	0	dimensionless	2. C.
no. of times to reset time step size	NDTCHG	0	dimensionless	4. A.
no. of time steps	NTI	0	dimensionless	4. A.
tolerance for nonlinear iteration	TOLAf	10^{-2}	m	3. A.
relaxation factor for nonlinear iteration	OMEf	1.0	dimensionless	2. C.
ρ_w	RHO	1.0×10^{3}	Kg/m^3	5.B. & 6.A.
μ_w	VISC	948.3264	Kg/m/day	5.B. & 6.A.
g	GRAV	7.316×10^{10}	m/day^2	6.A.

Table 4.6 Input Data Set for Example 3

```
    3 Three-Dimensional Pumping Flow Problem; L=M, T=DAY, M=KG
===== DATA SET 2: OPTION PARAMETERS
  10  0  1  0
 1 0.5D0 1.0d-4           NITRFT OMEFTF OMEFTT
 0 0 0 0 0 0 0 0 0 1 KSSF KSST ILUMP IMID IPNTSF IPNTST miconf nstrf nstrt
 1  1.0  1.0d0  1.5d0  0.0d0     KGRAV WF OMEF OMIF
 1 0  1  1  1  1                KVIT IWET IOPTIM ksorp lgrn
 1.0d0 0.5d0 1.0d0 1.0d0        WT WVT OMET OMIT
===== DATA SET 3: ITERATION PARAMETERS
 50 20 100 1.0d-2 1.0d-2       NITERF NCYLF NPITRF TOLAF TOLBF
  1 100 1.0d-3  1.0d-4         NITERT NPITRT TOLAT TOLBT
===== DATA SET 4: TIME CONTROL PARAMETERS
 0    0                        NTI NDTCHG
 0.05d0  0.00d0  1.0d0  20.0d0  DELT CHNG DELMAX TMAX
55                            KPR0 KPR(1..NTI)
00                            KDSK0 KDSK(1..NTI)
  0.0d0
===== DATA SET 5: MATERIAL PROPERTIES
1  7  0  1                    NMAT NMPPM
5.0D0  0.5D0  2.0D0   0.0D0  0.0D0  0.0D0   1.0d0   PROPF
0.0                                  RHOMU
 1.0d0
===== DATA SET 6: SOIL PROPERTIES
0    5    0    1.0d0  7.316D10  1.1232d4       KSP NSPPM KCP GRAV
   0.01250D0 0.250D0    0.00D0     0.5D0    2.0D0   THPROP
   0.000D0   0.000D0    0.00D0     0.0D0    0.0D0   AKPROP
===== DATA SET 7: NODE COORDINATES
  2079              NNP
    1 8 231  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.50D+02  0.00D+00
    2 8 231  0.00D+00  0.00D+00  0.15D+02  0.00D+00  0.50D+02  0.00D+00
    3 8 231  0.00D+00  0.00D+00  0.30D+02  0.00D+00  0.50D+02  0.00D+00
    4 8 231  0.00D+00  0.00D+00  0.35D+02  0.00D+00  0.50D+02  0.00D+00
    5 8 231  0.00D+00  0.00D+00  0.40D+02  0.00D+00  0.50D+02  0.00D+00
    6 8 231  0.00D+00  0.00D+00  0.45D+02  0.00D+00  0.50D+02  0.00D+00
    7 8 231  0.00D+00  0.00D+00  0.50D+02  0.00D+00  0.50D+02  0.00D+00
    8 8 231  0.00D+00  0.00D+00  0.55D+02  0.00D+00  0.50D+02  0.00D+00
    9 8 231  0.00D+00  0.00D+00  0.60D+02  0.00D+00  0.50D+02  0.00D+00
   10 8 231  0.00D+00  0.00D+00  0.66D+02  0.00D+00  0.50D+02  0.00D+00
   11 8 231  0.00D+00  0.00D+00  0.72D+02  0.00D+00  0.50D+02  0.00D+00
   12 8 231  0.70D+02  0.00D+00  0.00D+00  0.00D+00  0.50D+02  0.00D+00
   13 8 231  0.70D+02  0.00D+00  0.15D+02  0.00D+00  0.50D+02  0.00D+00
   14 8 231  0.70D+02  0.00D+00  0.30D+02  0.00D+00  0.50D+02  0.00D+00
   15 8 231  0.70D+02  0.00D+00  0.35D+02  0.00D+00  0.50D+02  0.00D+00
   16 8 231  0.70D+02  0.00D+00  0.40D+02  0.00D+00  0.50D+02  0.00D+00
   17 8 231  0.70D+02  0.00D+00  0.45D+02  0.00D+00  0.50D+02  0.00D+00
   18 8 231  0.70D+02  0.00D+00  0.50D+02  0.00D+00  0.50D+02  0.00D+00
   19 8 231  0.70D+02  0.00D+00  0.55D+02  0.00D+00  0.50D+02  0.00D+00
   20 8 231  0.70D+02  0.00D+00  0.60D+02  0.00D+00  0.50D+02  0.00D+00
   21 8 231  0.70D+02  0.00D+00  0.66D+02  0.00D+00  0.50D+02  0.00D+00
   22 8 231  0.70D+02  0.00D+00  0.72D+02  0.00D+00  0.50D+02  0.00D+00
   23 8 231  0.12D+03  0.00D+00  0.00D+00  0.00D+00  0.50D+02  0.00D+00
   24 8 231  0.12D+03  0.00D+00  0.15D+02  0.00D+00  0.50D+02  0.00D+00
   25 8 231  0.12D+03  0.00D+00  0.30D+02  0.00D+00  0.50D+02  0.00D+00
   26 8 231  0.12D+03  0.00D+00  0.35D+02  0.00D+00  0.50D+02  0.00D+00
   27 8 231  0.12D+03  0.00D+00  0.40D+02  0.00D+00  0.50D+02  0.00D+00
   28 8 231  0.12D+03  0.00D+00  0.45D+02  0.00D+00  0.50D+02  0.00D+00
   29 8 231  0.12D+03  0.00D+00  0.50D+02  0.00D+00  0.50D+02  0.00D+00
   30 8 231  0.12D+03  0.00D+00  0.55D+02  0.00D+00  0.50D+02  0.00D+00
   31 8 231  0.12D+03  0.00D+00  0.60D+02  0.00D+00  0.50D+02  0.00D+00
   32 8 231  0.12D+03  0.00D+00  0.66D+02  0.00D+00  0.50D+02  0.00D+00
```

```
33 8 231  0.12D+03  0.00D+00  0.72D+02  0.00D+00  0.50D+02  0.00D+00
34 8 231  0.16D+03  0.00D+00  0.00D+00  0.00D+00  0.50D+02  0.00D+00
35 8 231  0.16D+03  0.00D+00  0.15D+02  0.00D+00  0.50D+02  0.00D+00
36 8 231  0.16D+03  0.00D+00  0.30D+02  0.00D+00  0.50D+02  0.00D+00
37 8 231  0.16D+03  0.00D+00  0.35D+02  0.00D+00  0.50D+02  0.00D+00
38 8 231  0.16D+03  0.00D+00  0.40D+02  0.00D+00  0.50D+02  0.00D+00
39 8 231  0.16D+03  0.00D+00  0.45D+02  0.00D+00  0.50D+02  0.00D+00
40 8 231  0.16D+03  0.00D+00  0.50D+02  0.00D+00  0.50D+02  0.00D+00
41 8 231  0.16D+03  0.00D+00  0.55D+02  0.00D+00  0.50D+02  0.00D+00
42 8 231  0.16D+03  0.00D+00  0.60D+02  0.00D+00  0.50D+02  0.00D+00
43 8 231  0.16D+03  0.00D+00  0.66D+02  0.00D+00  0.50D+02  0.00D+00
44 8 231  0.16D+03  0.00D+00  0.72D+02  0.00D+00  0.50D+02  0.00D+00
45 8 231  0.20D+03  0.00D+00  0.00D+00  0.00D+00  0.50D+02  0.00D+00
46 8 231  0.20D+03  0.00D+00  0.15D+02  0.00D+00  0.50D+02  0.00D+00
47 8 231  0.20D+03  0.00D+00  0.30D+02  0.00D+00  0.50D+02  0.00D+00
48 8 231  0.20D+03  0.00D+00  0.35D+02  0.00D+00  0.50D+02  0.00D+00
49 8 231  0.20D+03  0.00D+00  0.40D+02  0.00D+00  0.50D+02  0.00D+00
50 8 231  0.20D+03  0.00D+00  0.45D+02  0.00D+00  0.50D+02  0.00D+00
51 8 231  0.20D+03  0.00D+00  0.50D+02  0.00D+00  0.50D+02  0.00D+00
52 8 231  0.20D+03  0.00D+00  0.55D+02  0.00D+00  0.50D+02  0.00D+00
53 8 231  0.20D+03  0.00D+00  0.60D+02  0.00D+00  0.50D+02  0.00D+00
54 8 231  0.20D+03  0.00D+00  0.66D+02  0.00D+00  0.50D+02  0.00D+00
55 8 231  0.20D+03  0.00D+00  0.72D+02  0.00D+00  0.50D+02  0.00D+00
56 8 231  0.28D+03  0.00D+00  0.00D+00  0.00D+00  0.50D+02  0.00D+00
57 8 231  0.28D+03  0.00D+00  0.15D+02  0.00D+00  0.50D+02  0.00D+00
58 8 231  0.28D+03  0.00D+00  0.30D+02  0.00D+00  0.50D+02  0.00D+00
59 8 231  0.28D+03  0.00D+00  0.35D+02  0.00D+00  0.50D+02  0.00D+00
60 8 231  0.28D+03  0.00D+00  0.40D+02  0.00D+00  0.50D+02  0.00D+00
61 8 231  0.28D+03  0.00D+00  0.45D+02  0.00D+00  0.50D+02  0.00D+00
62 8 231  0.28D+03  0.00D+00  0.50D+02  0.00D+00  0.50D+02  0.00D+00
63 8 231  0.28D+03  0.00D+00  0.55D+02  0.00D+00  0.50D+02  0.00D+00
64 8 231  0.28D+03  0.00D+00  0.60D+02  0.00D+00  0.50D+02  0.00D+00
65 8 231  0.28D+03  0.00D+00  0.66D+02  0.00D+00  0.50D+02  0.00D+00
66 8 231  0.28D+03  0.00D+00  0.72D+02  0.00D+00  0.50D+02  0.00D+00
67 8 231  0.35D+03  0.00D+00  0.00D+00  0.00D+00  0.50D+02  0.00D+00
68 8 231  0.35D+03  0.00D+00  0.15D+02  0.00D+00  0.50D+02  0.00D+00
69 8 231  0.35D+03  0.00D+00  0.30D+02  0.00D+00  0.50D+02  0.00D+00
70 8 231  0.35D+03  0.00D+00  0.35D+02  0.00D+00  0.50D+02  0.00D+00
71 8 231  0.35D+03  0.00D+00  0.40D+02  0.00D+00  0.50D+02  0.00D+00
72 8 231  0.35D+03  0.00D+00  0.45D+02  0.00D+00  0.50D+02  0.00D+00
73 8 231  0.35D+03  0.00D+00  0.50D+02  0.00D+00  0.50D+02  0.00D+00
74 8 231  0.35D+03  0.00D+00  0.55D+02  0.00D+00  0.50D+02  0.00D+00
75 8 231  0.35D+03  0.00D+00  0.60D+02  0.00D+00  0.50D+02  0.00D+00
76 8 231  0.35D+03  0.00D+00  0.66D+02  0.00D+00  0.50D+02  0.00D+00
77 8 231  0.35D+03  0.00D+00  0.72D+02  0.00D+00  0.50D+02  0.00D+00
78 8 231  0.40D+03  0.00D+00  0.00D+00  0.00D+00  0.50D+02  0.00D+00
79 8 231  0.40D+03  0.00D+00  0.15D+02  0.00D+00  0.50D+02  0.00D+00
80 8 231  0.40D+03  0.00D+00  0.30D+02  0.00D+00  0.50D+02  0.00D+00
81 8 231  0.40D+03  0.00D+00  0.35D+02  0.00D+00  0.50D+02  0.00D+00
82 8 231  0.40D+03  0.00D+00  0.40D+02  0.00D+00  0.50D+02  0.00D+00
83 8 231  0.40D+03  0.00D+00  0.45D+02  0.00D+00  0.50D+02  0.00D+00
84 8 231  0.40D+03  0.00D+00  0.50D+02  0.00D+00  0.50D+02  0.00D+00
85 8 231  0.40D+03  0.00D+00  0.55D+02  0.00D+00  0.50D+02  0.00D+00
86 8 231  0.40D+03  0.00D+00  0.60D+02  0.00D+00  0.50D+02  0.00D+00
87 8 231  0.40D+03  0.00D+00  0.66D+02  0.00D+00  0.50D+02  0.00D+00
88 8 231  0.40D+03  0.00D+00  0.72D+02  0.00D+00  0.50D+02  0.00D+00
89 8 231  0.45D+03  0.00D+00  0.00D+00  0.00D+00  0.50D+02  0.00D+00
90 8 231  0.45D+03  0.00D+00  0.15D+02  0.00D+00  0.50D+02  0.00D+00
91 8 231  0.45D+03  0.00D+00  0.30D+02  0.00D+00  0.50D+02  0.00D+00
92 8 231  0.45D+03  0.00D+00  0.35D+02  0.00D+00  0.50D+02  0.00D+00
93 8 231  0.45D+03  0.00D+00  0.40D+02  0.00D+00  0.50D+02  0.00D+00
94 8 231  0.45D+03  0.00D+00  0.45D+02  0.00D+00  0.50D+02  0.00D+00
```

```
 95 8 231  0.45D+03  0.00D+00  0.50D+02  0.00D+00  0.50D+02  0.00D+00
 96 8 231  0.45D+03  0.00D+00  0.55D+02  0.00D+00  0.50D+02  0.00D+00
 97 8 231  0.45D+03  0.00D+00  0.60D+02  0.00D+00  0.50D+02  0.00D+00
 98 8 231  0.45D+03  0.00D+00  0.66D+02  0.00D+00  0.50D+02  0.00D+00
 99 8 231  0.45D+03  0.00D+00  0.72D+02  0.00D+00  0.50D+02  0.00D+00
100 8 231  0.50D+03  0.00D+00  0.00D+00  0.00D+00  0.50D+02  0.00D+00
101 8 231  0.50D+03  0.00D+00  0.15D+02  0.00D+00  0.50D+02  0.00D+00
102 8 231  0.50D+03  0.00D+00  0.30D+02  0.00D+00  0.50D+02  0.00D+00
103 8 231  0.50D+03  0.00D+00  0.35D+02  0.00D+00  0.50D+02  0.00D+00
104 8 231  0.50D+03  0.00D+00  0.40D+02  0.00D+00  0.50D+02  0.00D+00
105 8 231  0.50D+03  0.00D+00  0.45D+02  0.00D+00  0.50D+02  0.00D+00
106 8 231  0.50D+03  0.00D+00  0.50D+02  0.00D+00  0.50D+02  0.00D+00
107 8 231  0.50D+03  0.00D+00  0.55D+02  0.00D+00  0.50D+02  0.00D+00
108 8 231  0.50D+03  0.00D+00  0.60D+02  0.00D+00  0.50D+02  0.00D+00
109 8 231  0.50D+03  0.00D+00  0.66D+02  0.00D+00  0.50D+02  0.00D+00
110 8 231  0.50D+03  0.00D+00  0.72D+02  0.00D+00  0.50D+02  0.00D+00
111 8 231  0.54D+03  0.00D+00  0.00D+00  0.00D+00  0.50D+02  0.00D+00
112 8 231  0.54D+03  0.00D+00  0.15D+02  0.00D+00  0.50D+02  0.00D+00
113 8 231  0.54D+03  0.00D+00  0.30D+02  0.00D+00  0.50D+02  0.00D+00
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119 8 231  0.54D+03  0.00D+00  0.60D+02  0.00D+00  0.50D+02  0.00D+00
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121 8 231  0.54D+03  0.00D+00  0.72D+02  0.00D+00  0.50D+02  0.00D+00
122 8 231  0.57D+03  0.00D+00  0.00D+00  0.00D+00  0.50D+02  0.00D+00
123 8 231  0.57D+03  0.00D+00  0.15D+02  0.00D+00  0.50D+02  0.00D+00
124 8 231  0.57D+03  0.00D+00  0.30D+02  0.00D+00  0.50D+02  0.00D+00
125 8 231  0.57D+03  0.00D+00  0.35D+02  0.00D+00  0.50D+02  0.00D+00
126 8 231  0.57D+03  0.00D+00  0.40D+02  0.00D+00  0.50D+02  0.00D+00
127 8 231  0.57D+03  0.00D+00  0.45D+02  0.00D+00  0.50D+02  0.00D+00
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131 8 231  0.57D+03  0.00D+00  0.66D+02  0.00D+00  0.50D+02  0.00D+00
132 8 231  0.57D+03  0.00D+00  0.72D+02  0.00D+00  0.50D+02  0.00D+00
133 8 231  0.60D+03  0.00D+00  0.00D+00  0.00D+00  0.50D+02  0.00D+00
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136 8 231  0.60D+03  0.00D+00  0.35D+02  0.00D+00  0.50D+02  0.00D+00
137 8 231  0.60D+03  0.00D+00  0.40D+02  0.00D+00  0.50D+02  0.00D+00
138 8 231  0.60D+03  0.00D+00  0.45D+02  0.00D+00  0.50D+02  0.00D+00
139 8 231  0.60D+03  0.00D+00  0.50D+02  0.00D+00  0.50D+02  0.00D+00
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143 8 231  0.60D+03  0.00D+00  0.72D+02  0.00D+00  0.50D+02  0.00D+00
144 8 231  0.65D+03  0.00D+00  0.00D+00  0.00D+00  0.50D+02  0.00D+00
145 8 231  0.65D+03  0.00D+00  0.15D+02  0.00D+00  0.50D+02  0.00D+00
146 8 231  0.65D+03  0.00D+00  0.30D+02  0.00D+00  0.50D+02  0.00D+00
147 8 231  0.65D+03  0.00D+00  0.35D+02  0.00D+00  0.50D+02  0.00D+00
148 8 231  0.65D+03  0.00D+00  0.40D+02  0.00D+00  0.50D+02  0.00D+00
149 8 231  0.65D+03  0.00D+00  0.45D+02  0.00D+00  0.50D+02  0.00D+00
150 8 231  0.65D+03  0.00D+00  0.50D+02  0.00D+00  0.50D+02  0.00D+00
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153 8 231  0.65D+03  0.00D+00  0.66D+02  0.00D+00  0.50D+02  0.00D+00
154 8 231  0.65D+03  0.00D+00  0.72D+02  0.00D+00  0.50D+02  0.00D+00
155 8 231  0.70D+03  0.00D+00  0.00D+00  0.00D+00  0.50D+02  0.00D+00
156 8 231  0.70D+03  0.00D+00  0.15D+02  0.00D+00  0.50D+02  0.00D+00
```

```
157 8 231  0.70D+03  0.00D+00  0.30D+02  0.00D+00  0.50D+02  0.00D+00
158 8 231  0.70D+03  0.00D+00  0.35D+02  0.00D+00  0.50D+02  0.00D+00
159 8 231  0.70D+03  0.00D+00  0.40D+02  0.00D+00  0.50D+02  0.00D+00
160 8 231  0.70D+03  0.00D+00  0.45D+02  0.00D+00  0.50D+02  0.00D+00
161 8 231  0.70D+03  0.00D+00  0.50D+02  0.00D+00  0.50D+02  0.00D+00
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163 8 231  0.70D+03  0.00D+00  0.60D+02  0.00D+00  0.50D+02  0.00D+00
164 8 231  0.70D+03  0.00D+00  0.66D+02  0.00D+00  0.50D+02  0.00D+00
165 8 231  0.70D+03  0.00D+00  0.72D+02  0.00D+00  0.50D+02  0.00D+00
166 8 231  0.75D+03  0.00D+00  0.00D+00  0.00D+00  0.50D+02  0.00D+00
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168 8 231  0.75D+03  0.00D+00  0.30D+02  0.00D+00  0.50D+02  0.00D+00
169 8 231  0.75D+03  0.00D+00  0.35D+02  0.00D+00  0.50D+02  0.00D+00
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183 8 231  0.80D+03  0.00D+00  0.50D+02  0.00D+00  0.50D+02  0.00D+00
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185 8 231  0.80D+03  0.00D+00  0.60D+02  0.00D+00  0.50D+02  0.00D+00
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187 8 231  0.80D+03  0.00D+00  0.72D+02  0.00D+00  0.50D+02  0.00D+00
188 8 231  0.85D+03  0.00D+00  0.00D+00  0.00D+00  0.50D+02  0.00D+00
189 8 231  0.85D+03  0.00D+00  0.15D+02  0.00D+00  0.50D+02  0.00D+00
190 8 231  0.85D+03  0.00D+00  0.30D+02  0.00D+00  0.50D+02  0.00D+00
191 8 231  0.85D+03  0.00D+00  0.35D+02  0.00D+00  0.50D+02  0.00D+00
192 8 231  0.85D+03  0.00D+00  0.40D+02  0.00D+00  0.50D+02  0.00D+00
193 8 231  0.85D+03  0.00D+00  0.45D+02  0.00D+00  0.50D+02  0.00D+00
194 8 231  0.85D+03  0.00D+00  0.50D+02  0.00D+00  0.50D+02  0.00D+00
195 8 231  0.85D+03  0.00D+00  0.55D+02  0.00D+00  0.50D+02  0.00D+00
196 8 231  0.85D+03  0.00D+00  0.60D+02  0.00D+00  0.50D+02  0.00D+00
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200 8 231  0.90D+03  0.00D+00  0.15D+02  0.00D+00  0.50D+02  0.00D+00
201 8 231  0.90D+03  0.00D+00  0.30D+02  0.00D+00  0.50D+02  0.00D+00
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203 8 231  0.90D+03  0.00D+00  0.40D+02  0.00D+00  0.50D+02  0.00D+00
204 8 231  0.90D+03  0.00D+00  0.45D+02  0.00D+00  0.50D+02  0.00D+00
205 8 231  0.90D+03  0.00D+00  0.50D+02  0.00D+00  0.50D+02  0.00D+00
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208 8 231  0.90D+03  0.00D+00  0.66D+02  0.00D+00  0.50D+02  0.00D+00
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212 8 231  0.95D+03  0.00D+00  0.30D+02  0.00D+00  0.50D+02  0.00D+00
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216 8 231  0.95D+03  0.00D+00  0.50D+02  0.00D+00  0.50D+02  0.00D+00
217 8 231  0.95D+03  0.00D+00  0.55D+02  0.00D+00  0.50D+02  0.00D+00
218 8 231  0.95D+03  0.00D+00  0.60D+02  0.00D+00  0.50D+02  0.00D+00
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  219 8 231  0.95D+03  0.00D+00  0.66D+02  0.00D+00  0.50D+02  0.00D+00
  220 8 231  0.95D+03  0.00D+00  0.72D+02  0.00D+00  0.50D+02  0.00D+00
  221 8 231  0.10D+04  0.00D+00  0.00D+00  0.00D+00  0.50D+02  0.00D+00
  222 8 231  0.10D+04  0.00D+00  0.15D+02  0.00D+00  0.50D+02  0.00D+00
  223 8 231  0.10D+04  0.00D+00  0.30D+02  0.00D+00  0.50D+02  0.00D+00
  224 8 231  0.10D+04  0.00D+00  0.35D+02  0.00D+00  0.50D+02  0.00D+00
  225 8 231  0.10D+04  0.00D+00  0.40D+02  0.00D+00  0.50D+02  0.00D+00
  226 8 231  0.10D+04  0.00D+00  0.45D+02  0.00D+00  0.50D+02  0.00D+00
  227 8 231  0.10D+04  0.00D+00  0.50D+02  0.00D+00  0.50D+02  0.00D+00
  228 8 231  0.10D+04  0.00D+00  0.55D+02  0.00D+00  0.50D+02  0.00D+00
  229 8 231  0.10D+04  0.00D+00  0.60D+02  0.00D+00  0.50D+02  0.00D+00
  230 8 231  0.10D+04  0.00D+00  0.66D+02  0.00D+00  0.50D+02  0.00D+00
  231 8 231  0.10D+04  0.00D+00  0.72D+02  0.00D+00  0.50D+02  0.00D+00
    0  0  0    0.0   0.0   0.0   0.0  0.0  0.0    END OF COORDINATES
===== DATA SET 8: SUBREGIONAL DATA
    9                  NREGN
    1    8    1  231    0
    0    0    0    0    0           END OF NNPLR(9)
    1  230    1    1    1
    0    0    0    0    0          END OF GNLR(I,1)
    1  230    1  232    1
    0    0    0    0    0          END OF GNLR(I,2)
    1  230    1  463    1
    0    0    0    0    0          END OF GNLR(I,3)
    1  230    1  694    1
    0    0    0    0    0          END OF GNLR(I,4)
    1  230    1  925    1
    0    0    0    0    0          END OF GNLR(I,5)
    1  230    1 1156    1
    0    0    0    0    0          END OF GNLR(I,6)
    1  230    1 1387    1
    0    0    0    0    0          END OF GNLR(I,7)
    1  230    1 1618    1
    0    0    0    0    0          END OF GNLR(I,8)
    1  230    1 1849    1
    0    0    0    0    0          END OF GNLR(I,9)
===== DATA SET 9 : ELEMENT INCIDENCES
  1600        NEL
    1    9    1    1   12  243  232    2   13  244  233    1
   11    9    1   12   23  254  243   13   24  255  244    1
   21    9    1   23   34  265  254   24   35  266  255    1
   31    9    1   34   45  276  265   35   46  277  266    1
   41    9    1   45   56  287  276   46   57  288  277    1
   51    9    1   56   67  298  287   57   68  299  288    1
   61    9    1   67   78  309  298   68   79  310  299    1
   71    9    1   78   89  320  309   79   90  321  310    1
   81    9    1   89  100  331  320   90  101  332  321    1
   91    9    1  100  111  342  331  101  112  343  332    1
  101    9    1  111  122  353  342  112  123  354  343    1
  111    9    1  122  133  364  353  123  134  365  354    1
  121    9    1  133  144  375  364  134  145  376  365    1
  131    9    1  144  155  386  375  145  156  387  376    1
  141    9    1  155  166  397  386  156  167  398  387    1
  151    9    1  166  177  408  397  167  178  409  398    1
  161    9    1  177  188  419  408  178  189  420  409    1
  171    9    1  188  199  430  419  189  200  431  420    1
  181    9    1  199  210  441  430  200  211  442  431    1
  191    9    1  210  221  452  441  211  222  453  442    1
  201    9    1  232  243  474  463  233  244  475  464    1
  211    9    1  243  254  485  474  244  255  486  475    1
  221    9    1  254  265  496  485  255  266  497  486    1
  231    9    1  265  276  507  496  266  277  508  497    1
```

241	9	1	276	287	518	507	277	288	519	508	1
251	9	1	287	298	529	518	288	299	530	519	1
261	9	1	298	309	540	529	299	310	541	530	1
271	9	1	309	320	551	540	310	321	552	541	1
281	9	1	320	331	562	551	321	332	563	552	1
291	9	1	331	342	573	562	332	343	574	563	1
301	9	1	342	353	584	573	343	354	585	574	1
311	9	1	353	364	595	584	354	365	596	585	1
321	9	1	364	375	606	595	365	376	607	596	1
331	9	1	375	386	617	606	376	387	618	607	1
341	9	1	386	397	628	617	387	398	629	618	1
351	9	1	397	408	639	628	398	409	640	629	1
361	9	1	408	419	650	639	409	420	651	640	1
371	9	1	419	430	661	650	420	431	662	651	1
381	9	1	430	441	672	661	431	442	673	662	1
391	9	1	441	452	683	672	442	453	684	673	1
401	9	1	463	474	705	694	464	475	706	695	1
411	9	1	474	485	716	705	475	486	717	706	1
421	9	1	485	496	727	716	486	497	728	717	1
431	9	1	496	507	738	727	497	508	739	728	1
441	9	1	507	518	749	738	508	519	750	739	1
451	9	1	518	529	760	749	519	530	761	750	1
461	9	1	529	540	771	760	530	541	772	761	1
471	9	1	540	551	782	771	541	552	783	772	1
481	9	1	551	562	793	782	552	563	794	783	1
491	9	1	562	573	804	793	563	574	805	794	1
501	9	1	573	584	815	804	574	585	816	805	1
511	9	1	584	595	826	815	585	596	827	816	1
521	9	1	595	606	837	826	596	607	838	827	1
531	9	1	606	617	848	837	607	618	849	838	1
541	9	1	617	628	859	848	618	629	860	849	1
551	9	1	628	639	870	859	629	640	871	860	1
561	9	1	639	650	881	870	640	651	882	871	1
571	9	1	650	661	892	881	651	662	893	882	1
581	9	1	661	672	903	892	662	673	904	893	1
591	9	1	672	683	914	903	673	684	915	904	1
601	9	1	694	705	936	925	695	706	937	926	1
611	9	1	705	716	947	936	706	717	948	937	1
621	9	1	716	727	958	947	717	728	959	948	1
631	9	1	727	738	969	958	728	739	970	959	1
641	9	1	738	749	980	969	739	750	981	970	1
651	9	1	749	760	991	980	750	761	992	981	1
661	9	1	760	771	1002	991	761	772	1003	992	1
671	9	1	771	782	1013	1002	772	783	1014	1003	1
681	9	1	782	793	1024	1013	783	794	1025	1014	1
691	9	1	793	804	1035	1024	794	805	1036	1025	1
701	9	1	804	815	1046	1035	805	816	1047	1036	1
711	9	1	815	826	1057	1046	816	827	1058	1047	1
721	9	1	826	837	1068	1057	827	838	1069	1058	1
731	9	1	837	848	1079	1068	838	849	1080	1069	1
741	9	1	848	859	1090	1079	849	860	1091	1080	1
751	9	1	859	870	1101	1090	860	871	1102	1091	1
761	9	1	870	881	1112	1101	871	882	1113	1102	1
771	9	1	881	892	1123	1112	882	893	1124	1113	1
781	9	1	892	903	1134	1123	893	904	1135	1124	1
791	9	1	903	914	1145	1134	904	915	1146	1135	1
801	9	1	925	936	1167	1156	926	937	1168	1157	1
811	9	1	936	947	1178	1167	937	948	1179	1168	1
821	9	1	947	958	1189	1178	948	959	1190	1179	1
831	9	1	958	969	1200	1189	959	970	1201	1190	1
841	9	1	969	980	1211	1200	970	981	1212	1201	1
851	9	1	980	991	1222	1211	981	992	1223	1212	1

861	9	1	991	1002	1233	1222	992	1003	1234	1223	1
871	9	1	1002	1013	1244	1233	1003	1014	1245	1234	1
881	9	1	1013	1024	1255	1244	1014	1025	1256	1245	1
891	9	1	1024	1035	1266	1255	1025	1036	1267	1256	1
901	9	1	1035	1046	1277	1266	1036	1047	1278	1267	1
911	9	1	1046	1057	1288	1277	1047	1058	1289	1278	1
921	9	1	1057	1068	1299	1288	1058	1069	1300	1289	1
931	9	1	1068	1079	1310	1299	1069	1080	1311	1300	1
941	9	1	1079	1090	1321	1310	1080	1091	1322	1311	1
951	9	1	1090	1101	1332	1321	1091	1102	1333	1322	1
961	9	1	1101	1112	1343	1332	1102	1113	1344	1333	1
971	9	1	1112	1123	1354	1343	1113	1124	1355	1344	1
981	9	1	1123	1134	1365	1354	1124	1135	1366	1355	1
991	9	1	1134	1145	1376	1365	1135	1146	1377	1366	1
1001	9	1	1156	1167	1398	1387	1157	1168	1399	1388	1
1011	9	1	1167	1178	1409	1398	1168	1179	1410	1399	1
1021	9	1	1178	1189	1420	1409	1179	1190	1421	1410	1
1031	9	1	1189	1200	1431	1420	1190	1201	1432	1421	1
1041	9	1	1200	1211	1442	1431	1201	1212	1443	1432	1
1051	9	1	1211	1222	1453	1442	1212	1223	1454	1443	1
1061	9	1	1222	1233	1464	1453	1223	1234	1465	1454	1
1071	9	1	1233	1244	1475	1464	1234	1245	1476	1465	1
1081	9	1	1244	1255	1486	1475	1245	1256	1487	1476	1
1091	9	1	1255	1266	1497	1486	1256	1267	1498	1487	1
1101	9	1	1266	1277	1508	1497	1267	1278	1509	1498	1
1111	9	1	1277	1288	1519	1508	1278	1289	1520	1509	1
1121	9	1	1288	1299	1530	1519	1289	1300	1531	1520	1
1131	9	1	1299	1310	1541	1530	1300	1311	1542	1531	1
1141	9	1	1310	1321	1552	1541	1311	1322	1553	1542	1
1151	9	1	1321	1332	1563	1552	1322	1333	1564	1553	1
1161	9	1	1332	1343	1574	1563	1333	1344	1575	1564	1
1171	9	1	1343	1354	1585	1574	1344	1355	1586	1575	1
1181	9	1	1354	1365	1596	1585	1355	1366	1597	1586	1
1191	9	1	1365	1376	1607	1596	1366	1377	1608	1597	1
1201	9	1	1387	1398	1629	1618	1388	1399	1630	1619	1
1211	9	1	1398	1409	1640	1629	1399	1410	1641	1630	1
1221	9	1	1409	1420	1651	1640	1410	1421	1652	1641	1
1231	9	1	1420	1431	1662	1651	1421	1432	1663	1652	1
1241	9	1	1431	1442	1673	1662	1432	1443	1674	1663	1
1251	9	1	1442	1453	1684	1673	1443	1454	1685	1674	1
1261	9	1	1453	1464	1695	1684	1454	1465	1696	1685	1
1271	9	1	1464	1475	1706	1695	1465	1476	1707	1696	1
1281	9	1	1475	1486	1717	1706	1476	1487	1718	1707	1
1291	9	1	1486	1497	1728	1717	1487	1498	1729	1718	1
1301	9	1	1497	1508	1739	1728	1498	1509	1740	1729	1
1311	9	1	1508	1519	1750	1739	1509	1520	1751	1740	1
1321	9	1	1519	1530	1761	1750	1520	1531	1762	1751	1
1331	9	1	1530	1541	1772	1761	1531	1542	1773	1762	1
1341	9	1	1541	1552	1783	1772	1542	1553	1784	1773	1
1351	9	1	1552	1563	1794	1783	1553	1564	1795	1784	1
1361	9	1	1563	1574	1805	1794	1564	1575	1806	1795	1
1371	9	1	1574	1585	1816	1805	1575	1586	1817	1806	1
1381	9	1	1585	1596	1827	1816	1586	1597	1828	1817	1
1391	9	1	1596	1607	1838	1827	1597	1608	1839	1828	1
1401	9	1	1618	1629	1860	1849	1619	1630	1861	1850	1
1411	9	1	1629	1640	1871	1860	1630	1641	1872	1861	1
1421	9	1	1640	1651	1882	1871	1641	1652	1883	1872	1
1431	9	1	1651	1662	1893	1882	1652	1663	1894	1883	1
1441	9	1	1662	1673	1904	1893	1663	1674	1905	1894	1
1451	9	1	1673	1684	1915	1904	1674	1685	1916	1905	1
1461	9	1	1684	1695	1926	1915	1685	1696	1927	1916	1
1471	9	1	1695	1706	1937	1926	1696	1707	1938	1927	1

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 1481    9    1 1706 1717 1948 1937 1707 1718 1949 1938    1
 1491    9    1 1717 1728 1959 1948 1718 1729 1960 1949    1
 1501    9    1 1728 1739 1970 1959 1729 1740 1971 1960    1
 1511    9    1 1739 1750 1981 1970 1740 1751 1982 1971    1
 1521    9    1 1750 1761 1992 1981 1751 1762 1993 1982    1
 1531    9    1 1761 1772 2003 1992 1762 1773 2004 1993    1
 1541    9    1 1772 1783 2014 2003 1773 1784 2015 2004    1
 1551    9    1 1783 1794 2025 2014 1784 1795 2026 2015    1
 1561    9    1 1794 1805 2036 2025 1795 1806 2037 2026    1
 1571    9    1 1805 1816 2047 2036 1806 1817 2048 2037    1
 1581    9    1 1816 1827 2058 2047 1817 1828 2059 2048    1
 1591    9    1 1827 1838 2069 2058 1828 1839 2070 2059    1
    0    0    0    0    0    0    0    0    0    0    0  END OF IE
===== DATA SET 10: MATERIAL CORRECTION
    0      NCM
===== DATA SET 11: INITIAL CONDITIONS
    1    8  231       0.60D+02  0.00D+00       0.0
    2    8  231       0.45D+02  0.00D+00       0.0
    3    8  231       0.30D+02  0.00D+00       0.0
    4    8  231       0.25D+02  0.00D+00       0.0
    5    8  231       0.20D+02  0.00D+00       0.0
    6    8  231       0.15D+02  0.00D+00       0.0
    7    8  231       0.10D+02  0.00D+00       0.0
    8    8  231       0.50D+01  0.00D+00       0.0
    9    8  231       0.00D+00  0.00D+00       0.0
   10    8  231      -0.60D+01  0.00D+00       0.0
   11    8  231      -0.12D+02  0.00D+00       0.0
   12    8  231       0.60D+02  0.00D+00       0.0
   13    8  231       0.45D+02  0.00D+00       0.0
   14    8  231       0.30D+02  0.00D+00       0.0
   15    8  231       0.25D+02  0.00D+00       0.0
   16    8  231       0.20D+02  0.00D+00       0.0
   17    8  231       0.15D+02  0.00D+00       0.0
   18    8  231       0.10D+02  0.00D+00       0.0
   19    8  231       0.50D+01  0.00D+00       0.0
   20    8  231       0.00D+00  0.00D+00       0.0
   21    8  231      -0.60D+01  0.00D+00       0.0
   22    8  231      -0.12D+02  0.00D+00       0.0
   23    8  231       0.60D+02  0.00D+00       0.0
   24    8  231       0.45D+02  0.00D+00       0.0
   25    8  231       0.30D+02  0.00D+00       0.0
   26    8  231       0.25D+02  0.00D+00       0.0
   27    8  231       0.20D+02  0.00D+00       0.0
   28    8  231       0.15D+02  0.00D+00       0.0
   29    8  231       0.10D+02  0.00D+00       0.0
   30    8  231       0.50D+01  0.00D+00       0.0
   31    8  231       0.00D+00  0.00D+00       0.0
   32    8  231      -0.60D+01  0.00D+00       0.0
   33    8  231      -0.12D+02  0.00D+00       0.0
   34    8  231       0.60D+02  0.00D+00       0.0
   35    8  231       0.45D+02  0.00D+00       0.0
   36    8  231       0.30D+02  0.00D+00       0.0
   37    8  231       0.25D+02  0.00D+00       0.0
   38    8  231       0.20D+02  0.00D+00       0.0
   39    8  231       0.15D+02  0.00D+00       0.0
   40    8  231       0.10D+02  0.00D+00       0.0
   41    8  231       0.50D+01  0.00D+00       0.0
   42    8  231       0.00D+00  0.00D+00       0.0
   43    8  231      -0.60D+01  0.00D+00       0.0
   44    8  231      -0.12D+02  0.00D+00       0.0
   45    8  231       0.60D+02  0.00D+00       0.0
   46    8  231       0.45D+02  0.00D+00       0.0
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47	8	231	0.30D+02	0.00D+00	0.0
48	8	231	0.25D+02	0.00D+00	0.0
49	8	231	0.20D+02	0.00D+00	0.0
50	8	231	0.15D+02	0.00D+00	0.0
51	8	231	0.10D+02	0.00D+00	0.0
52	8	231	0.50D+01	0.00D+00	0.0
53	8	231	0.00D+00	0.00D+00	0.0
54	8	231	-0.60D+01	0.00D+00	0.0
55	8	231	-0.12D+02	0.00D+00	0.0
56	8	231	0.60D+02	0.00D+00	0.0
57	8	231	0.45D+02	0.00D+00	0.0
58	8	231	0.30D+02	0.00D+00	0.0
59	8	231	0.25D+02	0.00D+00	0.0
60	8	231	0.20D+02	0.00D+00	0.0
61	8	231	0.15D+02	0.00D+00	0.0
62	8	231	0.10D+02	0.00D+00	0.0
63	8	231	0.50D+01	0.00D+00	0.0
64	8	231	0.00D+00	0.00D+00	0.0
65	8	231	-0.60D+01	0.00D+00	0.0
66	8	231	-0.12D+02	0.00D+00	0.0
67	8	231	0.60D+02	0.00D+00	0.0
68	8	231	0.45D+02	0.00D+00	0.0
69	8	231	0.30D+02	0.00D+00	0.0
70	8	231	0.25D+02	0.00D+00	0.0
71	8	231	0.20D+02	0.00D+00	0.0
72	8	231	0.15D+02	0.00D+00	0.0
73	8	231	0.10D+02	0.00D+00	0.0
74	8	231	0.50D+01	0.00D+00	0.0
75	8	231	0.00D+00	0.00D+00	0.0
76	8	231	-0.60D+01	0.00D+00	0.0
77	8	231	-0.12D+02	0.00D+00	0.0
78	8	231	0.60D+02	0.00D+00	0.0
79	8	231	0.45D+02	0.00D+00	0.0
80	8	231	0.30D+02	0.00D+00	0.0
81	8	231	0.25D+02	0.00D+00	0.0
82	8	231	0.20D+02	0.00D+00	0.0
83	8	231	0.15D+02	0.00D+00	0.0
84	8	231	0.10D+02	0.00D+00	0.0
85	8	231	0.50D+01	0.00D+00	0.0
86	8	231	0.00D+00	0.00D+00	0.0
87	8	231	-0.60D+01	0.00D+00	0.0
88	8	231	-0.12D+02	0.00D+00	0.0
89	8	231	0.60D+02	0.00D+00	0.0
90	8	231	0.45D+02	0.00D+00	0.0
91	8	231	0.30D+02	0.00D+00	0.0
92	8	231	0.25D+02	0.00D+00	0.0
93	8	231	0.20D+02	0.00D+00	0.0
94	8	231	0.15D+02	0.00D+00	0.0
95	8	231	0.10D+02	0.00D+00	0.0
96	8	231	0.50D+01	0.00D+00	0.0
97	8	231	0.00D+00	0.00D+00	0.0
98	8	231	-0.60D+01	0.00D+00	0.0
99	8	231	-0.12D+02	0.00D+00	0.0
100	8	231	0.60D+02	0.00D+00	0.0
101	8	231	0.45D+02	0.00D+00	0.0
102	8	231	0.30D+02	0.00D+00	0.0
103	8	231	0.25D+02	0.00D+00	0.0
104	8	231	0.20D+02	0.00D+00	0.0
105	8	231	0.15D+02	0.00D+00	0.0
106	8	231	0.10D+02	0.00D+00	0.0
107	8	231	0.50D+01	0.00D+00	0.0
108	8	231	0.00D+00	0.00D+00	0.0

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109    8  231      -0.60D+01  0.00D+00       0.0
110    8  231      -0.12D+02  0.00D+00       0.0
111    8  231       0.60D+02  0.00D+00       0.0
112    8  231       0.45D+02  0.00D+00       0.0
113    8  231       0.30D+02  0.00D+00       0.0
114    8  231       0.25D+02  0.00D+00       0.0
115    8  231       0.20D+02  0.00D+00       0.0
116    8  231       0.15D+02  0.00D+00       0.0
117    8  231       0.10D+02  0.00D+00       0.0
118    8  231       0.50D+01  0.00D+00       0.0
119    8  231       0.00D+00  0.00D+00       0.0
120    8  231      -0.60D+01  0.00D+00       0.0
121    8  231      -0.12D+02  0.00D+00       0.0
122    8  231       0.60D+02  0.00D+00       0.0
123    8  231       0.45D+02  0.00D+00       0.0
124    8  231       0.30D+02  0.00D+00       0.0
125    8  231       0.25D+02  0.00D+00       0.0
126    8  231       0.20D+02  0.00D+00       0.0
127    8  231       0.15D+02  0.00D+00       0.0
128    8  231       0.10D+02  0.00D+00       0.0
129    8  231       0.50D+01  0.00D+00       0.0
130    8  231       0.00D+00  0.00D+00       0.0
131    8  231      -0.60D+01  0.00D+00       0.0
132    8  231      -0.12D+02  0.00D+00       0.0
133    8  231       0.60D+02  0.00D+00       0.0
134    8  231       0.45D+02  0.00D+00       0.0
135    8  231       0.30D+02  0.00D+00       0.0
136    8  231       0.25D+02  0.00D+00       0.0
137    8  231       0.20D+02  0.00D+00       0.0
138    8  231       0.15D+02  0.00D+00       0.0
139    8  231       0.10D+02  0.00D+00       0.0
140    8  231       0.50D+01  0.00D+00       0.0
141    8  231       0.00D+00  0.00D+00       0.0
142    8  231      -0.60D+01  0.00D+00       0.0
143    8  231      -0.12D+02  0.00D+00       0.0
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145    8  231       0.45D+02  0.00D+00       0.0
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154    8  231      -0.12D+02  0.00D+00       0.0
155    8  231       0.60D+02  0.00D+00       0.0
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157    8  231       0.30D+02  0.00D+00       0.0
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159    8  231       0.20D+02  0.00D+00       0.0
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161    8  231       0.10D+02  0.00D+00       0.0
162    8  231       0.50D+01  0.00D+00       0.0
163    8  231       0.00D+00  0.00D+00       0.0
164    8  231      -0.60D+01  0.00D+00       0.0
165    8  231      -0.12D+02  0.00D+00       0.0
166    8  231       0.60D+02  0.00D+00       0.0
167    8  231       0.45D+02  0.00D+00       0.0
168    8  231       0.30D+02  0.00D+00       0.0
169    8  231       0.25D+02  0.00D+00       0.0
170    8  231       0.20D+02  0.00D+00       0.0
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171    8  231       0.15D+02  0.00D+00       0.0
172    8  231       0.10D+02  0.00D+00       0.0
173    8  231       0.50D+01  0.00D+00       0.0
174    8  231       0.00D+00  0.00D+00       0.0
175    8  231      -0.60D+01  0.00D+00       0.0
176    8  231      -0.12D+02  0.00D+00       0.0
177    8  231       0.60D+02  0.00D+00       0.0
178    8  231       0.45D+02  0.00D+00       0.0
179    8  231       0.30D+02  0.00D+00       0.0
180    8  231       0.25D+02  0.00D+00       0.0
181    8  231       0.20D+02  0.00D+00       0.0
182    8  231       0.15D+02  0.00D+00       0.0
183    8  231       0.10D+02  0.00D+00       0.0
184    8  231       0.50D+01  0.00D+00       0.0
185    8  231       0.00D+00  0.00D+00       0.0
186    8  231      -0.60D+01  0.00D+00       0.0
187    8  231      -0.12D+02  0.00D+00       0.0
188    8  231       0.60D+02  0.00D+00       0.0
189    8  231       0.45D+02  0.00D+00       0.0
190    8  231       0.30D+02  0.00D+00       0.0
191    8  231       0.25D+02  0.00D+00       0.0
192    8  231       0.20D+02  0.00D+00       0.0
193    8  231       0.15D+02  0.00D+00       0.0
194    8  231       0.10D+02  0.00D+00       0.0
195    8  231       0.50D+01  0.00D+00       0.0
196    8  231       0.00D+00  0.00D+00       0.0
197    8  231      -0.60D+01  0.00D+00       0.0
198    8  231      -0.12D+02  0.00D+00       0.0
199    8  231       0.60D+02  0.00D+00       0.0
200    8  231       0.45D+02  0.00D+00       0.0
201    8  231       0.30D+02  0.00D+00       0.0
202    8  231       0.25D+02  0.00D+00       0.0
203    8  231       0.20D+02  0.00D+00       0.0
204    8  231       0.15D+02  0.00D+00       0.0
205    8  231       0.10D+02  0.00D+00       0.0
206    8  231       0.50D+01  0.00D+00       0.0
207    8  231       0.00D+00  0.00D+00       0.0
208    8  231      -0.60D+01  0.00D+00       0.0
209    8  231      -0.12D+02  0.00D+00       0.0
210    8  231       0.60D+02  0.00D+00       0.0
211    8  231       0.45D+02  0.00D+00       0.0
212    8  231       0.30D+02  0.00D+00       0.0
213    8  231       0.25D+02  0.00D+00       0.0
214    8  231       0.20D+02  0.00D+00       0.0
215    8  231       0.15D+02  0.00D+00       0.0
216    8  231       0.10D+02  0.00D+00       0.0
217    8  231       0.50D+01  0.00D+00       0.0
218    8  231       0.00D+00  0.00D+00       0.0
219    8  231      -0.60D+01  0.00D+00       0.0
220    8  231      -0.12D+02  0.00D+00       0.0
221    8  231       0.60D+02  0.00D+00       0.0
222    8  231       0.45D+02  0.00D+00       0.0
223    8  231       0.30D+02  0.00D+00       0.0
224    8  231       0.25D+02  0.00D+00       0.0
225    8  231       0.20D+02  0.00D+00       0.0
226    8  231       0.15D+02  0.00D+00       0.0
227    8  231       0.10D+02  0.00D+00       0.0
228    8  231       0.50D+01  0.00D+00       0.0
229    8  231       0.00D+00  0.00D+00       0.0
230    8  231      -0.60D+01  0.00D+00       0.0
231    8  231      -0.12D+02  0.00D+00       0.0
  0    0    0   0.0D0     0.0D0     0.0D0    END OF IC FOR FLOW
```

```
===== DATA SET 12: ELEMENT(DISTRIBUTED) SOURCE/SINK OF FLOW
    0  0  0  0                    SELF NSPRF NSDPF KSAIF
===== DATA SET 13: POINT(WELL) SOURCE/SINK OF FLOW
    0  0  0  0                    NWNPF NWPRF NWDPF KWAIF
===== DATA SET 16: Rainfall/Evaporation-Seepage Boundary Conditions of Ffow
    0  0  0  0  0                 NVESF NVNPF NRPRF NRDPF KRAIF
===== DATA SET 17:  DIRICHLET BOUNDARY CONDITIONS OF FLOW
    165  2  2  0                  NDNPF NDPRF NDDPF KDAIF
     0.0D0    60.0D0    1.0D38    60.0D0  THDBFF HDBFF
     0.0D0    30.0D0    1.0D38    30.0D0  THDBFF HDBFF
   1  8  1  1  1
  10  8  1  232  1
  19  8  1  463  1
  28  8  1  694  1
  37  8  1  925  1
  46  8  1  1156 1
  55  8  1  1387 1
  64  8  1  1618 1
  73  8  1  1849 1
  82  8  1  221  1
  91  8  1  452  1
 100  8  1  683  1
 109  8  1  914  1
 118  8  1  1145 1
 127  8  1  1376 1
 136  8  1  1607 1
 145  8  1  1838 1
 154  8  1  2069 1
 163  2  1  111  1
  0   0  0  0    0
    1  161    1    1    0
  163    2    1    2    0
    0    0    0    0    0                 END OF IDTYPF
===== DATA SET 18: CAUCHY BOUNDARY CONDITIONS OF FLOW
    0  0  0  0  0                       NCESF NCNPF NCPRF NCDPF KCAIF
===== DATA SET 19: NEUMANN BOUNDARY CONDITIONS, FLOW
    0  0  0  0  0                       NNESF NNNPF NNPRF NNDPF KNAIF
    0           ====== END OF JOB ======
```

4.7 Example 4: One-Dimensional Single Component Transport Problem

A simple problem is presented here to illustrate the application of this model and show the improvement of results with the local grid refinement approach, LEZOOMPC. This is a one-dimensional transport problem between z = 0 and z = 200.0 (Figure 4.12). Initially, the concentration is zero throughout the region of interest. The concentration at x = 0.0 is maintained at $C = C_o = 1.0$ (Figure 4.12). The natural condition of zero gradient flux is imposed at z = 200.0 (Figure 4.12). A bulk density of 1.2, a dispersivity of 5.0, an effective porosity of 0.4 (not used in the program) are assumed.

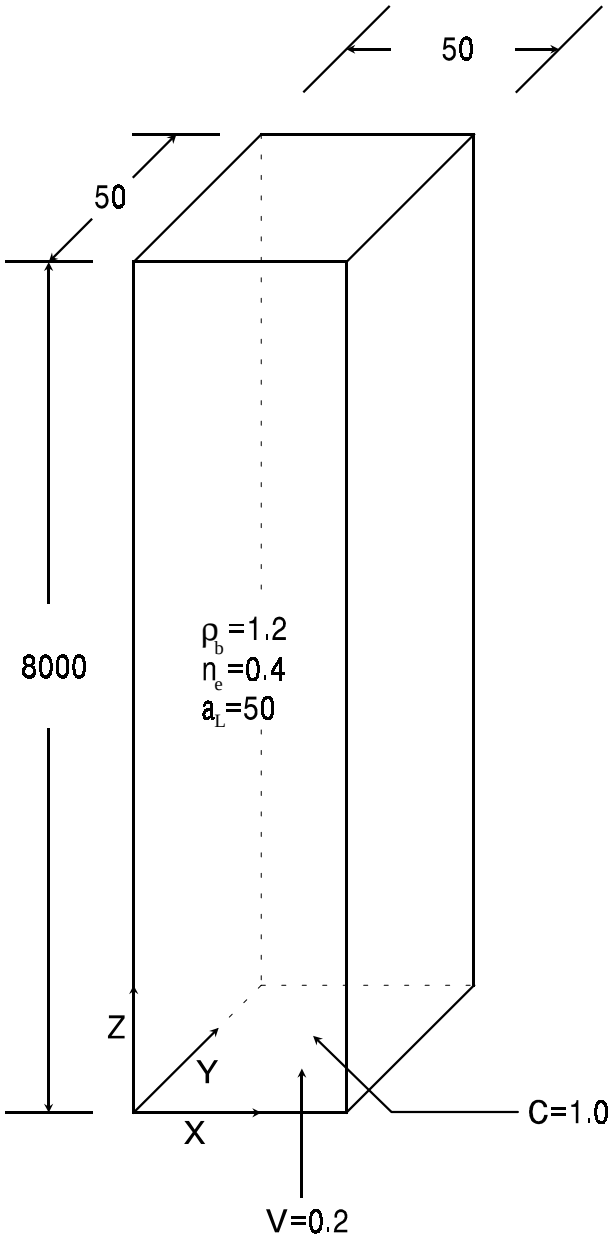


Figure 4.12 Problem definition and sketch for Example 4.

A specific discharge (Darcy velocity) of 2.0 is assumed and a moisture content of 0.4 is used. For numerical simulation the region is divided into 40 elements of equal size with 5.0 (Figure 4.13). A time step size of 0.5 is used and 44 time-step simulation is made. No adsorption is allowed. For this discretization, mesh Peclet number is $P_e = 1$ and Courant number $C_r = 0.5$.

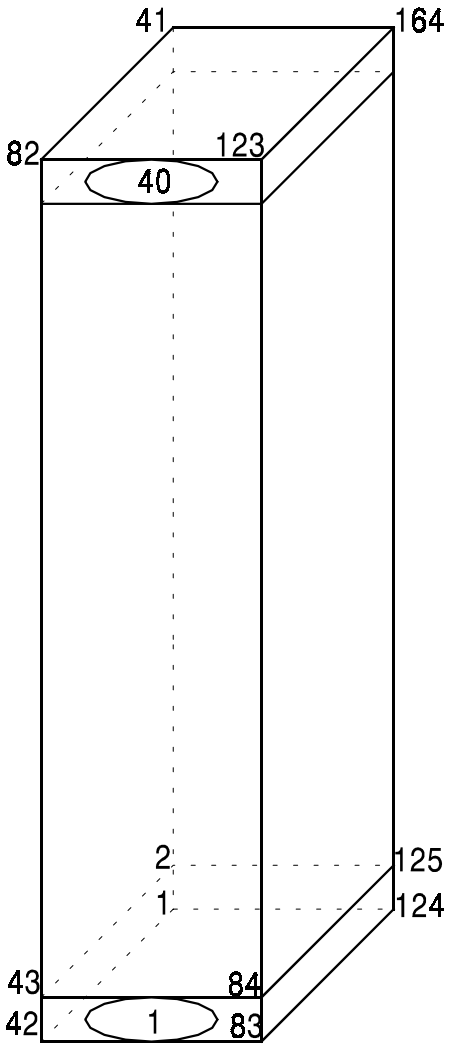


Figure 4.13 Finite element discretization for Example 4.

To execute the problem, the maximum control-integers in the MAIN must be specified as follows:

```
C----- For Example 1 through Example 5
c
      PARAMETER(MAXNPK=2079,MAXELK=1600,MXBNPK=999,MXBESK=999,
      >                MXTUBK=3008,MXADNK=maxnpk+0)
      PARAMETER(MXJBDK=35,MXKBDK=8,MXNTIK=100,MXDTCK=4)
      PARAMETER(LTMXNK=693,LMXNPK=231,LMXBWK=49,MXRGNK=9)
      PARAMETER(MXMATK=8,MXSPMK=5,MXMPMK=9)

C-------- 2.  For flow source/sink, boundary conditions, and materials

      PARAMETER(MXSELh=1,MXSPRh=1,MXSDPh=1,MXWNPh=4,MXWPRh=2,MXWDPh=3)
      PARAMETER(MXCNPh=110,MXCESh=90,MXCPRh=1,MXCDPh=2)
      PARAMETER(MXNNPh=1,MXNESh=1,MXNPRh=1,MXNDPh=1)
      PARAMETER(MXVNPh=198,MXVESh=170,MXVPRh=2,MXVDPh=4)
      PARAMETER(MXDNPh=165,MXDPRh=11,MXDDPh=2)

C -------- 3.  For transport source/sink, boundary conditions, and materials
C
      PARAMETER(MXSELc=1,MXSPRc=1,MXSDPc=1,MXWNPc=4,MXWPRc=2,MXWDPc=5)
      PARAMETER(MXCNPc=55,MXCESc=40,MXCPRc=2,MXCDPc=4)
      PARAMETER(MXNNPc=11,MXNESc=4,MXNPRc=1,MXNDPc=2)
      PARAMETER(MXVNPc=638,MXVESc=560,MXVPRc=1,MXVDPc=2)
      PARAMETER(MXDNPc=70,MXDPRc=6,MXDDPc=2)
C
      PARAMETER(MXNCCK=2)
C
      PARAMETER(MXLSVK=500,MXMSVK=500,MXKGLDK=2000,MXNDBK=2000)
      PARAMETER(MXNEPK=20,MXEPWK=20)
      PARAMETER(MXNPWK=99,MXELWK=27, mxnpws=1331,mxelws=1000)
      PARAMETER(MXNPFGK=2900,MXKGLK=2800)
C
```

Figure 4.14 depicts the concentration profiles along the z-axis at various times. It illustrates migration of the contamination with time. In the meantime, it shows the results obtained by the implementation of LEZOOMPC are almost the same as the exact solution. However, the Lagrangian-Eulerian approach, which is much better than conventional finite element scheme, still generates numerical dispersion even though the Courant number is less than 1 and Peclet number is only equal to one.

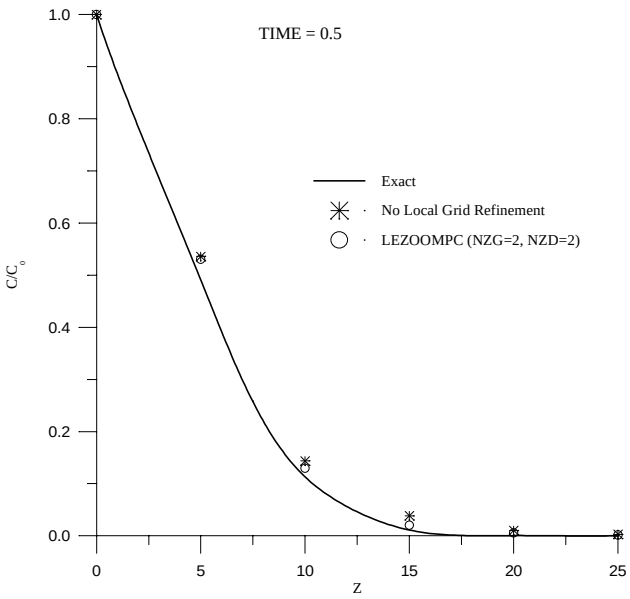


Figure 4.14a The concentration profile of Example 4 (1 of 6)

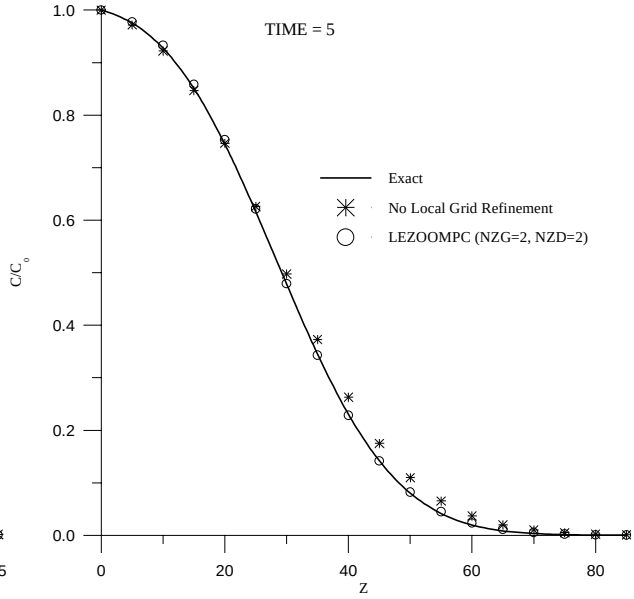


Figure 4.14b The concentration profile of Example 4 (2 of 6)

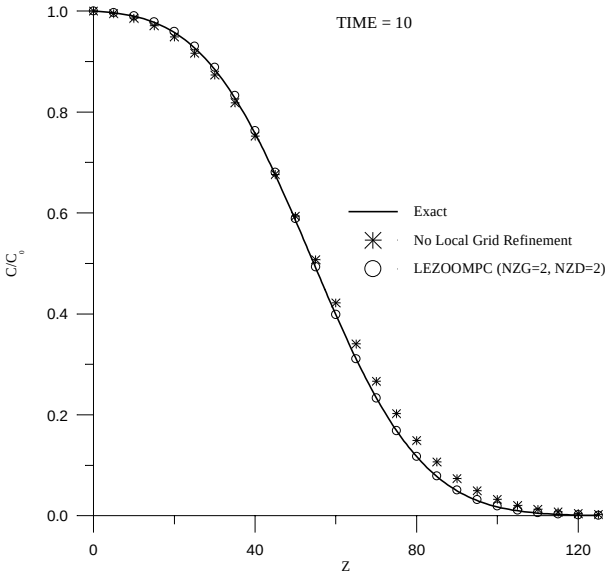


Figure 4.14c The concentration profile of Example 4 (3 0f 6)

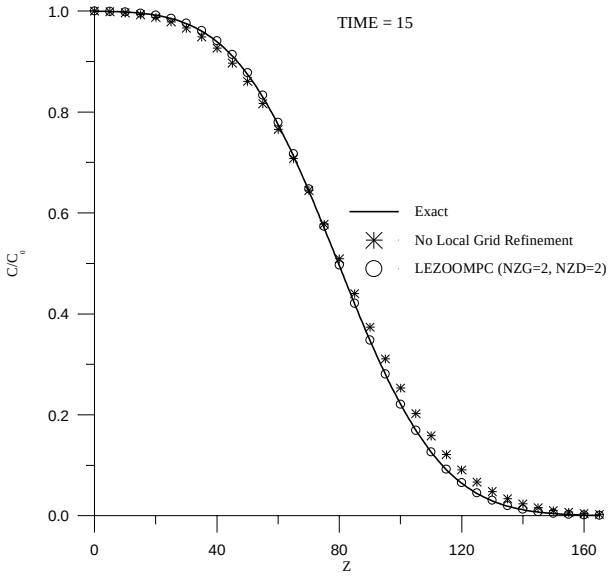


Figure4.14d The concentration profile of Example 4 (4 of 6)

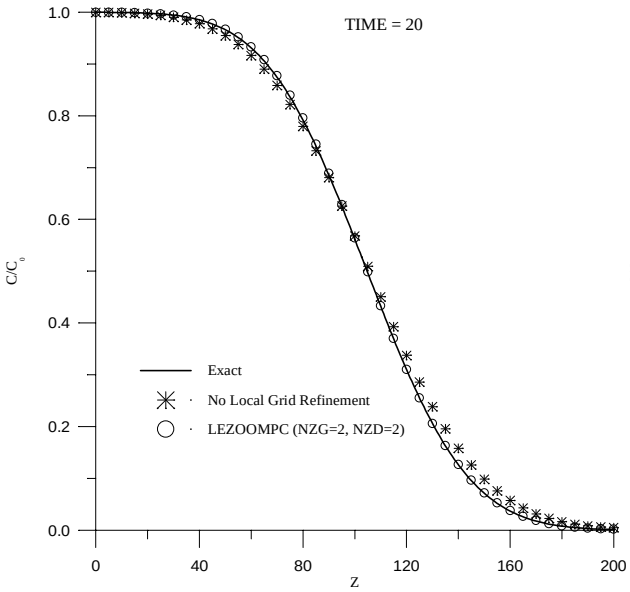


Figure 4.14e The concentration profile of Example 4 (5 of 6)

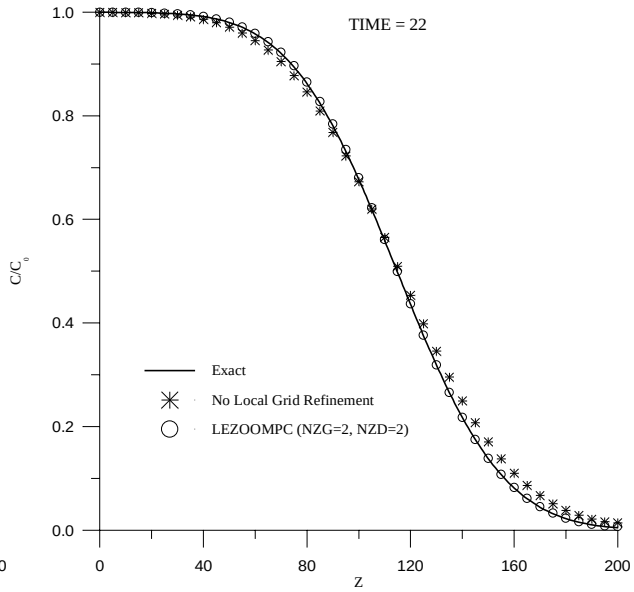


Figure 4.14f The concentration profile of Example 4 (6 of 6)

4.8 Input and Output for Example 4

Table 4.7 lists the input parameters and Table 4.8 shows the input data set for the sample problem described in the above section. The output is given in the attached floppy disk.

Table 4.7 The list of input parameters for Example 4

Parameters	Notation in the data input guide	Value	Unit	Data set
number of points	NNP	164	Dimensionless	7. A.
$\triangle x$	XAD	50	cm	7. B.
$\triangle y$	YAD	50	cm	7. B.
$\triangle z$	ZAD	5	cm	7. B.
K_d	RKD(1)	0	cm^3/g	5. F.
ρ_b	PROPt(1,1)	1.2	g/cm^3	5. E.

α_L	PROPt(1,2)	5.0	cm	5. E.
$\mu_o^{(1)}$	GRATE(1)	0.0	1/day	5. H.
$\mu_n^{(2)}$	GRATE(2)	0.0	1/day	5. H.
$\mu_o^{(3)}$	GRATE(3)	0.0	1/day	5. H.
$\mu_n^{(3)}$	GRATE(4)	0.0	1/day	5. H.
no. of elements	NEL	40	dimensionless	9. A.
θ	TH	0.4	dimensionless	25. B.
V_z	VZ	2.0	cm/day	25. A.
no. of subregion	NREGN	4	dimensionless	8. A.
no. of points in each subregion	NODES	41	dimensionless	8. B.
initial time step size	DELT	0.5	day	4. B.
time step size increment percentage	CHNG	0	dimensionless	4. B.
maximum time step size	DELMAX	0.5	day	4. B.
no. of times to reset time step size	NDTCHG	0	dimensionless	4. A.
Total simulation time	TMAX	22	day	4. B.
no. of time steps	NTI	44	dimensionless	4. A.
tolerance for nonlinear iteration	TOLBt	1×10^{-4}	dimensionless	3. B.
relaxation factor for nonlinear iteration	OMEt	1.0	dimensionless	2. E.

Table 4.8 Input Data Set for Example 4

```
    4 One-Dimensional Single Component Transport Problem; L=CM,T=DAY, M=G
========= data set 2: option parameters
  1  0  1  1
 100  0.5d0  1.0d-4
 1  1  1  0  0  0  0  0  0  2
 1  1.0  0.5d0  0.5d0  0.0d0
 -1  0  1  1  1  1
 1.0d0 0.5d0 1.0d0 1.0d0
========= data set 3: iteration parameters
 50 20 100 2.0d-2 2.0d-2
 50 100 1.0d-3  1.0d-4
========= data set 4: time control parameters
 44   2
```

```
 0.5d0    0.0d0    0.5d0    22.0d0
33       030003 0 0030   0 0 030 000 00 30003
0100000000100000000010000000001000000000010001
    1.0D01  2.0000D1
========= DATA SET 5:  MATERIAL PROPERTIES
1 7  1  1
     1.2d0    5.0d0      0.0d0     0.0d0     1.0d0    0.0d0  0.0d0
     0.0d0  0.0  0.0  0.0  0.0  0.0  0.0
     0.0d0  0.0  0.0  0.0  0.0  0.0  0.0
 0.0  0.0  0.0  0.0                    GRATE
 0.4  0.17 0.4  0.17                   YCOEFF
1.8D-2  1.8D-2  1.8D-2  1.8D-2        RTARDS   Kso, Ksn
3.0D-5  2.0D-5  3.0D-5  2.0D-5        RTARDO   Ko, Kn
3.0d-4  3.0D-4  3.0D-4  3.0D-4        RTARDN   Kpo, Kpn
1.0  0.375  1.0   0.375              SCOEFF   gammao, gamman
0.0    0.0    0.0    0.0             ECOEFF   alphao, alphan
0.0  0.0  0.0  0.0                   DCOEFF   lambdao, lambdan
3.0D-5  1.013D-4 3.0D-5 1.013D-4     SATURC   GAMMAo, GAMMAn
0.0  0.0   0.0  0.0                  PCOEFF   Epsilon
  1.1d-4                             COFK
========= DATA SET 6:  soil properties
    0    4    0    1.0d0    7.316d12    1.1232d2
   0.150D0   0.450D0    0.00D0    -1.0D2            THPROP
   0.000D0   0.000D0    0.00D0     0.0D0            AKPROP
C ******* DATA SET 7:  NODE COORDINATES
  164
    1   40    1   0.0D0    50.0D0     0.0D0     0.0D0     0.0D0     5.0D0
   42   40    1   0.0D0     0.0D0     0.0D0     0.0D0     0.0D0     5.0D0
   83   40    1   50.0D0     0.0D0     0.0D0     0.0D0     0.0D0     5.0D0
  124   40    1   50.0D0    50.0D0     0.0D0     0.0D0     0.0D0     5.0D0
    0    0    0   0.0     0.0       0.0       0.0       0.0       0.0
C ******* DATA SET 8:  SUBREGIONAL DATA
    4
  1  3  1  41  0
  0 0 0 0 0                          END OF NNPLR(K)
  1 40  1  1  1
  0 0 0 0 0                          END OF GNLR(I,1)
  1 40  1 42  1
  0 0 0 0 0                          END OF GNLR(I,2)
  1 40  1 83 1
 0 0 0 0 0                           END OF GNLR(I,3)
    1   40    1  124    1
 0 0 0 0 0                           END OF GNLR(I,4)
C ******* DATA SET 9:  ELEMENT INCIDENCES
   40
    1   39    1   42   83  124    1   43   84  125    2    1
    0    0    0    0    0    0    0    0    0   0    0   0   END OF IE
C ******* data set10: material correction
    0
C ******* DATA SET 11:  INITIAL CONDITIONS
    1    3   41         1.0d0      0.0d0     0.0
    2   38    1         0.0d0      0.0d0     0.0d0
   43   38    1         0.0d0      0.0d0     0.0d0
   84   38    1         0.0d0      0.0d0     0.0d0
  125   38    1         0.0d0      0.0d0     0.0d0
   41    3   41         0.0d0      0.0d0     0.0d0
    0    0    0         0.0d0      0.0d0     0.0d0   end of ic, transport
========= data set 14: element(distributed) source/sink, transport
    0 0 0 0
========= data set 15: point(well) source/sink, transport
    0 0 0 0
========= data set 20: run-in/seep-out boundary
```

```
    1 4 1 2 0
   0.0d0  0.0d0  1.0d38  0.0d0
    1   0   0   1   0
    0   0   0   0   0   end of irtyp
    1   0   0  82 123 164  41  0  0  0  0
    0   0   0   0   0   0   0  0  0  0  0   end fof isvt(j,i),j=1,4
    1   3   1  41  41
    0   0   0   0   0         end of npvbt
========= data set 21: dirichlet boundary conditions, transport
    4   1   2   0
   0.0d0    1.0d0    1.0d38    1.0d0
    1   3   1   1   41
    0   0   0   0   0
    1   3   1   1   0
    0   0   0   0   0     end of idtyp
========= data set 22: Cauchy boundary condition, transport
    0   0   0   0   0
========= data set 23: Neumann boundary condition, transport
    0   0   0   0   0
C ***** DATA SET 24 : PARAMETERS CONTROLLING TRACKING SCHEME
  1 1 0 2 1 2 1 1 1 2 1 2 2
  1.0d-4  1.0d-4
C ******* DATA SET 25:  HYDROLOGICAL BOUNDARY CONDITIONS
 1 163 1  0.0D0 0.0D0 2.0D0 0.0D0 0.0D0 0.0D0
 0   0 0    0.0   0.0   0.0   0.0   0.0   0.0  END OF VELOCITY
    1   39    1 0.4D0 0.0
    0    0    0    0.0      0.0                END OF TH
    0                  END OF JOB
----------------------------------------0000
```

4.9 Example 5: Two-Dimensional Single Component Transport Problem

This is a two-dimensional transport problem in a rectangular region of (x,y,z) = (0.0, 0.0, 0.0) and (x,y,z) = (540.0, 270.0, 1.0) (Figure 4.15). Initially, the concentration is zero throughout the region of interest. The concentration of 1.0 is maintained at x = 0.0 and $90 \leq y \leq 180$ (Figure 4.15).A concentration of 0.0 is maintained at x = 0.0 and $0.0 < y < 90.0$ or $180.0 < y < 270.0$ (Figure 4.15). A natural condition is imposed at x = 540. A bulk density of 1.2, a longitudinal dispersivity of 10.0, and a lateral dispersivity of 1.0 are assumed. A specific discharge (Darcy's velocity) of 2.0 is used and a moisture content of 0.2 is assumed. The region is divided into 9 x 9 x 1 = 81 elements resulting in 10 x 10 x 2 = 200 nodes (Figure 4.16). The element size is 60.0 x 30.0 x 1.0. A time-step size of 4.5 is used and a 40 time-step simulation is made to illustrate how to use 3DFATMIC. No adsorption is allowed.

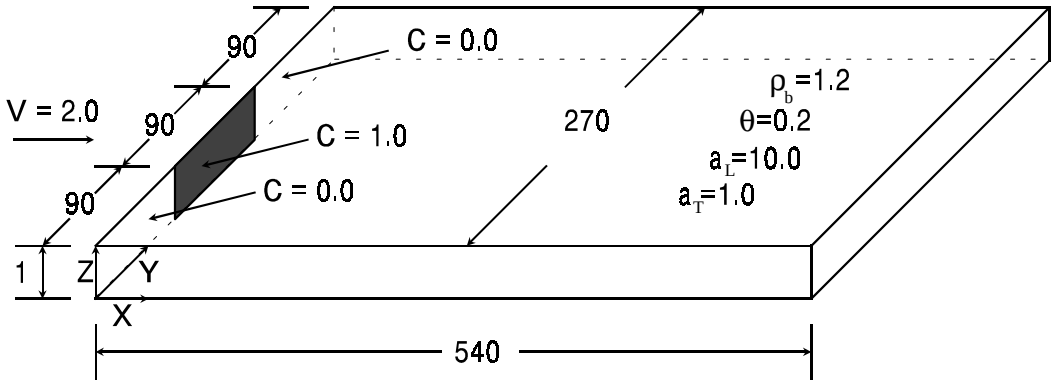


Figure 4.15 Problem definition and sketch for Example 5.

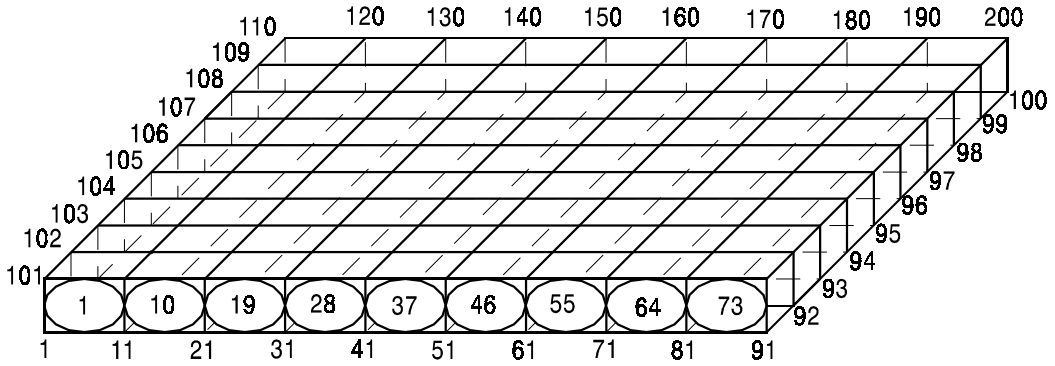


Figure 4.16 Finite element discretization for Example 5.

To execute the problem, the maximum control-integers in the MAIN should be specified as:

```
C----- For Example 1 through Example 5
c
      PARAMETER(MAXNPK=2079,MAXELK=1600,MXBNPK=999,MXBESK=999,
      >                MXTUBK=3008,MXADNK=maxnpk+0)
      PARAMETER(MXJBDK=35,MXKBDK=8,MXNTIK=100,MXDTCK=4)
      PARAMETER(LTMXNK=693,LMXNPK=231,LMXBWK=49,MXRGNK=9)
      PARAMETER(MXMATK=8,MXSPMK=5,MXMPMK=9)

C-------- 2.  For flow source/sink, boundary conditions, and materials

      PARAMETER(MXSELh=1,MXSPRh=1,MXSDPh=1,MXWNPh=4,MXWPRh=2,MXWDPh=3)
      PARAMETER(MXCNPh=110,MXCESh=90,MXCPRh=1,MXCDPh=2)
      PARAMETER(MXNNPh=1,MXNESh=1,MXNPRh=1,MXNDPh=1)
      PARAMETER(MXVNPh=198,MXVESh=170,MXVPRh=2,MXVDPh=4)
      PARAMETER(MXDNPh=165,MXDPRh=11,MXDDPh=2)

C -------- 3.  For transport source/sink, boundary conditions, and materials
```

```
C
      PARAMETER(MXSELc=1,MXSPRc=1,MXSDPc=1,MXWNPc=4,MXWPRc=2,MXWDPc=5)
      PARAMETER(MXCNPc=55,MXCESc=40,MXCPRc=2,MXCDPc=4)
      PARAMETER(MXNNPc=11,MXNESc=4,MXNPRc=1,MXNDPc=2)
      PARAMETER(MXVNPc=638,MXVESc=560,MXVPRc=1,MXVDPc=2)
      PARAMETER(MXDNPc=70,MXDPRc=6,MXDDPc=2)
C
      PARAMETER(MXNCCK=2)
C
      PARAMETER(MXLSVK=500,MXMSVK=500,MXKGLDK=2000,MXNDBK=2000)
      PARAMETER(MXNEPK=20,MXEPWK=20)
      PARAMETER(MXNPWK=99,MXELWK=27, mxnpws=1331,mxelws=1000)
      PARAMETER(MXNPFGK=2900,MXKGLK=2800)
C
```

Figure 4.17 depicts the 50% concentration contours at various times. It illustrates how the pollutant is moving through the medium with time.

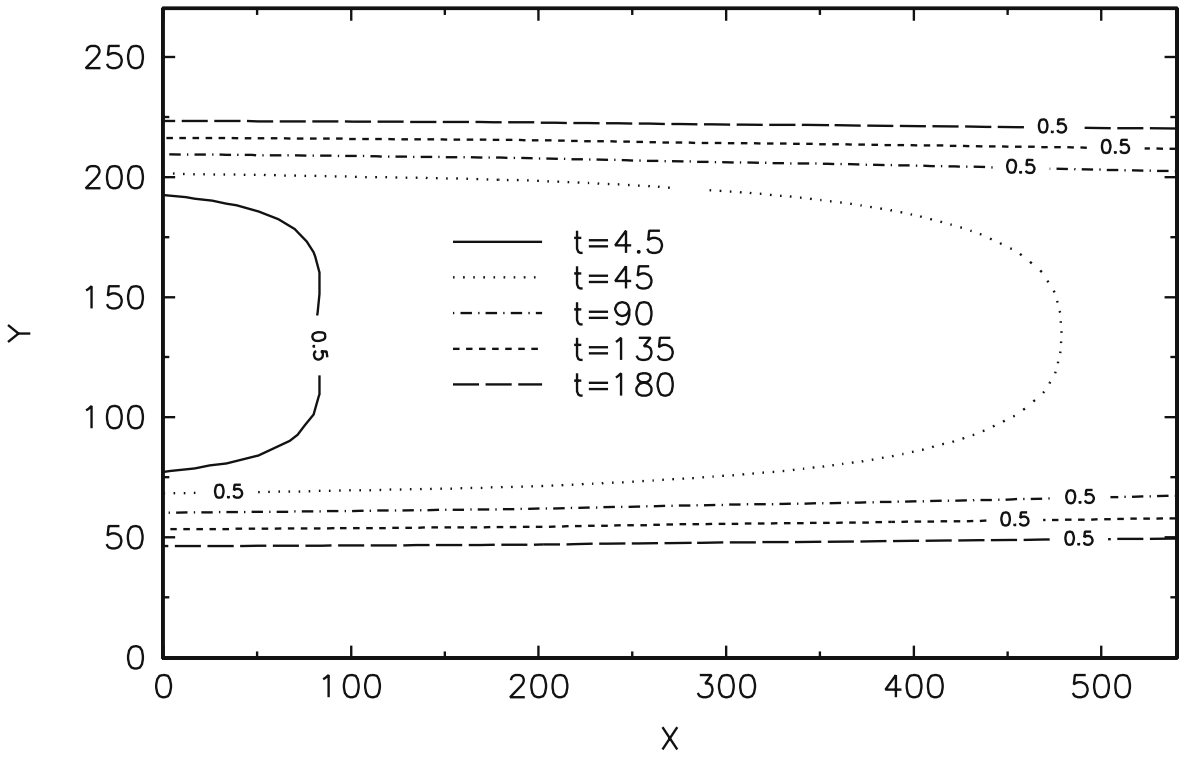


Figure 4.17 Contours of 50% concentration at various times**.**

4.10 Input and Output for Example 5

Table 4.9 lists the input parameters and Table 4.10 shows the input data set for the problem described in the above section. To save space, the output is available in electronic form.

Table 4.9 The list of input parameters for Example 5

Parameters	Notation in the data input guide	Value	Unit	Data set
number of points	NNP	200	Dimensionless	7. A.
Δx	XAD	60	cm	7. B.
Δy	YAD	30	cm	7. B.
Δz	ZAD	1	cm	7. B.
K_d	RKD(1)	0	cm^3/g	5. F.
ρ_b	PROPt(1,1)	1.2	g/cm^3	5. E.
α_L	PROPt(1,2)	10.0	cm	5. E.
α_T	PROPt(1,3)	1.0	cm	5. E.
$\mu_o^{(1)}$	GRATE(1)	0.0	1/day	5. H.
$\mu_n^{(2)}$	GRATE(2)	0.0	1/day	5. H.
$\mu_o^{(3)}$	GRATE(3)	0.0	1/day	5. H.
$\mu_n^{(3)}$	GRATE(4)	0.0	1/day	5. H.
no. of elements	NEL	81	dimensionless	9. A.
θ	TH	0.2	dimensionless	25. B.
V_x	VZ	2.0	cm/day	25. A.
no. of subregion	NREGN	2	dimensionless	8. A.
no. of points in each subregion	NODES	100	dimensionless	8. B.
initial time step size	DELT	4.5	day	4. B.
time step size increment percentage	CHNG	0	dimensionless	4. B.
maximum time step size	DELMAX	4.5	day	4. B.
no. of times to reset time step size	NDTCHG	0	dimensionless	4. A.
Total simulation time	TMAX	180	day	4. B.
no. of time steps	NTI	40	dimensionless	4. A.
tolerance for nonlinear iteration	TOLBt	10^{-4}	dimensionless	3. A.
relaxation factor for nonlinear iteration	OMEt	1.0	dimensionless	2. E.

Table 4.10 Input Data Set for Example 5

```
    5 Two-Dimensional Single Compoent Transport Problem; L=CM,T=DAY,M=G
===== DATA SET 2: OPTION PARAMETERS
  1  0  1  0
 50 0.5D0 1.0d-4                                NITRFT OMEFTF OMEFTT
 1  1  1  0  0  0 0 0 0  2        KSSF KSST ILUMP IMID IPNTSF IPNTST
 1  1.0  0.5d0  0.5d0   0.0d0      KGRAV WF OMEF OMIF
-1  0  1  1  1  0             KVIT IWET IOPTIM ksorp lgrn miconf
 1.0d0 0.5d0 1.0d0 1.00D0     WT WVT OMET OMIT
===== DATA SET 3: ITERATION PARAMETERS
 50 20 100 2.0d-2 2.0d-2      NITERF NCYLF NPITRF TOLAF TOLBF
 50 900 1.0d-3  1.0d-4        NITERT NPITRT TOLAT TOLBT
===== DATA SET 4: TIME CONTROL PARAMETERS
 40   0                        NTI NDTCHG
 4.50d0  0.00d0  4.5d0   1.8d2   DELT CHNG DELMAX TMAX
55000000005000000000500000000050000000005   KPR0 KPR(1..NTI)
00000000000000000000000000000000000000000   DSK0 KDSK(1..NTI)
  0.0d0
===== DATA SET 5: MATERIAL PROPERTIES
1  7   1   1                                  NMAT NMPPM
1.2d0  10.0d0    1.0d0   0.0d0   1.0d0   0.0d0   1.0d0   0.0d0 PROPT
0.0  0.0  0.0  0.0  0.0  0.0  0.0
0.0  0.0  0.0  0.0  0.0  0.0  0.0
 0.0  0.0  0.0  0.0                  GRATE
 0.4  0.17 0.4  0.17                 YCOEFF
1.8D-2  1.8D-2  1.8D-2  1.8D-2       RTARDS   Kso, Ksn
3.0D-5  2.0D-5  3.0D-5  2.0D-5       RTARDO   Ko, Kn
3.0d-4  3.0D-4  3.0D-4  3.0D-4       RTARDN   Kpo, Kpn
1.0  0.375  1.0   0.375              SCOEFF   gammao, gamman
0.0    0.0    0.0    0.0            ECOEFF   alphao, alphan
0.0  0.0  0.0  0.0                  DCOEFF   lambdao, lambdan
3.0D-5  1.013D-4 3.0D-5 1.013D-4     SATURC   GAMMAo, GAMMAn
0.0  0.0   0.0  0.0                 PCOEFF   Epsilon
  1.1d-4                            COFK
===== DATA SET 6: SOIL PROPERTIES
0    1    0    1.0D0  1.0d0  1.0d0   KSP NSPPM KCP GRAV
   0.000D0                         THPROP
   0.000D0                         AKPROP
===== DATA SET 7: NODE COORDINATES
  200                              NNP
  1 9  10  0.0D0  0.0D0 0.0D0 6.0D1 0.0D0 0.0D0
  2 9  10  0.0D0  3.0D1 0.0D0 6.0D1 0.0D0 0.0D0
  3 9  10  0.0D0  6.0D1 0.0D0 6.0D1 0.0D0 0.0D0
  4 9  10  0.0D0  9.0D1 0.0D0 6.0D1 0.0D0 0.0D0
  5 9  10  0.0D0 12.0D1 0.0D0 6.0D1 0.0D0 0.0D0
  6 9  10  0.0D0 15.0D1 0.0D0 6.0D1 0.0D0 0.0D0
  7 9  10  0.0D0 18.0D1 0.0D0 6.0D1 0.0D0 0.0D0
  8 9  10  0.0D0 21.0D1 0.0D0 6.0D1 0.0D0 0.0D0
  9 9  10  0.0D0 24.0D1 0.0D0 6.0D1 0.0D0 0.0D0
 10 9  10  0.0D0 27.0D1 0.0D0 6.0D1 0.0D0 0.0D0
 101 9  10  0.0D0  0.0D0 1.0D0 6.0D1 0.0D0 0.0D0
 102 9  10  0.0D0  3.0D1 1.0D0 6.0D1 0.0D0 0.0D0
 103 9  10  0.0D0  6.0D1 1.0D0 6.0D1 0.0D0 0.0D0
 104 9  10  0.0D0  9.0D1 1.0D0 6.0D1 0.0D0 0.0D0
 105 9  10  0.0D0 12.0D1 1.0D0 6.0D1 0.0D0 0.0D0
 106 9  10  0.0D0 15.0D1 1.0D0 6.0D1 0.0D0 0.0D0
 107 9  10  0.0D0 18.0D1 1.0D0 6.0D1 0.0D0 0.0D0
 108 9  10  0.0D0 21.0D1 1.0D0 6.0D1 0.0D0 0.0D0
 109 9  10  0.0D0 24.0D1 1.0D0 6.0D1 0.0D0 0.0D0
 110 9  10  0.0D0 27.0D1 1.0D0 6.0D1 0.0D0 0.0D0
  0  0   0  0.0    0.0   0.0   0.0   0.0   0.0 END OF COORDINATES
```

```
===== DATA SET 8: SUBREGIONAL DATA
    2                NREGN
  1  1  1  100 0
  0  0  0    0 0    END OF NNPLR(K)
  1 99  1    1 1
  0  0  0    0 0    END OF GNLR(I,1)
  1 99  1  101 1
  0  0  0    0 0    END OF GNLR(I,2)
===== DATA SET 9 : ELEMENT INCIDENCES
  81                 NEL
   1 8  1  1 11 12  2  101 111 112 102  1
  10 8  1 11 21 22 12  111 121 122 112  1
  19 8  1 21 31 32 22  121 131 132 122  1
  28 8  1 31 41 42 32  131 141 142 132  1
  37 8  1 41 51 52 42  141 151 152 142  1
  46 8  1 51 61 62 52  151 161 162 152  1
  55 8  1 61 71 72 62  161 171 172 162  1
  64 8  1 71 81 82 72  171 181 182 172  1
  73 8  1 81 91 92 82  181 191 192 182  1
   0 0  0  0  0  0  0    0   0   0   0  0 END OF IE
===== DATA SET 10: MATERIAL CORRECTION
    0                                     NCM
===== DATA SET 11: INITIAL CONDITIONS
    1  199    1          0.0D0     0.0D0  0.0
    0    0    0          0.0       0.0    0.0 END OF IC FOR TRANSPORT
===== DATA SET 14: ELEMENT(DISTRIBUTED) SOURCE/SINK OF TRANSPORT
    0  0  0  0             NSELT NSPRT NSDPT KSAIT
===== DATA SET 15: POINT(WELL) SOURCE/SINK OF TRANSPORT
    0  0  0  0             NWNPT NWPRT NWDPT KWAIT
===== DATA SET 20: VARIABLE BOUNDARY CONDITIONS OF TRANSPORT
    9 20  1  2  0          NVEST NVNPT NRPRT NRDPT KRAIT
0.0D0 0.0D0    1.0D38  0.0D0         TCVBFT CVBFT
    1    8    1    1    0
    0    0    0    0    0       END OF IVTYPT
    1    8    1   91   92  192  191    1    1    1    1
    0    0    0    0    0    0  0  0  0  0  0 END OF ISVT(J,I) J=1,4
    1    9    1   91    1
   11    9    1  191    1
    0    0    0    0    0          END OF NPVBT
===== DATA SET 21:  DIRICHLET BOUNDARY CONDITIONS OF TRANSPORT
   20  2  2  0                     NDNPT NDPRT NDDPT KDAIT
     0.0D0     1.0D0    1.0D38     1.0D0  TCDBFT CDBFT
     0.0d0     0.0d0    1.0d38     0.0d0
    1   3   1  4   1                   NPDBT(1..NDNPT)
    5   3   1  104  1
    9   2   1  1    1
    12  2   1  8    1
    15  2   1  101  1
    18  2   1  108  1
    0   0   0   0   0
    1    7    1    1    0
    9   11    1    2    0
    0    0    0    0    0               END OF IDTYPT
===== DATA SET 22: CAUCHY BOUNDARY CONDITIONS OF TRANSPORT
    0  0  0  0  0                     NCEST NCNPT NCPRT NCDPT KCAIT
===== DATA SET 23: NEUMANN BOUNDARY CONDITIONS, TRANSPORT
    0  0  0  0  0                     NNEST NNNPT NNPRT NNDPT KNAIT
C ***** DATA SET 24 : PARAMETERS CONTROLLING TRACKING SCHEME
  1 1 0 2 2 1 1 1 1 2 2 1 2
  1.0d-4  1.0d-4
===== DATA SET 25: HYDROLOGICAL VARIABLES
 1 199 1    2.0D0  0.0D0  0.0  0.0  0.0  0.0
```

```
0   0 0    0.0    0.0    0.0  0.0  0.0  0.0  END OF X-VELOCITY
1  80 1    0.2D0  0.0    0.0
0   0 0    0.0    0.0    0.0                 END OF TH
   0           ====== END OF JOB ======
```

4.11 Example 6: Two-Dimensional Multicomponent Transport in a Uniform Flow Field

This problem is used to illustrate the behavior of a dissolved organic plume undergoing natural biodegradation in a uniform ground-water flow field. The kinetic and microbial parameters for the simulation are the same as those published by Macquarrie et al. (1990). But with the different setup of governing equations in the system, the equivalent parameters in 3DFATMIC are adjusted and shown in Table 4.11. Figure 4.18 shows the x-z cross section of the region of interest and the remaining transport parameters. Substrate and oxygen are assumed to be at 0 and 3.5 mg/L everywhere in the domain at time zero, respectively. The initial condition is comprised of a square patch, which is placed far enough from the domain limits to avoid boundary effects, and shown in Figure 4.18. The concentrations in the initial patch are 3 mg/L for substrate and 1 mg/L for oxygen. The total background concentration of microbial #1 population is 0.23 mg/L and the retardation factor associated with microbes is 1000. Although the nitrate, nutrient, microbe #2, and microbe #3 are included in the input data, the simulations for these four components are not performed. Therefore, the initial and boundary conditions for these four components are set to zero in the input data file. Because of the implementation of the developed Lagrangian-Eulerian finite element numerical scheme with adapted local refinement, the Courant and Peclet criteria are not needed. Therefore, the nodal spacing is greater than that specified by Macquarrie et al. and shown in Figure 4.19.

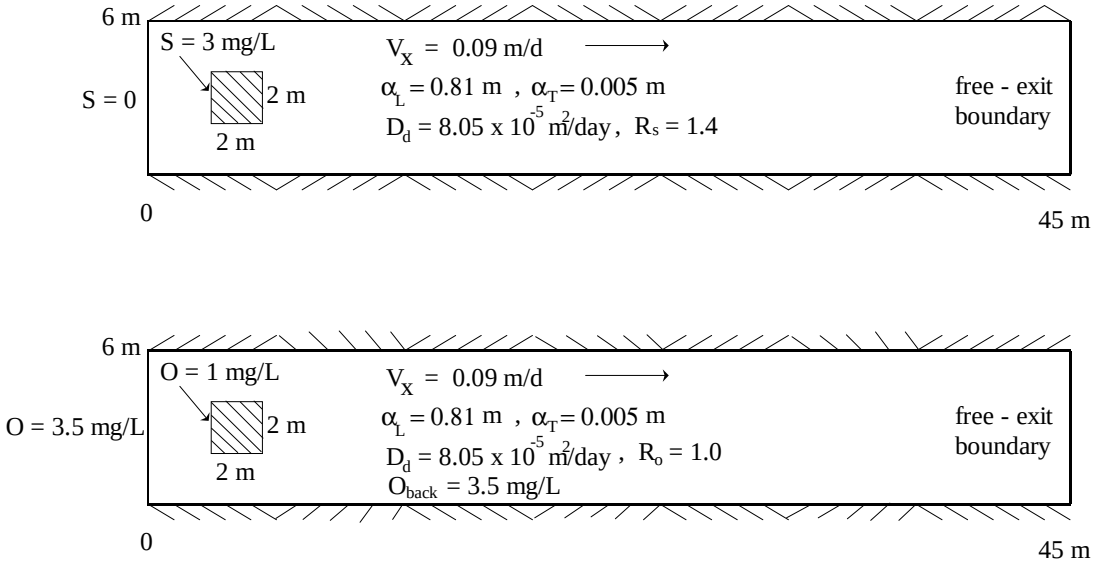


Figure 4.18 The x-z crosssection of region of interest and the associated physical parameters.

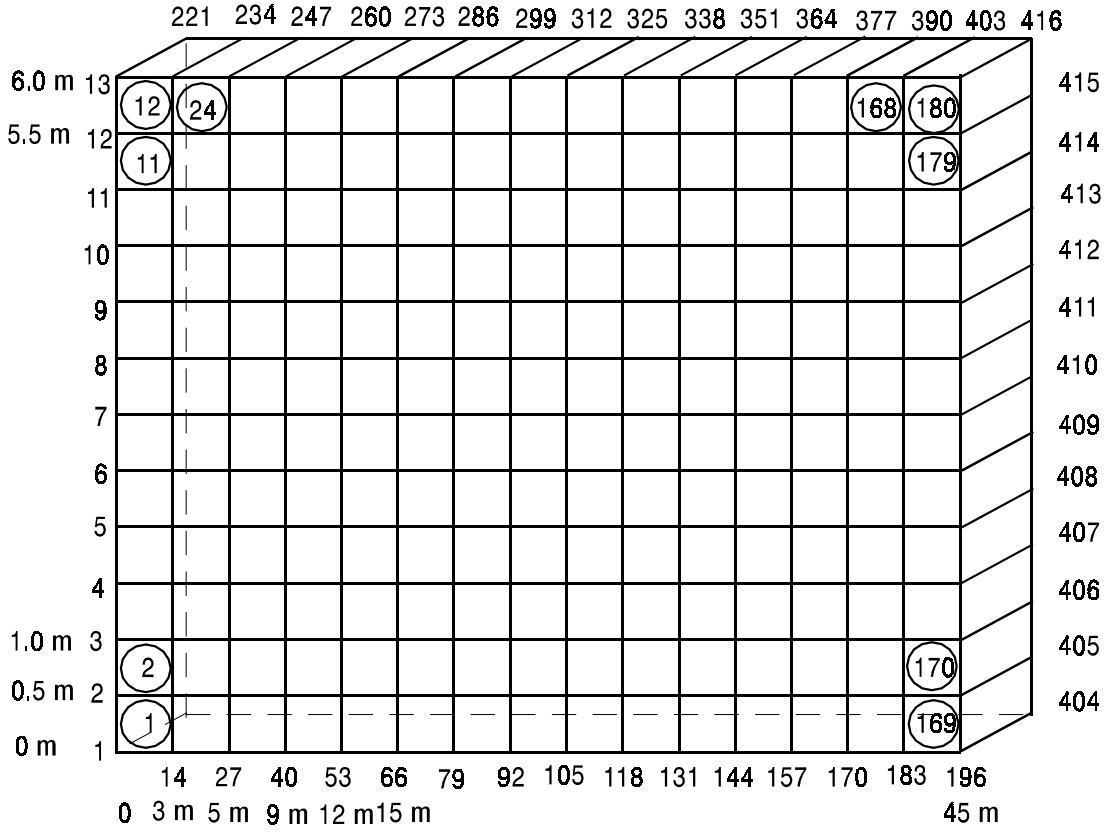


Figure 4.19 The discretization of the region of interest

To execute the problem, the maximum control-integers in the MAIN should be specified as

```
C----- For Example 6 &Example 8
c
      PARAMETER(MAXNPK=2288,MAXELK=1800,MXBNPK=1999,MXBESK=1999,
      >                MXTUBK=2640,MXADNK=maxnpk+14000)
      PARAMETER(MXJBDK=85,MXKBDK=8,MXNTIK=100,MXDTCK=4)
      PARAMETER(LTMXNK=693,LMXNPK=231,LMXBWK=49,MXRGNK=11)
      PARAMETER(MXMATK=1,MXSPMK=2,MXMPMK=7)

C-------- 2.  For flow source/sink, boundary conditions, and materials

      PARAMETER(MXSELh=1,MXSPRh=1,MXSDPh=1,MXWNPh=1,MXWPRh=1,MXWDPh=1)
      PARAMETER(MXCNPh=1,MXCESh=1,MXCPRh=1,MXCDPh=1)
      PARAMETER(MXNNPh=1,MXNESh=1,MXNPRh=1,MXNDPh=1)
      PARAMETER(MXVNPh=1,MXVESh=1,MXVPRh=1,MXVDPh=1)
      PARAMETER(MXDNPh=1,MXDPRh=1,MXDDPh=1)

C -------- 3.  For transport source/sink, boundary conditions, and materials
C
      PARAMETER(MXSELc=1,MXSPRc=1,MXSDPc=1,MXWNPc=1,MXWPRc=1,MXWDPc=1)
      PARAMETER(MXCNPc=1,MXCESc=1,MXCPRc=1,MXCDPc=1)
      PARAMETER(MXNNPc=1,MXNESc=1,MXNPRc=1,MXNDPc=1)
      PARAMETER(MXVNPc=143,MXVESc=120,MXVPRc=1,MXVDPc=2)
      PARAMETER(MXDNPc=143,MXDPRc=2,MXDDPc=2)
C
      PARAMETER(MXNCCK=7)
C
      PARAMETER(MXLSVK=5000,MXMSVK=5000,MXKGLDK=29999,MXNDBK=9999)
      PARAMETER(MXNEPK=1,MXEPWK=1)
      PARAMETER(MXNPWK=48,MXELWK=15, mxnpws=1,mxelws=1)
      PARAMETER(MXNPFGK=260000,MXKGLK=140000)
C
```

4.12 Input and Output for Example 6

Table 4.11 lists the input parameters and Table 4.12 shows the input data set for the sample problem described in the above section. The output isavailable in electronic form.

Table 4.11 The list of input parameters for Example 6

Parameters	Notation in the data input guide	Value	Unit	Data set
number of points	NNP	416	Dimensionless	7. A.

$\triangle x$	XAD	3.0 (except arround x = 5.0)	m	7. B.
$\triangle y$	YAD	0.5	m	7. B.
$\triangle z$	ZAD	0.5	m	7. B.
α_L	PROP(1,2)	0.81	m	5. E.
α_T	PROP(1,3)	5.0×10^{-3}	m	5. E.
D_m	PROP(1,4)	8.05×10^{-5}	m^2/day	5. E.
K_{d1}	RKD(1)	1000	m^3/mg	5. F.
K_{ds}	RKD(4)	0.4	m^3/mg	5. F.
$\mu_o^{(1)}$	GRATE(1)	0.21	1/day	5. H.
$\mu_n^{(2)}$	GRATE(2)	0..0	1/day	5. H.
$\mu_o^{(3)}$	GRATE(3)	0.0	1/day	5. H.
$\mu_n^{(3)}$	GRATE(4)	0.0	1/day	5. H.
$Y_o^{(1)}$	YCOEFF(1)	0.426	mg/mg	5. H.
$Y_n^{(2)}$	YCOEFF(2)	0.17	mg/mg	5. H.
$Y_o^{(3)}$	YCOEFF(3)	0.4	mg/mg	5. H.
$Y_n^{(3)}$	YCOEFF(4)	0.17	mg/mg	5. H.
$K_{so}^{(1)}$	RTARDS(1)	654	mg/m^3	5. H.
$K_{sn}^{(2)}$	RTARDS(2)	0.018	mg/m^3	5. H.
$K_{so}^{(3)}$	RTARDS(3)	0.018	mg/m^3	5. H.
$K_{sn}^{(3)}$	RTARDS(4)	0.018	mg/m^3	5. H.
$K_o^{(1)}$	RTARDO(1)	1.0×10^{2}	mg/m^3	5. H.
$K_n^{(2)}$	RTARDO(2)	2.0×10^{-5}	mg/m^3	5. H.
$K_o^{(3)}$	RTARDO(3)	3.0×10^{-5}	mg/m^3	5. H.
$K_n^{(3)}$	RTARDO(4)	2.0×10^{-5}	mg/m^3	5. H.
$K_{po}^{(1)}$	RTARDN(1)	3.0×10^{-4}	mg/m^3	5. H.
$K_{pn}^{(2)}$	RTARDN(2)	0.0	mg/m^3	5. H.
$K_{po}^{(3)}$	RTARDN(3)	0.0	mg/m^3	5. H.
$K_{pn}^{(3)}$	RTARDN(4)	0.0	mg/m^3	5. H.
$\gamma_o^{(1)}$	SCOEFF(1)	7.044	dimensionless	5. H.
$\gamma_n^{(2)}$	SCOEFF(2)	0.0	dimensionless	5. H.

$\gamma_o^{(3)}$	SCOEFF(3)	0.0	dimensionless	5. H.
$\gamma_n^{(3)}$	SCOEFF(4)	0.0	dimensionless	5. H.
$\alpha_o^{(1)}$	ECOEFF(1)	0.0	dimensionless	5. H.
$\alpha_n^{(2)}$	ECOEFF(2)	0.0	dimensionless	5. H.
$\alpha_o^{(3)}$	ECOEFF(3)	0.0	dimensionless	5. H.
$\alpha_n^{(3)}$	ECOEFF(4)	0.0	dimensionless	5. H.
$\lambda_o^{(1)}$	DCOEFF(1)	0.0	1/day	5. H.
$\lambda_n^{(2)}$	DCOEFF(2)	0.0	1/day	5. H.
$\lambda_o^{(3)}$	DCOEFF(3)	0.0	1/day	5. H.
$\lambda_n^{(3)}$	DCOEFF(4)	0.0	1/day	5. H.
$\Gamma_o^{(1)}$	SATURC(1)	0.0	mg/m^3	5. H.
$\Gamma_n^{(2)}$	SATURC(2)	0.0	mg/m^3	5. H.
$\Gamma_o^{(3)}$	SATURC(3)	0.0	mg/m^3	5. H.
$\Gamma_n^{(3)}$	SATURC(4)	0.0	mg/m^3	5. H.
$\epsilon_o^{(1)}$	PCOEFF(1)	0.0	dimensionless	5. H.
$\epsilon_n^{(2)}$	PCOEFF(2)	0.0	dimensionless	5. H.
$\epsilon_o^{(3)}$	PCOEFF(3)	0.0	dimensionless	5. H.
$\epsilon_n^{(3)}$	PCOEFF(4)	0.0	dimensionless	5. H.
K_c	COFK	0.0	mg/m^3	5. H.
no. of elements	NEL	180	dimensionless	9. A.
no. of subregion	NREGN	2	dimensionless	8. A.
no. of points in each subregion	NODES	208	dimensionless	8. B.
Velocity	V_x	0.09	m/day	25. A.
transient-state for transport	KSSt	1	dimensionless	2. B.
initial time step size	DELT	2.0	day	4. B.
time step size increment percentage	CHNG	0	dimensionless	4. B.
maximum time step size	DELMAX	2.0	day	4. B.
no. of times to reset time step size	NDTCHG	0	dimensionless	4. A.
Total simulation time	TMAX	200	day	4. B.

no. of time steps	NTI	100	dimensionless	4. A.
tolerance for transport nonlinear iteration	TOLBt	1×10^{-4}	dimensionless	3. B.
relaxation factor for transport nonlinear iteration	OMEt	1.0	dimensionless	2. E.
ρ_w	RHO	10^9	mg/m^3	5.B. & 6.A.
μ_w	VISC	94832640	mg/m/day	5.B. & 6.A.
g	GRAV	7.316×10^{10}	m/day^2	6.A.

Table 4.12 Input Data Set for Example 6

```
    6 Two-D Multicomponent Transport in a Uniform Flow Field: mg,m,day
===== DATA SET 2: OPTION PARAMETERS
  1  0  1  0
 50 0.5D0 1.0D-4          NITRFT OMEFTF OMEFTT
 1  1  1  0  0  1  0  0  1  1   KSSF KSST ILUMP IMID IPNTSF IPNTST
 1  1.0  1.0d0  1.0d0 0.0d0     KGRAV WF OMEF OMIF
 -1  1  0  1  1                 KVIT IWET IOPTIM KSORP LGRAN
 1.0d0 1.0d0 1.0d0 1.0d0        WT WVT OMET OMIT
===== DATA SET 3: ITERATION PARAMETERS
 50 20 100 1.0d-2 1.0d-2        NITERF NCYLF NPITRF TOLAF TOLBF
 500 100 1.0d-2  1.0d-4         NITERT NPITRT TOLAT TOLBT ALLOW
===== DATA SET 4: TIME CONTROL PARAMETERS
 100  0                         NTI NDTCHG
 2.0d0  0.00d0  2.0d0   2.0d2   DELT CHNG DELMAX TMAX
55        0         0         0         0         5         0         0
0         0         5
1                                                   1
0                   1
  0.0d0
===== DATA SET 5: MATERIAL PROPERTIES
 1  7  7  1                    NMAT NMPPM
 1.00d0 8.1d-1   5.0d-3  8.05D-5 1.0d0   0.0d0   1.0d0    PROPT
 1.0d3  0.0d0  0.0   0.4D0  0.0D0  0.0D0  0.0D0
 0.0d0  0.0d0  0.0   0.0    0.0    0.0    0.0
 0.21 0.0  0.0  0.0                  GRATE
 0.426 0.17 0.4  0.17                 YCOEFF
6.54D2   1.8D-2  1.8D-2  1.8D-2      RTARDS   Kso, Ksn
1.0D2   2.0D-5  3.0D-5  2.0D-5       RTARDO   Ko, Kn
0.0d0   0.0D0   0.0D0   0.0D0       RTARDN   Kpo, Kpn
7.044  0.0    0.0   0.0             SCOEFF   gammao, gamman
0.0    0.0    0.0    0.0           ECOEFF   alphao, alphan
0.0  0.0  0.0  0.0                 DCOEFF   lambdao, lambdan
0.0D0   0.0D0 0.0D0 0.0D0      SATURC   GAMMAo, GAMMAn
0.0  0.0   0.0  0.0                 PCOEFF   Epsilon
  0.0d0                             COFK
===== DATA SET 6: SOIL PROPERTIES
1    2    0   1.0d0  9.8D0  1.0D0          KSP NSPPM KCP GRAV
-1000.0    1000.0                      PRESSURE
    0.1       0.1                      WATER CONTENT
    1.0       1.0                      RELATIVE CONDUCTIVITY
```

```
    0.0       0.0                          WATER CAPACITY
===== DATA SET 7: NODE COORDINATES
  416                                      NNP
  1  1   13  0.0  0.0  0.0  3.0  0.0   0.0
 27  0    0  5.0  0.0  0.0  0.0  0.0   0.0
 40  12  13  9.0  0.0  0.0  3.0  0.0   0.0
  2  1   13  0.0  0.0  0.5  3.0  0.0   0.0
 28  0    0  5.0  0.0  0.5  0.0  0.0   0.0
 41  12  13  9.0  0.0  0.5  3.0  0.0   0.0
  3  1   13  0.0  0.0  1.0  3.0  0.0   0.0
 29  0    0  5.0  0.0  1.0  0.0  0.0   0.0
 42  12  13  9.0  0.0  1.0  3.0  0.0   0.0
  4  1   13  0.0  0.0  1.5  3.0  0.0   0.0
 30  0    0  5.0  0.0  1.5  0.0  0.0   0.0
 43  12  13  9.0  0.0  1.5  3.0  0.0   0.0
  5  1   13  0.0  0.0  2.0  3.0  0.0   0.0
 31  0    0  5.0  0.0  2.0  0.0  0.0   0.0
 44  12  13  9.0  0.0  2.0  3.0  0.0   0.0
  6  1   13  0.0  0.0  2.5  3.0  0.0   0.0
 32  0    0  5.0  0.0  2.5  0.0  0.0   0.0
 45  12  13  9.0  0.0  2.5  3.0  0.0   0.0
  7  1   13  0.0  0.0  3.0  3.0  0.0   0.0
 33  0    0  5.0  0.0  3.0  0.0  0.0   0.0
 46  12  13  9.0  0.0  3.0  3.0  0.0   0.0
  8  1   13  0.0  0.0  3.5  3.0  0.0   0.0
 34  0    0  5.0  0.0  3.5  0.0  0.0   0.0
 47  12  13  9.0  0.0  3.5  3.0  0.0   0.0
  9  1   13  0.0  0.0  4.0  3.0  0.0   0.0
 35  0    0  5.0  0.0  4.0  0.0  0.0   0.0
 48  12  13  9.0  0.0  4.0  3.0  0.0   0.0
 10  1   13  0.0  0.0  4.5  3.0  0.0   0.0
 36  0    0  5.0  0.0  4.5  0.0  0.0   0.0
 49  12  13  9.0  0.0  4.5  3.0  0.0   0.0
 11  1   13  0.0  0.0  5.0  3.0  0.0   0.0
 37  0    0  5.0  0.0  5.0  0.0  0.0   0.0
 50  12  13  9.0  0.0  5.0  3.0  0.0   0.0
 12  1   13  0.0  0.0  5.5  3.0  0.0   0.0
 38  0    0  5.0  0.0  5.5  0.0  0.0   0.0
 51  12  13  9.0  0.0  5.5  3.0  0.0   0.0
 13  1   13  0.0  0.0  6.0  3.0  0.0   0.0
 39  0    0  5.0  0.0  6.0  0.0  0.0   0.0
 52  12  13  9.0  0.0  6.0  3.0  0.0   0.0
209  1   13  0.0  0.5  0.0  3.0  0.0   0.0
235  0    0  5.0  0.5  0.0  0.0  0.0   0.0
248  12  13  9.0  0.5  0.0  3.0  0.0   0.0
210  1   13  0.0  0.5  0.5  3.0  0.0   0.0
236  0    0  5.0  0.5  0.5  0.0  0.0   0.0
249  12  13  9.0  0.5  0.5  3.0  0.0   0.0
211  1   13  0.0  0.5  1.0  3.0  0.0   0.0
237  0    0  5.0  0.5  1.0  0.0  0.0   0.0
250  12  13  9.0  0.5  1.0  3.0  0.0   0.0
212  1   13  0.0  0.5  1.5  3.0  0.0   0.0
238  0    0  5.0  0.5  1.5  0.0  0.0   0.0
251  12  13  9.0  0.5  1.5  3.0  0.0   0.0
213  1   13  0.0  0.5  2.0  3.0  0.0   0.0
239  0    0  5.0  0.5  2.0  0.0  0.0   0.0
252  12  13  9.0  0.5  2.0  3.0  0.0   0.0
214  1   13  0.0  0.5  2.5  3.0  0.0   0.0
240  0    0  5.0  0.5  2.5  0.0  0.0   0.0
253  12  13  9.0  0.5  2.5  3.0  0.0   0.0
215  1   13  0.0  0.5  3.0  3.0  0.0   0.0
241  0    0  5.0  0.5  3.0  0.0  0.0   0.0
```

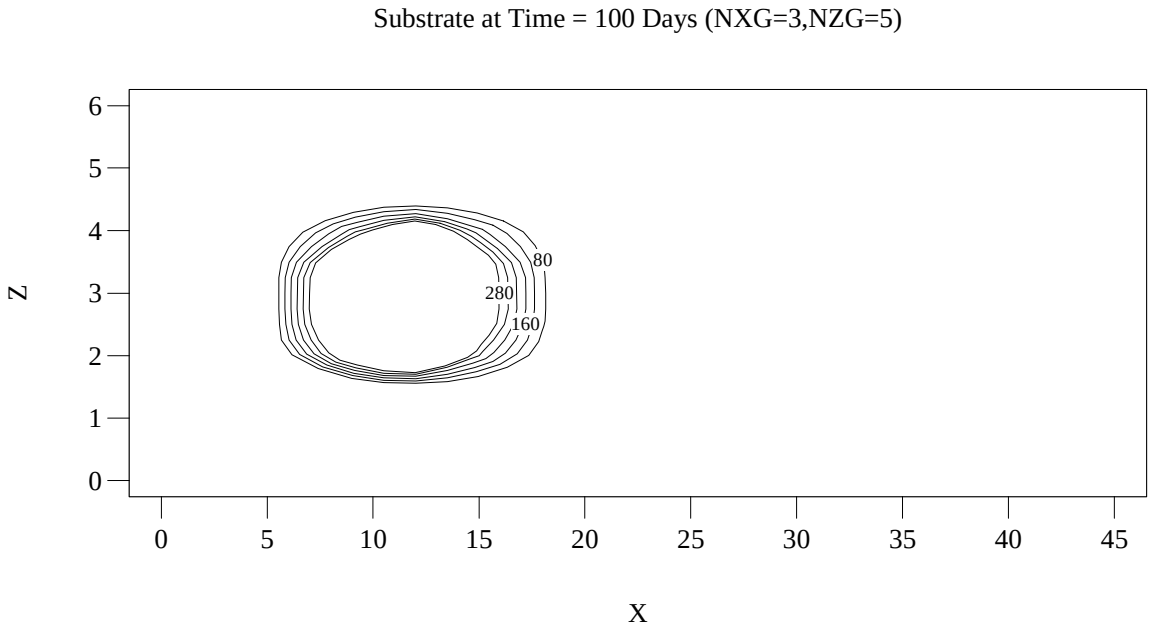
```
 254 12  13  9.0  0.5  3.0  3.0  0.0   0.0
 216 1   13  0.0  0.5  3.5  3.0  0.0   0.0
 242 0    0  5.0  0.5  3.5  0.0  0.0   0.0
 255 12  13  9.0  0.5  3.5  3.0  0.0   0.0
 217 1   13  0.0  0.5  4.0  3.0  0.0   0.0
 243 0    0  5.0  0.5  4.0  0.0  0.0   0.0
 256 12  13  9.0  0.5  4.0  3.0  0.0   0.0
 218 1   13  0.0  0.5  4.5  3.0  0.0   0.0
 244 0    0  5.0  0.5  4.5  0.0  0.0   0.0
 257 12  13  9.0  0.5  4.5  3.0  0.0   0.0
 219 1   13  0.0  0.5  5.0  3.0  0.0   0.0
 245 0    0  5.0  0.5  5.0  0.0  0.0   0.0
 258 12  13  9.0  0.5  5.0  3.0  0.0   0.0
 220 1   13  0.0  0.5  5.5  3.0  0.0   0.0
 246 0    0  5.0  0.5  5.5  0.0  0.0   0.0
 259 12  13  9.0  0.5  5.5  3.0  0.0   0.0
 221 1   13  0.0  0.5  6.0  3.0  0.0   0.0
 247 0    0  5.0  0.5  6.0  0.0  0.0   0.0
 260 12  13  9.0  0.5  6.0  3.0  0.0   0.0
  0  0 0  0.0    0.0   0.0   0.0   0.0   0.0  END OF COORDINATES
===== DATA SET 9 : ELEMENT INCIDENCES
  180                                          NEL
    1   14   12    1   14  222  209   2    15  223  210   13
    2   14   12    2   15  223  210   3    16  224  211   13
    3   14   12    3   16  224  211   4    17  225  212   13
    4   14   12    4   17  225  212   5    18  226  213   13
    5   14   12    5   18  226  213   6    19  227  214   13
    6   14   12    6   19  227  214   7    20  228  215   13
    7   14   12    7   20  228  215   8    21  229  216   13
    8   14   12    8   21  229  216   9    22  230  217   13
    9   14   12    9   22  230  217  10    23  231  218   13
   10   14   12   10   23  231  218  11    24  232  219   13
   11   14   12   11   24  232  219  12    25  233  220   13
   12   14   12   12   25  233  220  13    26  234  221   13
    0    0    0    0    0    0    0    0    0    0    0   0  END OF IE
===== DATA SET 10: MATERIAL CORRECTION
    0                                                      NCM
===== DATA SET 11 : INITIAL CONDIDTIONS
 1  415  1  2.3D-2 0.0D0  0.0D0
 0   0   0  0.0D0  0.0D0  0.0D0
 1  415  1  0.0D0  0.0D0  0.0D0
 0   0   0  0.0D0  0.0D0  0.0D0
 1  415  1  0.0D0  0.0D0  0.0D0
 0   0   0  0.0D0  0.0D0  0.0D0
 1  16   1  0.0D0  0.0D0  0.0D0
 18  4   1  3.0d3 0.0d0  0.0d0
 23  7   1  0.0d0  0.0d0  0.0d0
 31  4   1  3.0d3 0.0d0  0.0d0
 36 189  1  0.0d0  0.0d0  0.0d0
 226 4   1  3.0d3 0.0d0  0.0d0
 231 7   1  0.0d0  0.0d0  0.0d0
 239 4   1  3.0d3 0.0d0  0.0d0
 244 172 1  0.0d0  0.0d0  0.0d0
 0   0   0  0.0d0  0.0d0  0.0d0
 1  16   1  3.5D3 0.0D0  0.0D0
 18  4   1  1.0d3 0.0d0  0.0d0
 23  7   1  3.5d3 0.0d0  0.0d0
 31  4   1  1.0d3 0.0d0  0.0d0
 36 189  1  3.5d3 0.0d0  0.0d0
 226 4   1  1.0d3 0.0d0  0.0d0
 231 7   1  3.5d3 0.0d0  0.0d0
 239 4   1  1.0d3 0.0d0  0.0d0
```

```
 244 172 1  3.5d3 0.0d0  0.0d0
  0  0   0  0.0d0  0.0d0  0.0d0
  1  415 1  0.0d0  0.0d0  0.0d0
  0  0   0  0.0d0  0.0d0  0.0d0
  1  415 1  0.0d0  0.0d0  0.0d0
  0  0   0  0.0d0  0.0d0  0.0d0
===== DATA SET 14: ELEMENT(DISTRIBUTED) SOURCE/SINK OF TRANSPORT
    0  0  0  0                  NSELT NSPRT NSDPT KSAIT
===== DATA SET 15: POINT(WELL) SOURCE/SINK OF TRANSPORT
    0  0  0  0                  NWNPT NWPRT NWDPT KWAIT
===== DATA SET 20: VARIABLE BOUNDARY CONDITIONS OF TRANSPORT
    12  26   1  2  0            NVEST NVNPT NRPRT NRDPT KRAIT
    0.0D0  0.0D0  1.0D38  0.0D0
    1  11  1  1  0
    0  0   0  0  0
    1  11  1  1  0
    0  0   0  0  0
    1  11  1  1  0
    0  0   0  0  0
    1  11  1  1  0
    0  0   0  0  0
    1  11  1  1  0
    0  0   0  0  0
    1  11  1  1  0
    0  0   0  0  0
    1  11  1  1  0
    0  0   0  0  0
   1  11  1  196  404  405  197  1   1  1  1
  0    0  0   0   0     0    0   0  0  0  0
  1  12   1  196  1
  14 12   1  404  1
   0  0   0    0  0
===== DATA SET 21:  DIRICHLET BOUNDARY CONDITIONS OF TRANSPORT
   26  2  2  0             NDNPT NDPRT NDDPT KDAIT
   0.0D0  0.0D0  1.0D38  0.0D0
   0.0D0  3.5D3  1.0D38  3.5D3
   1  12  1  1  1
  14  12  1  209  1
   0   0   0  0  0
   1  25   1  1  0
   0  0    0  0  0
   1  25   1  1  0
   0  0    0  0  0
   1  25   1  1  0
   0  0    0  0  0
   1  25   1  1  0
   0  0    0  0  0
   1  25   1  2  0
   0  0    0  0  0
   1  25   1  1  0
   0   0   0  0  0
   1  25   1  1  0
   0   0   0  0  0
===== DATA SET 22: CAUCHY BOUNDARY CONDITIONS OF TRANSPORT
   0  0   0  0  0             NCEST NCNPT NCPRT NCDPT KCAIT
===== DATA SET 23: NEUMANN BOUNDARY CONDITIONS, TRANSPORT
    0  0  0  0  0             NNEST NNNPT NNPRT NNDPT KNAIT
===== DATA SET 24 : PARAMETERS CONTROLLOING TRACKING SCHEME
  1  1  0  3  1  5  1  1  1   3  1  5   2
  1.0d-4  1.0d-4
===== DATA SET 25 : VELOCITY AND MOISTURE CONTENT
  1  415  1  9.0D-2 0.0D0  0.0D0  0.0D0  0.0D0  0.0D0  0.0D0
```

```
0   0   0  0.0D0  0.0D0  0.0D0  0.0D0  0.0D0  0.0D0
1  179  1  1.0D0  0.0D0
0   0   0  0.0D0  0.0D0
  0          ====== END OF JOB ======
```

Figure 4.20, Figure 4.21, and Figure 4.22 show the simulation results of substrate, oxygen, and total microbial mass distributions at 100 days and 200 days, respectively.

(a)



(b)

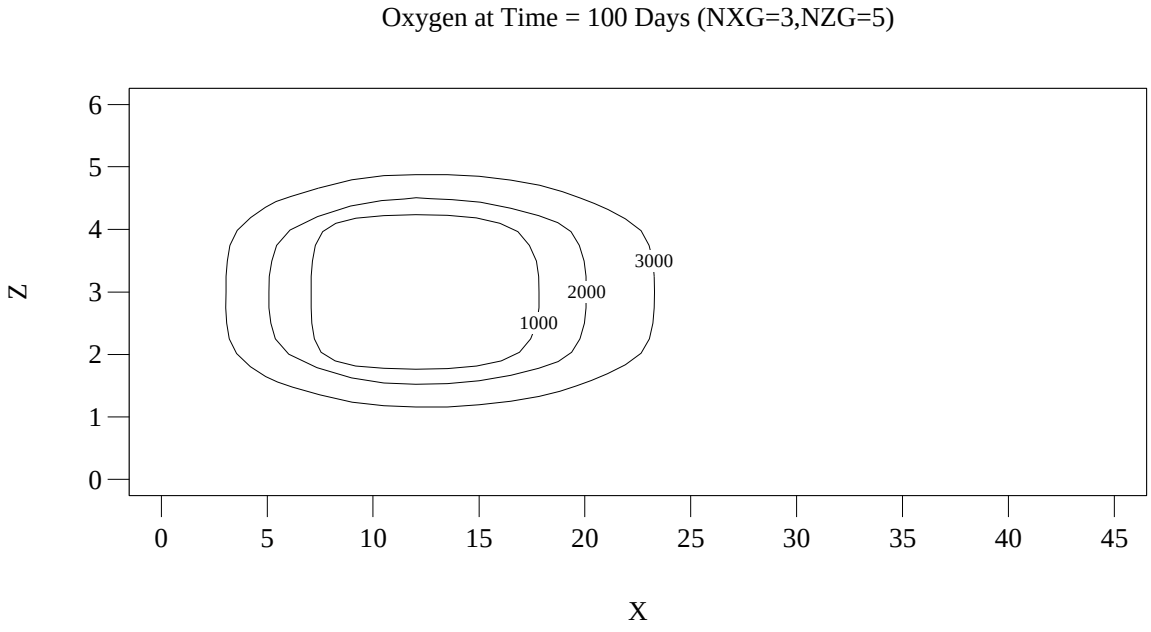
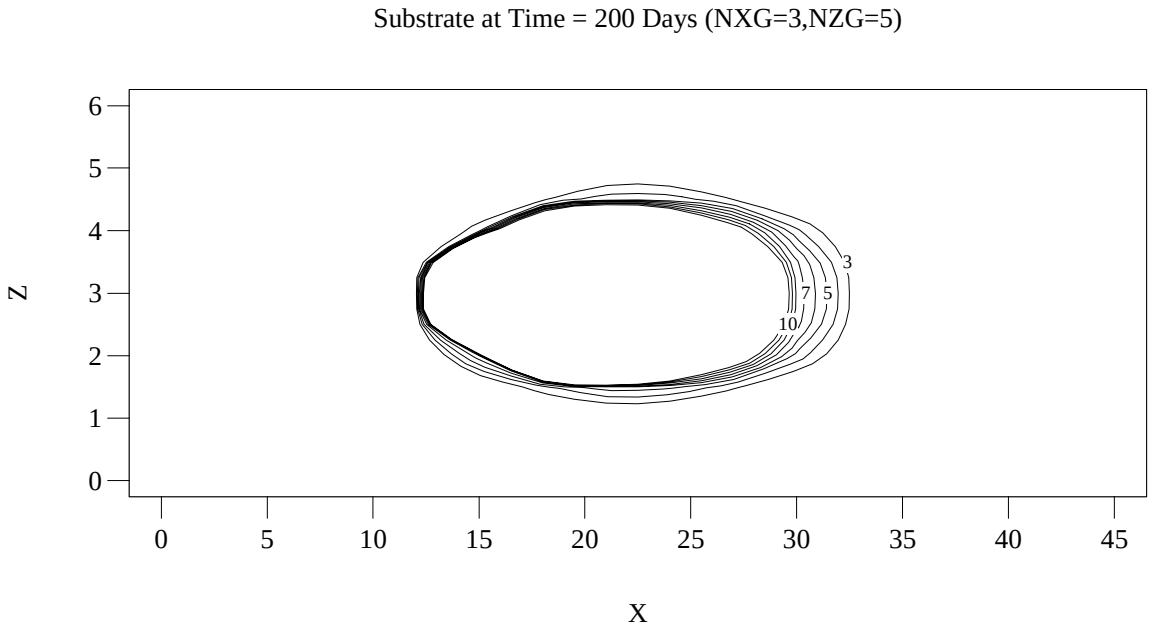


Figure 4.20 Dissolved plumes at 100 days: (a) substrate and (b) oxygen. Concentration isolines are in micrograms per liter

(a)



(b)

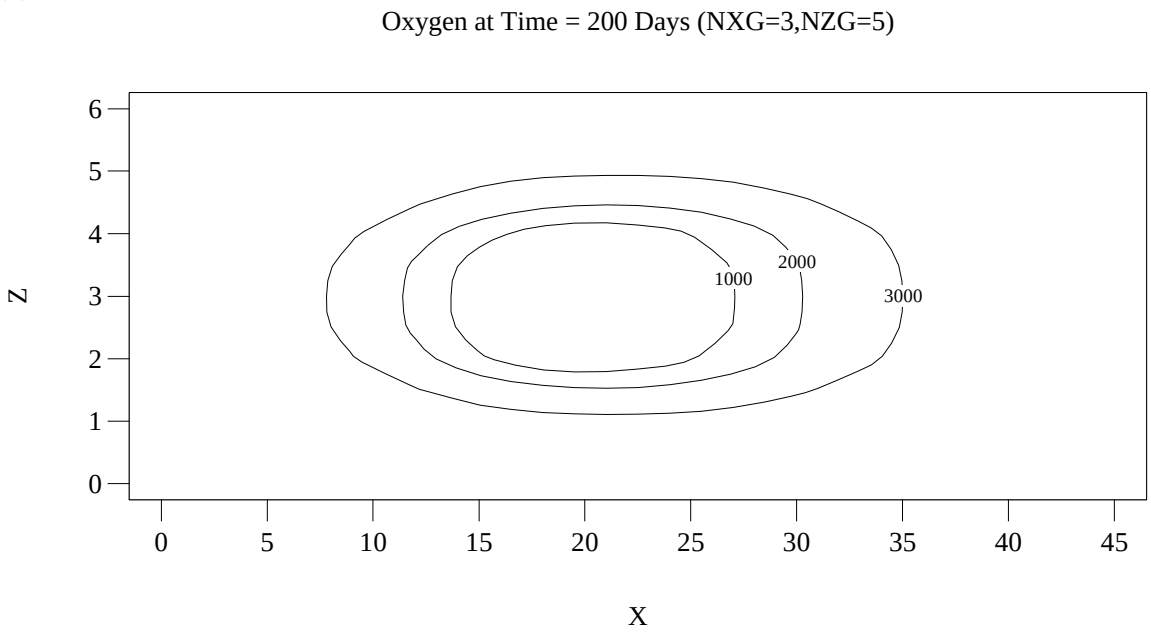
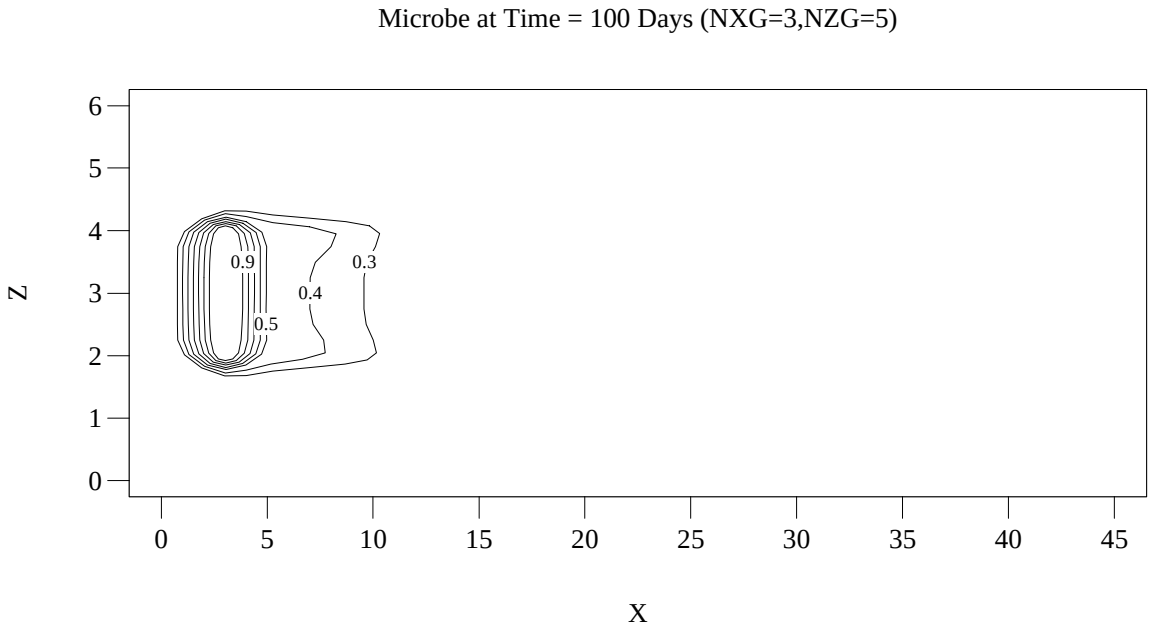


Figure 4.21 Dissolved plumes at 200 days: (a) substrate and (b) oxygen. Concentration isolines are in micrograms per liter

(a)



(b)

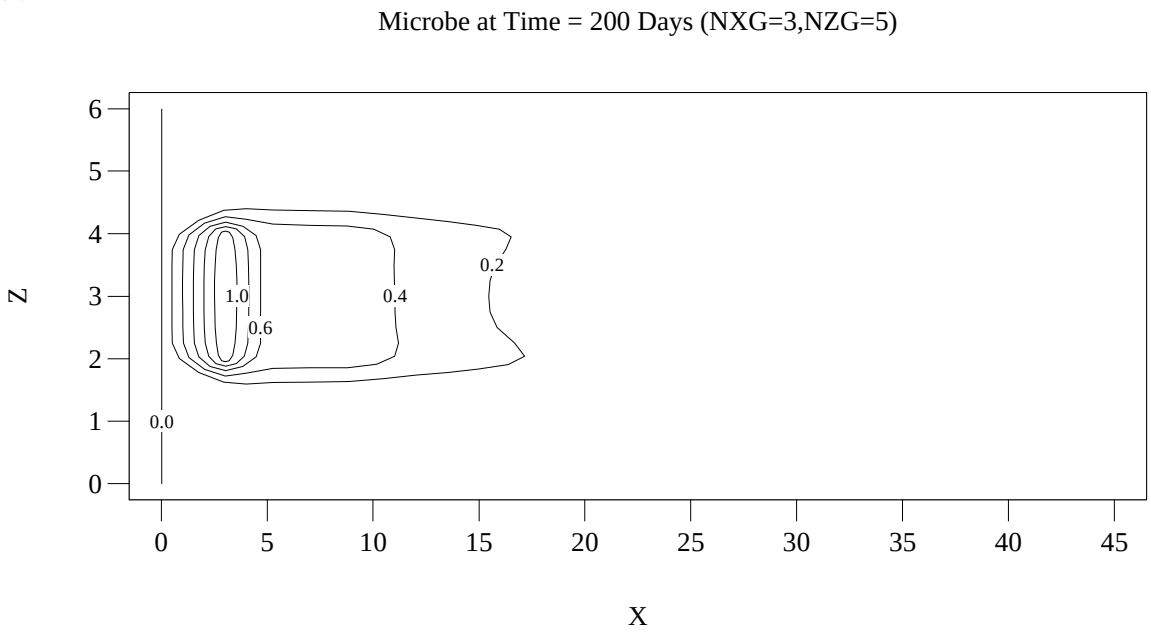


Figure 4.22 Total microbial mass distributions: (a) 100 and (b) 200 days. Concentration isolines are in mg/1000 cm^3 of aquifer material

4.13 Example 7: Two-Dimensional Coupled Flow and Multicomponent Transport Problem

This problem is presented in "Denitrification in nonhomogeneous laboratory scale aquifers: 5: user's manual for the mathematical model LT3VSI" by G.A. Bachelor et al. reported in 1990. The example aquifer used for this problem is 1.4 meters long with 15 nodes in the X direction, 1.6 meters thick with 17 nodes in the Z direction, 1 meter wide in the Y direction, and shown in Figure 4.23 and Figure 4.24. This aquifer has 8 different materials, two injection wells at (0.1,0.0,0.1) and (0.1,1.0,0.1), and two extraction wells at (1.3,0.0,1.5) and (1.3,1.0,1.5). The hydrological and microbial dynamical data are all from this report. The initial condition of the flow field is obtained by simulating steady state of flow field without sources and sinks. Then the flow field and concentration distribution are updated at each time step. There are two type of microbes included in the system, say microbe #1 and microbe #3 with 1.77×10^{-4} Kg/m^3 initially. The initial concentrations of the chemicals are 5×10^{-3} Kg/m^3 of substrate, 5×10^{-3} Kg/m^3 of oxygen, 5×10^{-3} Kg/m^3 of nitrate, and 3×10^{-3} Kg/m^3 of nutrient. The daily injection and withdrawal rates of water are 3.75×10^{-3} and 3.75×10^{-3} m^3, respectively. The total hydraulic head is 1.0 m at the upstream boundary AB (Figure 4.23) and 0.0 m at the downstream boundary CD (Figure 4.23). For transport simulation, variable boundary condition is implemented at the downstream boundary CD (Figure 4.23) and 1.77×10^{-4} Kg/m^3 of microbe #1, 1.77×10^{-4} Kg/m^3 of microbe #3, 1.5×10^{-2} Kg/m^3 of substrate, 5.0×10^{-3} Kg/m^3 of oxygen, 5.0×10^{-3} Kg/m^3 of nitrate, and 3.0×10^{-3} Kg/m^3 of nutrient influents through the upstream boundary. Because microbe #2 does not exist in this environment, the initial and boundary conditions for this component is set to zero in this simulation. This problem is set up for 4 days simulation.

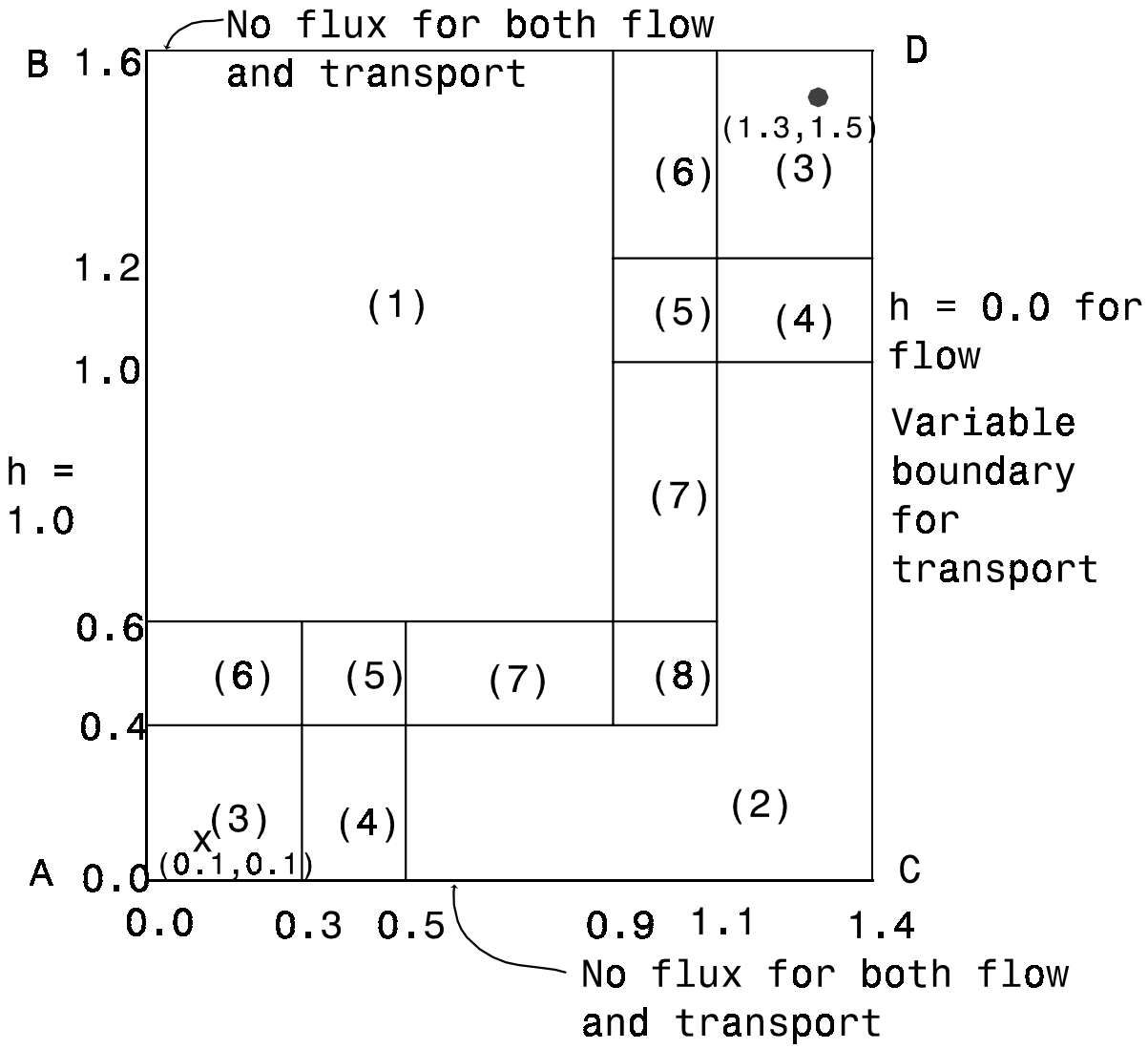
To execute the problem, the maximum control-integers in the MAIN should be specified as

```
C----- For Example7
c
      PARAMETER(MAXNPK=510,MAXELK=224,MXBNPK=510,MXBESK=508,
     >                MXTUBK=3552,MXADNK=MAXNPK+20000)
      PARAMETER(MXJBDK=45,MXKBDK=8,MXNTIK=80,MXDTCK=1)
      PARAMETER(LTMXNK=1,LMXNPK=1,LMXBWK=1,MXRGNK=1)
      PARAMETER(MXMATK=8,MXSPMK=2,MXMPMK=8)
```

```
C-------- 2.  For flow source/sink, boundary conditions, and materials

      PARAMETER(MXSELh=1,MXSPRh=1,MXSDPh=1,MXWNPh=4,MXWPRh=2,MXWDPh=3)
      PARAMETER(MXCNPh=1,MXCESh=1,MXCPRh=1,MXCDPh=1)
      PARAMETER(MXNNPh=1,MXNESh=1,MXNPRh=1,MXNDPh=1)
      PARAMETER(MXVNPh=1,MXVESh=1,MXVPRh=1,MXVDPh=1)
      PARAMETER(MXDNPh=68,MXDPRh=2,MXDDPh=2)

C -------- 3.  For transport source/sink, boundary conditions, and materials
C
      PARAMETER(MXSELc=1,MXSPRc=1,MXSDPc=1,MXWNPc=4,MXWPRc=2,MXWDPc=3)
      PARAMETER(MXCNPc=55,MXCESc=40,MXCPRc=2,MXCDPc=4)
      PARAMETER(MXNNPc=11,MXNESc=4,MXNPRc=1,MXNDPc=2)
      PARAMETER(MXVNPc=34,MXVESc=16,MXVPRc=1,MXVDPc=2)
      PARAMETER(MXDNPc=34,MXDPRc=5,MXDDPc=2)
C
      PARAMETER(MXNCCK=7)
C
      PARAMETER(MXLSVK=5000,MXMSVK=5000,MXKGLDK=39900,MXNDBK=9600)
      PARAMETER(MXNEPK=1,MXEPWK=1)
      PARAMETER(MXNPWK=27,MXELWK=8, mxnpws=27,mxelws=8)
      PARAMETER(MXNPFGK=190000,MXKGLK=99999)
C
```



(1) : material type 1

x : injection well

● : extraction well

Figure 4.23 The x-z crosssection of the region of interest.

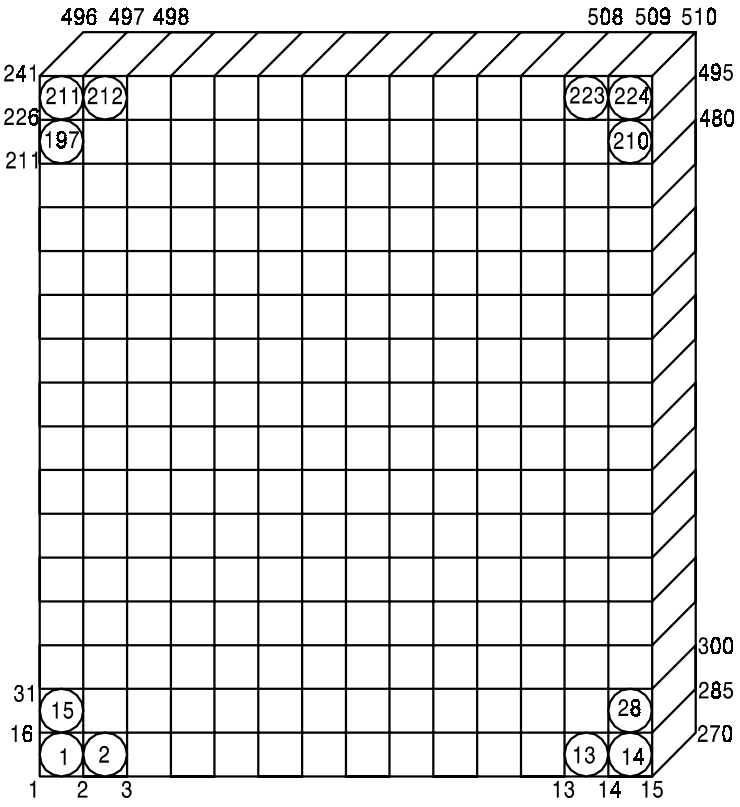


Figure 4.24 The Discretization of Example 7.

Because the soil properties are input by tabular form, the specificcation of soil property functions in subroutine SPFUNC is not needed.

4.14 Input and Output for Example 7

Table 4.13 lists the input parameters and Table 4.14 shows the input data set for the sample problem described in the above section. The output is available in electronic form.

Table 4.13 The list of input parameters for Example 7

Parameters	Notation in the data input guide	Value	Unit	Data set
number of points	NNP	510	Dimensionless	7. A.

$\triangle x$	XAD	0.1	m	7. B.
$\triangle y$	YAD	1.0	m	7. B.
$\triangle z$	ZAD	0.1	m	7. B.
no. of materials	NMAT	8	dimensionless	5. A.
$\mu_o^{(1)}$	GRATE(1)	4.0	1/day	5. H.
$\mu_n^{(2)}$	GRATE(2)	0.0	1/day	5. H.
$\mu_o^{(3)}$	GRATE(3)	4.0	1/day	5. H.
$\mu_n^{(3)}$	GRATE(4)	2.5	1/day	5. H.
$Y_o^{(1)}$	YCOEFF(1)	0.4	Kg/Kg	5. H.
$Y_n^{(2)}$	YCOEFF(2)	0.17	Kg/Kg	5. H.
$Y_o^{(3)}$	YCOEFF(3)	0.4	Kg/Kg	5. H.
$Y_n^{(3)}$	YCOEFF(4)	0.17	Kg/Kg	5. H.
$K_{so}^{(1)}$	RTARDS(1)	0.018	Kg/m^3	5. H.
$K_{sn}^{(2)}$	RTARDS(2)	0.018	Kg/m^3	5. H.
$K_{so}^{(3)}$	RTARDS(3)	0.018	Kg/m^3	5. H.
$K_{sn}^{(3)}$	RTARDS(4)	0.018	Kg/m^3	5. H.
$K_o^{(1)}$	RTARDO(1)	3.0×10^{-5}	Kg/m^3	5. H.
$K_n^{(2)}$	RTARDO(2)	2.0×10^{-5}	Kg/m^3	5. H.
$K_o^{(3)}$	RTARDO(3)	3.0×10^{-5}	Kg/m^3	5. H.
$K_n^{(3)}$	RTARDO(4)	2.0×10^{-5}	Kg/m^3	5. H.
$K_{po}^{(1)}$	RTARDN(1)	3.0×10^{-4}	Kg/m^3	5. H.
$K_{pn}^{(2)}$	RTARDN(2)	3.0×10^{-4}	Kg/m^3	5. H.
$K_{po}^{(3)}$	RTARDN(3)	3.0×10^{-4}	Kg/m^3	5. H.
$K_{pn}^{(3)}$	RTARDN(4)	3.0×10^{-4}	Kg/m^3	5. H.
$\gamma_o^{(1)}$	SCOEFF(1)	1.0	dimensionless	5. H.
$\gamma_n^{(2)}$	SCOEFF(2)	0.375	dimensionless	5. H.
$\gamma_o^{(3)}$	SCOEFF(3)	1.0	dimensionless	5. H.
$\gamma_n^{(3)}$	SCOEFF(4)	0.375	dimensionless	5. H.
$\alpha_o^{(1)}$	ECOEFF(1)	0.004	dimensionless	5. H.
$\alpha_n^{(2)}$	ECOEFF(2)	0.002	dimensionless	5. H.
$\alpha_o^{(3)}$	ECOEFF(3)	0.004	dimensionless	5. H.

$\alpha_n^{(3)}$	ECOEFF(4)	0.002	dimensionless	5. H.
$\lambda_o^{(1)}$	DCOEFF(1)	0.02	1/day	5. H.
$\lambda_n^{(2)}$	DCOEFF(2)	0.02	1/day	5. H.
$\lambda_o^{(3)}$	DCOEFF(3)	0.02	1/day	5. H.
$\lambda_n^{(3)}$	DCOEFF(4)	0.02	1/day	5. H.
$\Gamma_o^{(1)}$	SATURC(1)	3.0×10^{-5}	Kg/m^3	5. H.
$\Gamma_n^{(2)}$	SATURC(2)	2.0×10^{-5}	Kg/m^3	5. H.
$\Gamma_o^{(3)}$	SATURC(3)	3.0×10^{-5}	Kg/m^3	5. H.
$\Gamma_n^{(3)}$	SATURC(4)	2.0×10^{-5}	Kg/m^3	5. H.
$\epsilon_o^{(1)}$	PCOEFF(1)	0.05	dimensionless	5. H.
$\epsilon_n^{(2)}$	PCOEFF(2)	0.021	dimensionless	5. H.
$\epsilon_o^{(3)}$	PCOEFF(3)	0.05	dimensionless	5. H.
$\epsilon_n^{(3)}$	PCOEFF(4)	0.021	dimensionless	5. H.
K_c	COFK	1.1×10^{-4}	Kg/m^3	5. H.
no. of elements	NEL	224	dimensionless	9. A.
no. of materials to be corrected	NCM	134	dimensionless	10. A.
ICP solver	IPNTSf IPNTSt	3	dimensionless	2. B.
steady-state for flow	KSSf	0	dimensionless	2. B.
transient-state for transport	KSSt	1	dimensionless	2. B.
initial time step size	DELT	0.05	day	4. B.
time step size increment percentage	CHNG	0	dimensionless	4. B.
maximum time step size	DELMAX	0.05	day	4. B.
no. of times to reset time step size	NDTCHG	0	dimensionless	4. A.
Total simulation time	TMAX	4	day	4. B.
no. of time steps	NTI	80	dimensionless	4. A.
tolerance for flow nonlinear iteration	TOLAf	1×10^{-2}	m	3. A.
relaxation factor for flow nonlinear iteration	OMEf	1.0	dimensionless	2. C

tolerance for transport nonlinear iteration	TOLBt	1×10^{-4}	dimensionless	3. B.
relaxation factor for transport nonlinear iteration	OMEt	1.0	dimensionless	2. E.
ρ_w	RHO	1000.0	Kg/m^3	5.B. & 6.A.
μ_w	VISC	948.3264	Kg/m/day	5.B. & 6.A.
g	GRAV	7.316×10^{10}	m/day^2	6.A.

Table 4.14 Input Data Set for Example 7

```
    7 2-D Coupled Flow and Multicomponent Transport, L= M, M=KG, T=DAY
===== DATA SET 2: OPTION PARAMETERS
 11  0  1  0                                        IMOD,IGEOM,IBUG,ICHNG
 1 0.5D0 1.0D-4                                     NITRFs,OMEFTs,ALLOW
 0 1 1 0 3 3 0 0 0 1 KSSf,KSSt,ILUMP,IMID,IPNTSf,IPNTSt,NSTRf,NSTRt,MICONF,IQUAR
 1  1.0  1.0d0  0.5d0  0.0d0                       KGRAV,Wf,OMEf,OMIf
 2  1  0  1  1                                     KVIt,IWET,IOPTIM,KSORP,LGRAN
 1.0d0 1.0d0 1.0d0 1.0d0                          Wt,WVt,OMEt,OMIt  WT WVT OMET OMIT
  1   1.0d0                                       IEIGEN,GG
===== DATA SET 3: ITERATION PARAMETERS
 50 20 999 1.0d-2 1.0d-2                          NITERf,NCYLf,NPITER,TOLAf,TOLBf
 50 200 1.0d-3  1.0d-4                            NITERt,NPITERt,TOLAt,TOLBt
===== DATA SET 4: TIME CONTROL PARAMETERS
 80   0                                           NTI,NDTCHG
 5.0d-2  0.00d0  5.0d-2  4.0d0                    DELT,CHNG,DELMAX,TMAX
55        5         5         5         5         5         5         5
5
1         1         1         1         1         1         1         1
1
===== DATA SET 5: MATERIAL PROPERTIES
  8  7  7  1                                      NMAT,NMPPM,NCC,IRXN
 1.0d-2  0.0d0 1.0d-2 0.0D0 0.0D0 0.0D0 1.0D3         PROPf
 1.0d0   0.0d0 1.0d0  0.0D0 0.0D0 0.0D0 1.0D3         PROPf
 1.0d-1  0.0d0 1.0d-1 0.0D0 0.0D0 0.0D0 1.0D3         PROPf
 3.16d-1 0.0d0 3.16d-1 0.0D0 0.0D0 0.0D0 1.0D3        PROPf
 5.62d-2 0.0d0 5.62d-2 0.0D0 0.0D0 0.0D0 1.0D3        PROPf
 3.16d-2 0.0d0 3.16d-2 0.0D0 0.0D0 0.0D0 1.0D3        PROPf
 1.0d-1  0.0d0 1.00d-1 0.0D0 0.0D0 0.0D0 1.0D3        PROPf
 3.16d-1 0.0d0 3.16d-1 0.0D0 0.0D0 0.0D0 1.0D3        PROPf
 1.0d3  1.0d3  1.0d3  1.0d3  1.0d3  1.0d3  1.0d3      DINTS
 0.0    0.0d0  0.0d0  0.0d0  0.0d0  0.0d0  0.0d0      RHOMU
 1.414d3 0.0d0   0.0d0   0.0  1.0d0   0.0d0   1.0d0              PROPt
 0.0d0  0.0d0  0.0d0  0.0d0  0.0d0  0.0d0  0.0d0      RKD
 1.0d-2 1.0d-2 1.0d-2 1.0d-2 1.0d-2 1.0d-2 1.0d-2     TRANC
 1.9019d3 0.0d0    0.0d0   0.0     1.0d0   0.0d0   1.0d0              PROPT
 0.0d0  0.0d0  0.0d0  0.0d0  0.0d0  0.0d0  0.0d0      RKD
 0.0d0  0.0d0  0.0d0  0.0d0  0.0d0  0.0d0  0.0d0      TRANC
 1.6895d3  0.0d0    0.0d0   0.0     1.0d0   0.0d0   1.0d0               PROPT
 0.0d0  0.0d0  0.0d0  0.0d0  0.0d0  0.0d0  0.0d0      RKD
 1.0d-4 1.0d-4 1.0d-4 1.0d-4 1.0d-4 1.0d-4 1.0d-4     TRANC
 1.7558d3 0.0d0    0.0d0   0.0     1.0d0   0.0d0   1.0d0              PROPT
 0.0d0  0.0d0  0.0d0  0.0d0  0.0d0  0.0d0  0.0d0      RKD
```

```
 0.0d0  0.0d0  0.0d0  0.0d0  0.0d0  0.0d0  0.0d0      TRANC
 1.4728d3 0.0d0    0.0d0   0.0     1.0d0   0.0d0   1.0d0              PROPT
 0.0d0  0.0d0  0.0d0  0.0d0  0.0d0  0.0d0  0.0d0      RKD
 0.0d0  0.0d0  0.0d0  0.0d0  0.0d0  0.0d0  0.0d0      TRANC
 1.5158d3  0.0d0    0.0d0   0.0     1.0d0   0.0d0   1.0d0              PROPT
 0.0d0  0.0d0  0.0d0  0.0d0  0.0d0  0.0d0  0.0d0      RKD
 1.0d-3 1.0d-3 1.0d-3 1.0d-3 1.0d-3 1.0d-3 1.0d-3     TRANC
 1.5124d3 0.0d0    0.0d0   0.0     1.0d0   0.0d0   1.0d0              PROPT
 0.0d0  0.0d0  0.0d0  0.0d0  0.0d0  0.0d0  0.0d0      RKD
 0.0d0  0.0d0  0.0d0  0.0d0  0.0d0  0.0d0  0.0d0      TRANC
 1.7061d3 0.0d0    0.0d0   0.0     1.0d0   0.0d0   1.0d0              PROPT
 0.0d0  0.0d0  0.0d0  0.0d0  0.0d0  0.0d0  0.0d0      RKD
 0.0d0  0.0d0  0.0d0  0.0d0  0.0d0  0.0d0  0.0d0      TRANC
 4.0  0.0  4.0  2.5                    GRATE
 0.4  0.4  0.4  0.17                   YCOEFF
1.8D-2  1.8d-2  1.8D-2  1.8D-2         RTARDS   Kso, Ksn
3.0D-5  3.0d-5  3.0D-5  2.0D-5         RTARDO   Ko, Kn
3.0d-4  3.0d-4  3.0D-4  3.0D-4         RTARDN   Kpo, Kpn
1.0  0.375  1.0   0.375                SCOEFF   gammao, gamman
0.004  0.002  0.004  0.002            ECOEFF   alphao, alphan
0.02 0.02 0.02 0.02                   DCOEFF   lambdao, lambdan
3.0D-5  2.0d-5   3.0D-5 2.0D-5        SATURC   GAMMAo, GAMMAn
0.05 0.021 0.05 0.021                 PCOEFF   Epsilon
  1.1d-4                              COFK
===== DATA SET 6: SOIL PROPERTIES
  1  2    0   1.0d0  9.8D0  1.0D0     KSP,NSPPM,KCP,RHO,GRAV,VISC
 -1000.0  1000.0                      PRESUURE
 -1000.0  1000.0
 -1000.0  1000.0
 -1000.0  1000.0
 -1000.0  1000.0
 -1000.0  1000.0
 -1000.0  1000.0
 -1000.0  1000.0
 0.465    0.465                       MOISTURE CONTENT
  0.285   0.285
  0.365   0.365
  0.323   0.323
  0.387   0.387
  0.412   0.412
  0.364   0.364
  0.322   0.322
  1.0     1.0                         RELATIVE HYDRAULIC CONDUCTIVITY
  1.0     1.0
  1.0     1.0
  1.0     1.0
  1.0     1.0
  1.0     1.0
  1.0     1.0
  1.0     1.0
  0.0     0.0                         D(THETA)/DH
  0.0     0.0
  0.0     0.0
  0.0     0.0
  0.0     0.0
  0.0     0.0
  0.0     0.0
  0.0     0.0
===== DATA SET 7: NODE COORDINATES
  510                                 NNP
  1  16  15  0.0  0.0  0.0  0.0  0.0  0.1
  2  16  15  0.1  0.0  0.0  0.0  0.0  0.1
```

```
  3  16  15  0.2  0.0  0.0  0.0  0.0  0.1
  4  16  15  0.3  0.0  0.0  0.0  0.0  0.1
  5  16  15  0.4  0.0  0.0  0.0  0.0  0.1
  6  16  15  0.5  0.0  0.0  0.0  0.0  0.1
  7  16  15  0.6  0.0  0.0  0.0  0.0  0.1
  8  16  15  0.7  0.0  0.0  0.0  0.0  0.1
  9  16  15  0.8  0.0  0.0  0.0  0.0  0.1
 10  16  15  0.9  0.0  0.0  0.0  0.0  0.1
 11  16  15  1.0  0.0  0.0  0.0  0.0  0.1
 12  16  15  1.1  0.0  0.0  0.0  0.0  0.1
 13  16  15  1.2  0.0  0.0  0.0  0.0  0.1
 14  16  15  1.3  0.0  0.0  0.0  0.0  0.1
 15  16  15  1.4  0.0  0.0  0.0  0.0  0.1
256  16  15  0.0  1.0  0.0  0.0  0.0  0.1
257  16  15  0.1  1.0  0.0  0.0  0.0  0.1
258  16  15  0.2  1.0  0.0  0.0  0.0  0.1
259  16  15  0.3  1.0  0.0  0.0  0.0  0.1
260  16  15  0.4  1.0  0.0  0.0  0.0  0.1
261  16  15  0.5  1.0  0.0  0.0  0.0  0.1
262  16  15  0.6  1.0  0.0  0.0  0.0  0.1
263  16  15  0.7  1.0  0.0  0.0  0.0  0.1
264  16  15  0.8  1.0  0.0  0.0  0.0  0.1
265  16  15  0.9  1.0  0.0  0.0  0.0  0.1
266  16  15  1.0  1.0  0.0  0.0  0.0  0.1
267  16  15  1.1  1.0  0.0  0.0  0.0  0.1
268  16  15  1.2  1.0  0.0  0.0  0.0  0.1
269  16  15  1.3  1.0  0.0  0.0  0.0  0.1
270  16  15  1.4  1.0  0.0  0.0  0.0  0.1
  0   0  0   0.0  0.0  0.0  0.0  0.0  0.0
===== DATA SET 9 : ELEMENT INCIDENCES
  224                                          NEL
   1   15  14  1  2  257  256  16  17  272  271  15
   2   15  14  2  3  258  257  17  18  273  272  15
   3   15  14  3  4  259  258  18  19  274  273  15
   4   15  14  4  5  260  259  19  20  275  274  15
   5   15  14  5  6  261  260  20  21  276  275  15
   6   15  14  6  7  262  261  21  22  277  276  15
   7   15  14  7  8  263  262  22  23  278  277  15
   8   15  14  8  9  264  263  23  24  279  278  15
   9   15  14  9  10  265  264  24  25  280  279  15
  10   15  14  10 11  266  265  25  26  281  280  15
  11   15  14  11 12  267  266  26  27  282  281  15
  12   15  14  12 13  268  267  27  28  283  282  15
  13   15  14  13 14  269  268  28  29  284  283  15
  14   15  14  14 15  270  269  29  30  285  284  15
    0    0    0    0    0    0    0    0    0    0   0      END OF IE
===== DATA SET 10: MATERIAL CORRECTION
134                      NCM
1  3  14 3  0
2  3  14 3  0
3  3  14 3  0
6  8  1  2  0
20 8  1  2  0
34 8  1  2  0
48 8  1  2  0
68 5  14 2 0
69 5  14 2 0
70 5  14 2 0
180  3  14 3  0
181  3  14 3  0
182  3  14 3  0
152 2 1  4  0
```

```
166 2 1  4  0
4   3 14 4  0
5   3 14 4  0
57  2 1  6  0
71  2 1  6  0
60  1 1  5  0
74  1 1  5  0
62  3 1  7  0
76  3 1  7  0
66  1 1  8  0
80  1 1  8  0
94  3 14 7  0
95  3 14 7  0
153 1 1  5  0
167 1 1  5  0
181 3 14 6  0
182 3 14 6  0
0  0  0  0  0
===== DATA SET 11 : INITIAL CONDIDTIONS
 0 IHTR
 1  509  1  0.0d0  0.0d0  0.0d0          I.C. FOR FLOW
 0   0   0  0.0D0  0.0D0  0.0D0
 1  509  1  1.77D-4  0.0D0  0.0D0        I.C. FOR MICROBE 1
 0   0   0  0.0D0  0.0D0  0.0D0
 1  509  1  0.0D0  0.0D0  0.0D0          I.C. FOR MICROBE 2
 0   0   0  0.0D0  0.0D0  0.0D0
 1  509  1  1.77D-4  0.0D0  0.0D0        I.C. FOR MICROBE 3
 0   0   0  0.0D0  0.0D0  0.0D0
 1  509  1  5.0D-3   0.0D0  0.0D0        I.C. FOR SUBSTRATE
 0   0   0  0.0D0  0.0D0  0.0D0
 1  509  1  5.0D-3   0.0D0  0.0D0        I.C. FOR OXYGEN
 0   0   0  0.0D0  0.0D0  0.0D0
 1  509  1  5.0D-3   0.0D0  0.0D0        I.C. FOR NITRATE
 0   0   0  0.0D0  0.0D0  0.0D0
 1  509  1  3.0D-3   0.0D0  0.0D0        I.C. FOR NUTRIENT
 0   0   0  0.0D0  0.0D0  0.0D0
===== DATA SET 12: ELEMENT(DISTRIBUTED) SOURCE/SINK OF FLOW
    0  0  0  0                          NSELF,NSPRF,NSDPF,KSAIF
===== DATA SET 13: POINT(WELL) SOURCE/SINK OF FLOW
    4  2  3  0                          NWNPF,NWPRF,NWDPF,KWAIF
    0.0d0  0.0 1.0d-6  3.75d-3  1.0d38  3.75d-3
    0.0d0  0.0 1.0d-6  -2.0d-3   1.0d38 -2.0d-3
    17  239  272  494
    1  1  2  1  0
    2  1  2  2  0
    0  0  0  0  0
===== DATA SET 14: ELEMENT(DISTRIBUTED) SOURCE/SINK OF TRANSPORT
    0  0  0  0                          NSELT,NSPRT,NSDPT,KSAIT
===== DATA SET 15: POINT(WELL) SOURCE/SINK OF TRANSPORT
    4  2  3  0                          NWNPF,NWPRF,NWDPF,KWAIF
    0.0d0  0.0 0.0d0  1.0d-6  3.75d-3  0.0d0  1.0d38  3.75d-3  0.0d0
    0.0d0  0.0 0.0d0  1.0d-6  -2.0d-3  0.0d0  1.0d38 -2.0d-3   0.0d0
    17  239  272  494
    1  1  2  1  0
    2  1  2  2  0
    0  0  0  0  0
    1  1  2  1  0
    2  1  2  2  0
    0  0  0  0  0
    1  1  2  1  0
    2  1  2  2  0
    0  0  0  0  0
```

```
    1  1  2  1  0
    2  1  2  2  0
    0  0  0  0  0
    1  1  2  1  0
    2  1  2  2  0
    0  0  0  0  0
    1  1  2  1  0
    2  1  2  2  0
    0  0  0  0  0
    1  1  2  1  0
    2  1  2  2  0
    0  0  0  0  0
===== DATA SET 16: RAINFALL/EVAPORATION-SEEPAGE BOUNDARY CONDITIONS OF FLOW
    0  0  0  0  0                    NVESF,NVNPF,NRPRF,NRDPF,KRAIF
===== DATA SET 17:  DIRICHLET BOUNDARY CONDITIONS OF FLOW
  68   2  2  0                       NDNPF,NDPRF,NDDPF,KDAIF
  0.0d0   1.0   1.0d38   1.0
  0.0d0   0.0   1.0d38   0.0
  1   16   1  1   15
 18   16   1  256 15
 35   16   1  15  15
 52   16   1  270 15
  0   0  0   0    0
  1   33    1   1  0
 35   33    1   2  0
  0    0    0   0  0
===== DATA SET 18: CAUCHY BOUNDARY CONDITIONS OF FLOW
    0    0  0  0  0                  NCESF,NCNPF,NCPRF,NCDPF,KCAIF
===== DATA SET 19: NEUMANN BOUNDARY CONDITIONS, FLOW
    0  0  0  0  0                    NNESF,NNNPF,NNPRF,NNDPF,KNAIF
===== DATA SET 20: VARIABLE BOUNDARY CONDITIONS OF TRANSPORT
   16 34 1 2 0                       NVESF,NVNPF,NVPRF,NVDPF,KVAIF
   0.0d0  0.0d0  1.0d38  0.0d0
    1  15   1   1   0
    0   0   0   0   0   end of irtyp
    1  15   1   1   0
    0   0   0   0   0   end of irtyp
    1  15   1   1   0
    0   0   0   0   0   end of irtyp
    1  15   1   1   0
    0   0   0   0   0   end of irtyp
    1  15   1   1   0
    0   0   0   0   0   end of irtyp
    1  15   1   1   0
    0   0   0   0   0   end of irtyp
    1   15  1  15  270 285 30  15 15 15 15
    0   0   0   0   0   0   0  0  0  0  0   end fof isvt(j,i),j=1,4
    1   16  1  15  15
   18   16  1  270 15
     0    0  0  0  0                    NVEST,NVNPT,NVPRT,NVDPT,NVAIT
===== DATA SET 21:  DIRICHLET BOUNDARY CONDITIONS OF TRANSPORT
  34   5  2  0                         NDNPT,NDPRT,NDDPT,KDAIT
  0.0  1.77d-4  1.0d38  1.77d-4
  0.0  0.0      1.0d38  0.0
  0.0  1.5d-2   1.0d38  1.5d-2
  0.0  5.0d-3   1.0d38  5.0d-3
  0.0  3.0d-3   1.0d38  3.0d-3
  1   16   1  1   15
 18   16   1  256 15
  0   0  0   0    0
```

```
  1   33   1  1   0
  0   0    0  0   0
  1   33   1  2   0
  0   0    0  0   0
  1   33   1  1   0
  0   0    0  0   0
  1   33   1  3   0
  0   0    0  0   0
  1   33   1  4   0
  0   0    0  0   0
  1   33   1  4   0
  0   0    0  0   0
  1   33   1  5   0
  0   0    0  0   0
===== DATA SET 22: CAUCHY BOUNDARY CONDITIONS OF TRANSPORT
    0    0   0  0  0                  NCEST,NCNPT,NCPRT,NCDPT,KCAIT
===== DATA SET 23: NEUMANN BOUNDARY CONDITIONS, TRANSPORT
    0  0  0  0  0                     NNEST,NNNPT,NNPRT,NNDPT,KNAIT
===== DATA SET 24 : PARAMETERS CONTROLLOING TRACKING SCHEME
 1 1 0 2 1 2 2 1 2 2 1 2 1 IZOOM,IDZOOM,IEPC,NXA,NYA,NZA,NXW,NYW,NZW,NXD,NYD,NZD
  1.0d-4     1.0d-4        ADPEPS,ADPARM
    0           ====== END OF JOB ======
```

Figure 4.25 depicts the simulation results of velocity field and Figures 4.26a through 4.26c show concentration contours of microbes, substrate and oxygen, and nitrate and nutrient, respectively.

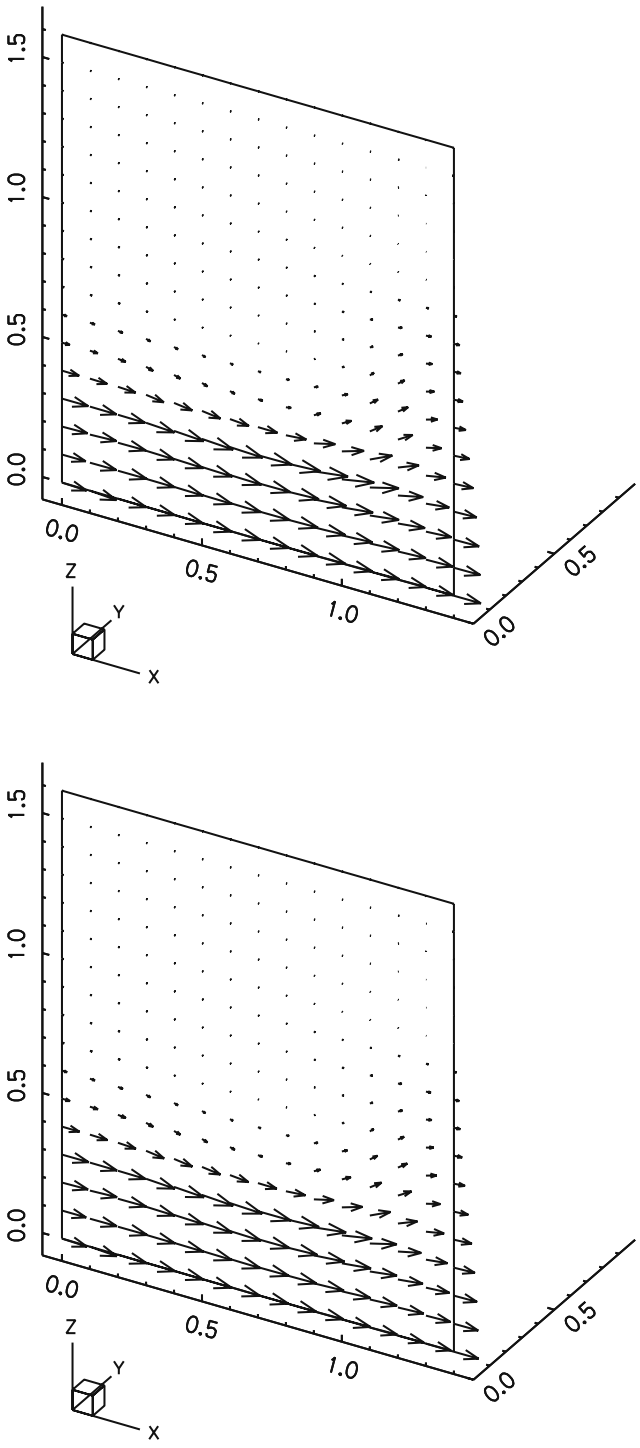


Figure 4.25 The velocity field at (a) time = 2 days and (b) time = 4 days

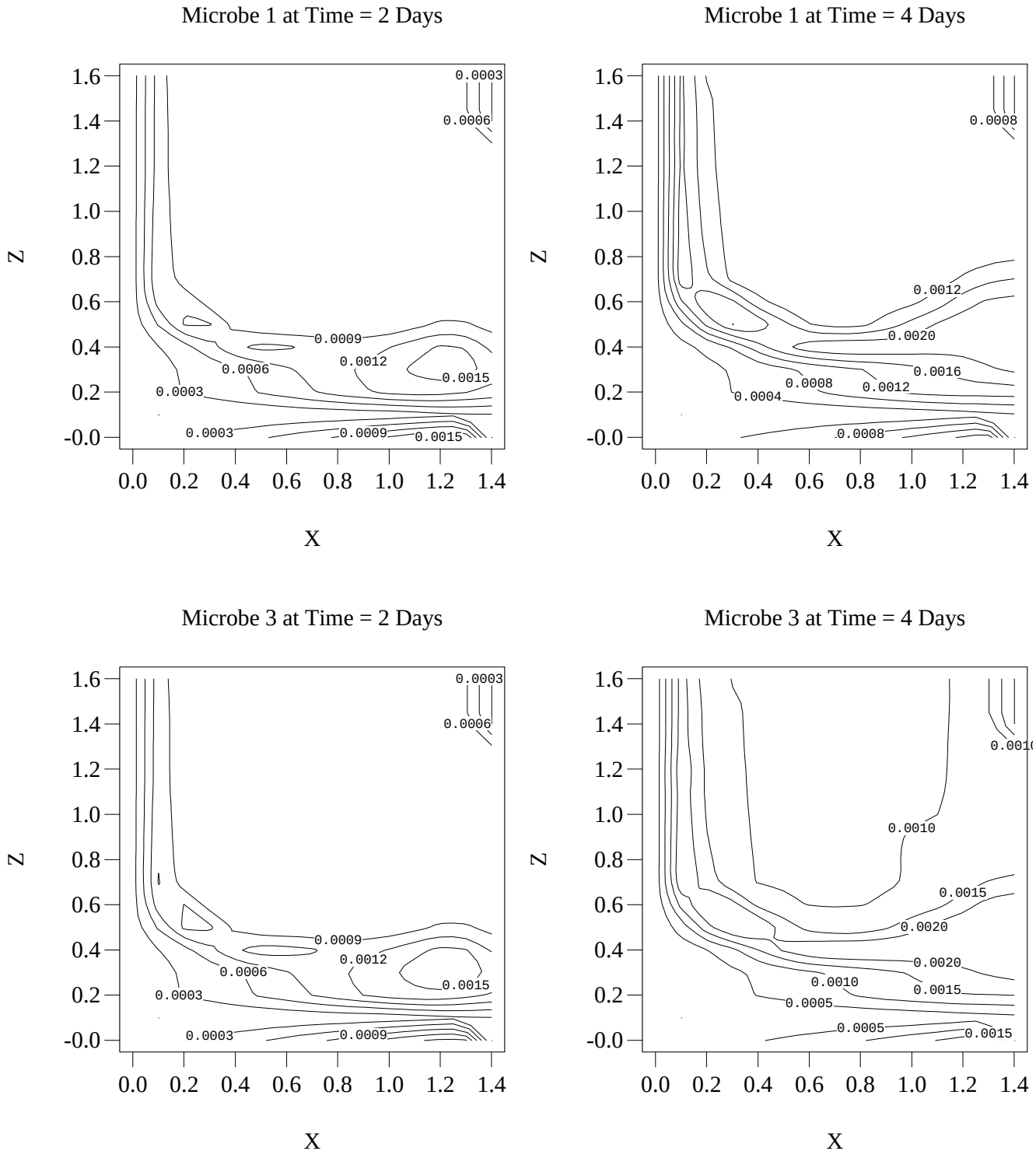


Fig. 4.26a Concentration contours of microbe #1 and microbe #3 at time = 2 days and 4 days, respectively.

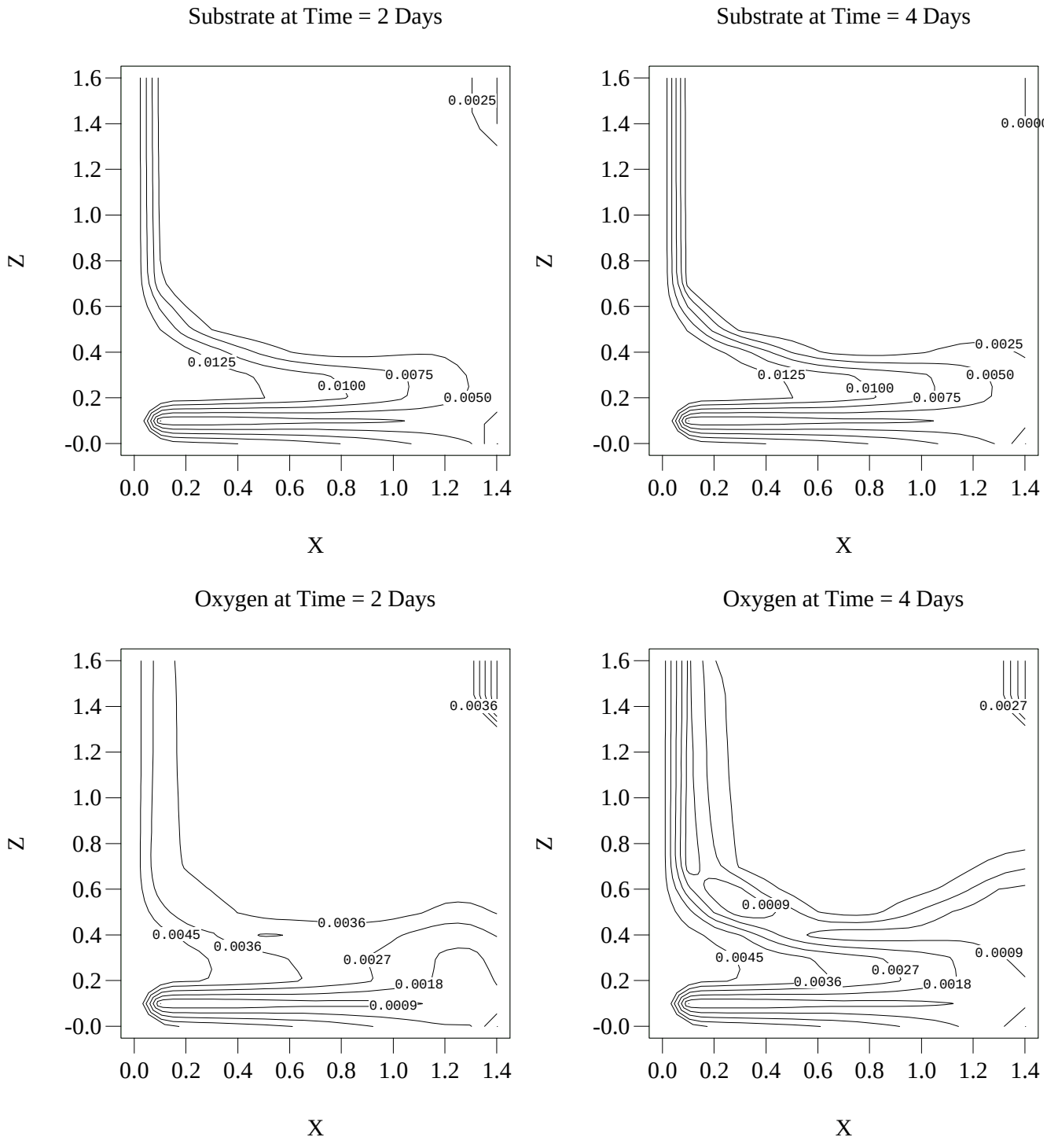


Fig. 4.26b Concentration contours of substrate and oxygen at time = 2 days and 4 days, respectively.

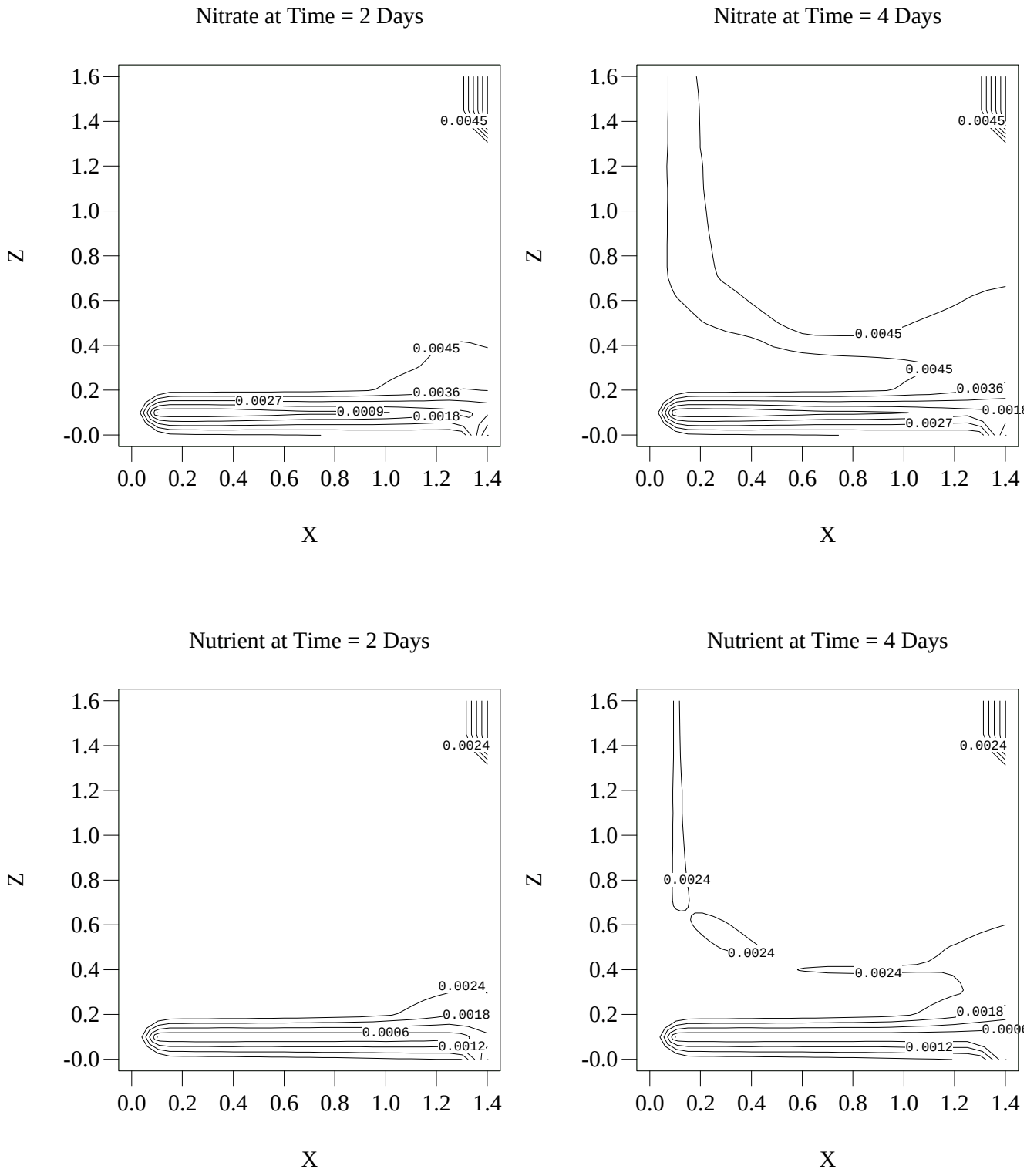


Fig. 4.26c Concentration contours of nitrate and nutrient at time = 2 days and 4 days, respectively.

4.15 Example 8: Three-Dimensional Multicomponent Transport in a Uniform Flow Field

This problem is used to demonstrate the 3-D multicomponent transport behavior. The kinetic and microbial parameters for the simulation are the same as those adopted by the previous example. The region is taken as $0 < x < 45$ m, $0 < y < 5$ m, and $0 < z < 6$ m and discretized to 15x10x12 = 1800 elements resulting in 16x11x 13 = 2288 nodal points (Figure 4.27). The initial condition is comprised of a patch with 2mx1mx2m (Figure 4.27), which is placed far enough from the domain limits to avoid boundary effects. The concentrations in the initial patch are 3 mg/L for substrate and 1 mg/L for oxygen. The total background concentration of microbial #1 population is 0.23 mg/L and the retardation factor associated with microbes is 1000. The boundary conditions and physical parameters are shown in Figure 4.18. Although the nitrate, nutrient, microbe #2, and microbe # 3 must be included in the input data, the simulation for these four components is not performed. Therefore, the initial and boundary conditions for these four components are set to zero in the input data file.

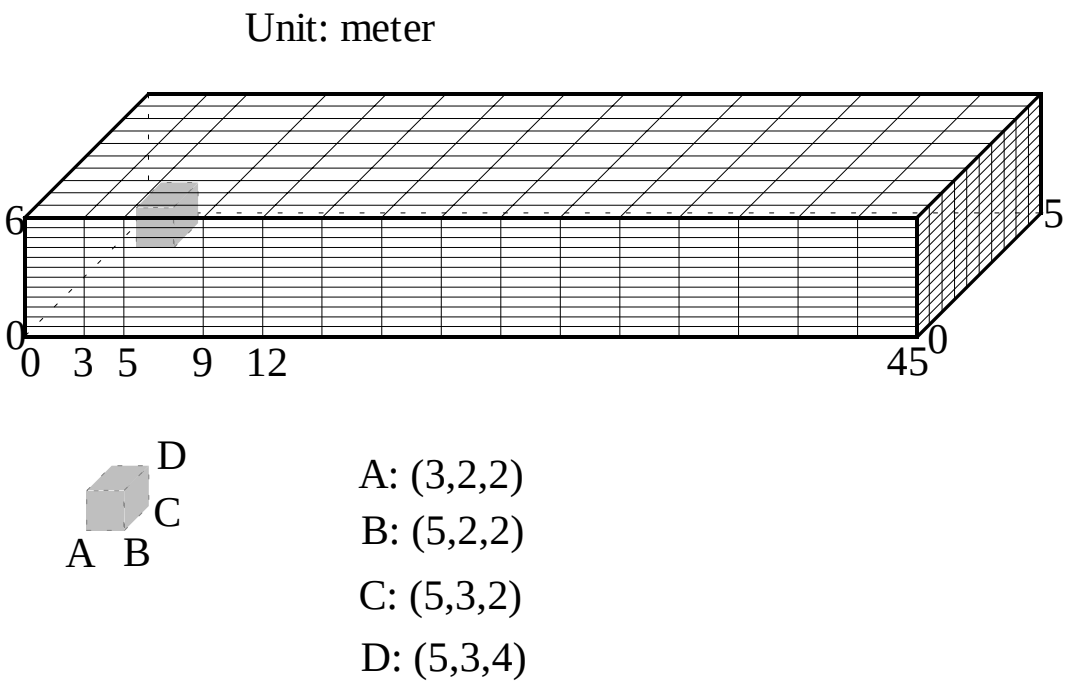


Figure 4.27 The region of interest for Example 8

To execute the problem, the maximum control-integers in the MAIN should be specified as

```
C----- For Example 6 & Example8
c
      PARAMETER(MAXNPK=2288,MAXELK=1800,MXBNPK=1999,MXBESK=1999,
      >                MXTUBK=2640,MXADNK=maxnpk+14000)
      PARAMETER(MXJBDK=85,MXKBDK=8,MXNTIK=100,MXDTCK=4)
      PARAMETER(LTMXNK=693,LMXNPK=231,LMXBWK=49,MXRGNK=11)
      PARAMETER(MXMATK=1,MXSPMK=2,MXMPMK=7)

C-------- 2.  For flow source/sink, boundary conditions, and materials

      PARAMETER(MXSELh=1,MXSPRh=1,MXSDPh=1,MXWNPh=1,MXWPRh=1,MXWDPh=1)
      PARAMETER(MXCNPh=1,MXCESh=1,MXCPRh=1,MXCDPh=1)
      PARAMETER(MXNNPh=1,MXNESh=1,MXNPRh=1,MXNDPh=1)
      PARAMETER(MXVNPh=1,MXVESh=1,MXVPRh=1,MXVDPh=1)
      PARAMETER(MXDNPh=1,MXDPRh=1,MXDDPh=1)

C -------- 3.  For transport source/sink, boundary conditions, and materials
C
      PARAMETER(MXSELc=1,MXSPRc=1,MXSDPc=1,MXWNPc=1,MXWPRc=1,MXWDPc=1)
      PARAMETER(MXCNPc=1,MXCESc=1,MXCPRc=1,MXCDPc=1)
      PARAMETER(MXNNPc=1,MXNESc=1,MXNPRc=1,MXNDPc=1)
      PARAMETER(MXVNPc=143,MXVESc=120,MXVPRc=1,MXVDPc=2)
      PARAMETER(MXDNPc=143,MXDPRc=2,MXDDPc=2)
C
      PARAMETER(MXNCCK=7)
C
      PARAMETER(MXLSVK=5000,MXMSVK=5000,MXKGLDK=29999,MXNDBK=9999)
      PARAMETER(MXNEPK=1,MXEPWK=1)
      PARAMETER(MXNPWK=48,MXELWK=15, mxnpws=1,mxelws=1)
      PARAMETER(MXNPFGK=260000,MXKGLK=140000)
C
```

4.16 Input and Output for Example 8

Table 4.15 lists the input parameters and Table 4.16 shows the input data set for the sample problem described in the above section. The output isavailable in electronic form.

Table 4.15 The list of input parameters for Example 8

Parameters	Notation in the data input guide	Value	Unit	Data set
number of points	NNP	2288	Dimensionless	7. A.
Δx	XAD	3.0 (except arround x = 5.0)	m	7. B.
Δy	YAD	0.5	m	7. B.
Δz	ZAD	0.5	m	7. B.
α_L	PROP(1,2)	0.81	m	5. E.
α_T	PROP(1,3)	5.0×10^{-3}	m	5. E.
D_m	PROP(1,4)	8.05×10^{-5}	m^2/day	5. E.
K_{d1}	RKD(1)	1000	m^3/mg	5. F.
K_{ds}	RKD(4)	0.4	m^3/mg	5. F.
$\mu_o^{(1)}$	GRATE(1)	0.21	1/day	5. H.
$\mu_n^{(2)}$	GRATE(2)	0..0	1/day	5. H.
$\mu_o^{(3)}$	GRATE(3)	0.0	1/day	5. H.
$\mu_n^{(3)}$	GRATE(4)	0.0	1/day	5. H.
$Y_o^{(1)}$	YCOEFF(1)	0.426	mg/mg	5. H.
$Y_n^{(2)}$	YCOEFF(2)	0.17	mg/mg	5. H.
$Y_o^{(3)}$	YCOEFF(3)	0.4	mg/mg	5. H.
$Y_n^{(3)}$	YCOEFF(4)	0.17	mg/mg	5. H.
$K_{so}^{(1)}$	RTARDS(1)	654	mg/m^3	5. H.
$K_{sn}^{(2)}$	RTARDS(2)	0.018	mg/m^3	5. H.
$K_{so}^{(3)}$	RTARDS(3)	0.018	mg/m^3	5. H.
$K_{sn}^{(3)}$	RTARDS(4)	0.018	mg/m^3	5. H.
$K_o^{(1)}$	RTARDO(1)	1.0×10^{2}	mg/m^3	5. H.
$K_n^{(2)}$	RTARDO(2)	2.0×10^{-5}	mg/m^3	5. H.
$K_o^{(3)}$	RTARDO(3)	3.0×10^{-5}	mg/m^3	5. H.
$K_n^{(3)}$	RTARDO(4)	2.0×10^{-5}	mg/m^3	5. H.
$K_{po}^{(1)}$	RTARDN(1)	3.0×10^{-4}	mg/m^3	5. H.
$K_{pn}^{(2)}$	RTARDN(2)	0.0	mg/m^3	5. H.

$K_{po}^{(3)}$	RTARDN(3)	0.0	mg/m^3	5. H.
$K_{pn}^{(3)}$	RTARDN(4)	0.0	mg/m^3	5. H.
$\gamma_o^{(1)}$	SCOEFF(1)	7.044	dimensionless	5. H.
$\gamma_n^{(2)}$	SCOEFF(2)	0.0	dimensionless	5. H.
$\gamma_o^{(3)}$	SCOEFF(3)	0.0	dimensionless	5. H.
$\gamma_n^{(3)}$	SCOEFF(4)	0.0	dimensionless	5. H.
$\alpha_o^{(1)}$	ECOEFF(1)	0.0	dimensionless	5. H.
$\alpha_n^{(2)}$	ECOEFF(2)	0.0	dimensionless	5. H.
$\alpha_o^{(3)}$	ECOEFF(3)	0.0	dimensionless	5. H.
$\alpha_n^{(3)}$	ECOEFF(4)	0.0	dimensionless	5. H.
$\lambda_o^{(1)}$	DCOEFF(1)	0.0	1/day	5. H.
$\lambda_n^{(2)}$	DCOEFF(2)	0.0	1/day	5. H.
$\lambda_o^{(3)}$	DCOEFF(3)	0.0	1/day	5. H.
$\lambda_n^{(3)}$	DCOEFF(4)	0.0	1/day	5. H.
$\Gamma_o^{(1)}$	SATURC(1)	0.0	mg/m^3	5. H.
$\Gamma_n^{(2)}$	SATURC(2)	0.0	mg/m^3	5. H.
$\Gamma_o^{(3)}$	SATURC(3)	0.0	mg/m^3	5. H.
$\Gamma_n^{(3)}$	SATURC(4)	0.0	mg/m^3	5. H.
$\epsilon_o^{(1)}$	PCOEFF(1)	0.0	dimensionless	5. H.
$\epsilon_n^{(2)}$	PCOEFF(2)	0.0	dimensionless	5. H.
$\epsilon_o^{(3)}$	PCOEFF(3)	0.0	dimensionless	5. H.
$\epsilon_n^{(3)}$	PCOEFF(4)	0.0	dimensionless	5. H.
K_c	COFK	0.0	mg/m^3	5. H.
no. of elements	NEL	1800	dimensionless	9. A.
no. of subregion	NREGN	11	dimensionless	8. A.
no. of points in each subregion	NODES	208	dimensionless	8. B.
Velocity	V_x	0.09	m/day	25. A.
transient-state for transport	KSSt	1	dimensionless	2. B.
initial time step size	DELT	2.0	day	4. B.
time step size increment percentage	CHNG	0	dimensionless	4. B.

maximum time step size	DELMAX	2.0	day	4. B.
no. of times to reset time step size	NDTCHG	0	dimensionless	4. A.
Total simulation time	TMAX	200	day	4. B.
no. of time steps	NTI	100	dimensionless	4. A.
tolerance for transport nonlinear iteration	TOLBt	1×10^{-4}	dimensionless	3. B.
relaxation factor for transport nonlinear iteration	OMEt	1.0	dimensionless	2. E.
ρ_w	RHO	10^9	mg/m^3	5.B. & 6.A.
μ_w	VISC	94832640	mg/m/day	5.B. & 6.A.
g	GRAV	7.316×10^{10}	m/day^2	6.A.

Table 4.16 Input Data Set for Example 8

```
    8 3-d multicomponent transport in uniform flow field,mg,m,day
===== DATA SET 2: OPTION PARAMETERS
  1   0   1  0
 50 0.5D0 1.0D-4                NITRFT OMEFTF OMEFTT
 1  1  1  0  0  0  0  0  1  1   KSSF KSST ILUMP IMID IPNTSF IPNTST
 1  1.0  1.0d0  1.0d0  0.0d0    KGRAV WF OMEF OMIF
 -1  1  0  1  1                 KVIT IWET IOPTIM KSORP LGRAN
 1.0d0 1.0d0 1.0d0 1.0d0        WT WVT OMET OMIT
===== DATA SET 3: ITERATION PARAMETERS
 50 20 100 1.0d-2 1.0d-2        NITERF NCYLF NPITRF TOLAF TOLBF
 50 100 1.0d-2  1.0d-4          NITERT NPITRT TOLAT TOLBT ALLOW
===== DATA SET 4: TIME CONTROL PARAMETERS
 100  3                         NTI NDTCHG
 2.0d0  0.00d0  2.0d0   2.0d2   DELT CHNG DELMAX TMAX
55        0         0         0         0         5         0         0
0         0         5
1                                                   1
0                   1
1.0d5  2.0d4  1.0D38            TDTCH
===== DATA SET 5: MATERIAL PROPERTIES
 1  7  7  1                    NMAT NMPPM
 1.00d0 8.1d-1   5.0d-3  8.05D-5 1.0d0   0.0d0   1.0d0 PROPT
 1.0d3  0.0d0  0.0   0.4D0  0.0D0  0.0D0  0.0D0
 0.0d0  0.0d0  0.0   0.0    0.0    0.0    0.0
 0.21 0.0  0.0  0.0                  GRATE
 0.426 0.17 0.4  0.17                 YCOEFF
6.54D2   1.8D-2  1.8D-2  1.8D-2       RTARDS   Kso, Ksn
1.0D2   2.0D-5  3.0D-5  2.0D-5       RTARDO   Ko, Kn
0.0d0   0.0D0   0.0D0   0.0D0        RTARDN   Kpo, Kpn
7.044  0.0    0.0   0.0              SCOEFF   gammao, gamman
0.0    0.0    0.0    0.0            ECOEFF   alphao, alphan
0.0  0.0  0.0  0.0                  DCOEFF   lambdao, lambdan
0.0D0   0.0D0 0.0D0 0.0D0      SATURC   GAMMAo, GAMMAn
```

```
0.0  0.0   0.0  0.0                    PCOEFF   Epsilon
  0.0d0                                COFK
===== DATA SET 6: SOIL PROPERTIES
1    2    0   1.0d0  9.8D0  1.0D0              KSP NSPPM KCP GRAV
-1000.0    1000.0                             PRESSURE
    0.1       0.1                             WATER CONTENT
    1.0       1.0                             RELATIVE CONDUCTIVITY
    0.0       0.0                             WATER CAPACITY
===== DATA SET 7: NODE COORDINATES
  2288                NNP
  1  1   13  0.0  0.0  0.0  3.0  0.0   0.0
 27  0    0  5.0  0.0  0.0  0.0  0.0   0.0
 40  12  13  9.0  0.0  0.0  3.0  0.0   0.0
  2  1   13  0.0  0.0  0.5  3.0  0.0   0.0
 28  0    0  5.0  0.0  0.5  0.0  0.0   0.0
 41  12  13  9.0  0.0  0.5  3.0  0.0   0.0
  3  1   13  0.0  0.0  1.0  3.0  0.0   0.0
 29  0    0  5.0  0.0  1.0  0.0  0.0   0.0
 42  12  13  9.0  0.0  1.0  3.0  0.0   0.0
  4  1   13  0.0  0.0  1.5  3.0  0.0   0.0
 30  0    0  5.0  0.0  1.5  0.0  0.0   0.0
 43  12  13  9.0  0.0  1.5  3.0  0.0   0.0
  5  1   13  0.0  0.0  2.0  3.0  0.0   0.0
 31  0    0  5.0  0.0  2.0  0.0  0.0   0.0
 44  12  13  9.0  0.0  2.0  3.0  0.0   0.0
  6  1   13  0.0  0.0  2.5  3.0  0.0   0.0
 32  0    0  5.0  0.0  2.5  0.0  0.0   0.0
 45  12  13  9.0  0.0  2.5  3.0  0.0   0.0
  7  1   13  0.0  0.0  3.0  3.0  0.0   0.0
 33  0    0  5.0  0.0  3.0  0.0  0.0   0.0
 46  12  13  9.0  0.0  3.0  3.0  0.0   0.0
  8  1   13  0.0  0.0  3.5  3.0  0.0   0.0
 34  0    0  5.0  0.0  3.5  0.0  0.0   0.0
 47  12  13  9.0  0.0  3.5  3.0  0.0   0.0
  9  1   13  0.0  0.0  4.0  3.0  0.0   0.0
 35  0    0  5.0  0.0  4.0  0.0  0.0   0.0
 48  12  13  9.0  0.0  4.0  3.0  0.0   0.0
 10  1   13  0.0  0.0  4.5  3.0  0.0   0.0
 36  0    0  5.0  0.0  4.5  0.0  0.0   0.0
 49  12  13  9.0  0.0  4.5  3.0  0.0   0.0
 11  1   13  0.0  0.0  5.0  3.0  0.0   0.0
 37  0    0  5.0  0.0  5.0  0.0  0.0   0.0
 50  12  13  9.0  0.0  5.0  3.0  0.0   0.0
 12  1   13  0.0  0.0  5.5  3.0  0.0   0.0
 38  0    0  5.0  0.0  5.5  0.0  0.0   0.0
 51  12  13  9.0  0.0  5.5  3.0  0.0   0.0
 13  1   13  0.0  0.0  6.0  3.0  0.0   0.0
 39  0    0  5.0  0.0  6.0  0.0  0.0   0.0
 52  12  13  9.0  0.0  6.0  3.0  0.0   0.0
 209 1   13  0.0  0.5  0.0  3.0  0.0   0.0
 235 0    0  5.0  0.5  0.0  0.0  0.0   0.0
 248 12  13  9.0  0.5  0.0  3.0  0.0   0.0
 210 1   13  0.0  0.5  0.5  3.0  0.0   0.0
 236 0    0  5.0  0.5  0.5  0.0  0.0   0.0
 249 12  13  9.0  0.5  0.5  3.0  0.0   0.0
 211 1   13  0.0  0.5  1.0  3.0  0.0   0.0
 237 0    0  5.0  0.5  1.0  0.0  0.0   0.0
 250 12  13  9.0  0.5  1.0  3.0  0.0   0.0
 212 1   13  0.0  0.5  1.5  3.0  0.0   0.0
 238 0    0  5.0  0.5  1.5  0.0  0.0   0.0
 251 12  13  9.0  0.5  1.5  3.0  0.0   0.0
 213 1   13  0.0  0.5  2.0  3.0  0.0   0.0
```

```
239 0    0  5.0  0.5  2.0  0.0  0.0   0.0
252 12  13  9.0  0.5  2.0  3.0  0.0   0.0
214 1   13  0.0  0.5  2.5  3.0  0.0   0.0
240 0    0  5.0  0.5  2.5  0.0  0.0   0.0
253 12  13  9.0  0.5  2.5  3.0  0.0   0.0
215 1   13  0.0  0.5  3.0  3.0  0.0   0.0
241 0    0  5.0  0.5  3.0  0.0  0.0   0.0
254 12  13  9.0  0.5  3.0  3.0  0.0   0.0
216 1   13  0.0  0.5  3.5  3.0  0.0   0.0
242 0    0  5.0  0.5  3.5  0.0  0.0   0.0
255 12  13  9.0  0.5  3.5  3.0  0.0   0.0
217 1   13  0.0  0.5  4.0  3.0  0.0   0.0
243 0    0  5.0  0.5  4.0  0.0  0.0   0.0
256 12  13  9.0  0.5  4.0  3.0  0.0   0.0
218 1   13  0.0  0.5  4.5  3.0  0.0   0.0
244 0    0  5.0  0.5  4.5  0.0  0.0   0.0
257 12  13  9.0  0.5  4.5  3.0  0.0   0.0
219 1   13  0.0  0.5  5.0  3.0  0.0   0.0
245 0    0  5.0  0.5  5.0  0.0  0.0   0.0
258 12  13  9.0  0.5  5.0  3.0  0.0   0.0
220 1   13  0.0  0.5  5.5  3.0  0.0   0.0
246 0    0  5.0  0.5  5.5  0.0  0.0   0.0
259 12  13  9.0  0.5  5.5  3.0  0.0   0.0
221 1   13  0.0  0.5  6.0  3.0  0.0   0.0
247 0    0  5.0  0.5  6.0  0.0  0.0   0.0
260 12  13  9.0  0.5  6.0  3.0  0.0   0.0
417 1   13  0.0  1.0  0.0  3.0  0.0   0.0
443 0    0  5.0  1.0  0.0  0.0  0.0   0.0
456 12  13  9.0  1.0  0.0  3.0  0.0   0.0
418 1   13  0.0  1.0  0.5  3.0  0.0   0.0
444 0    0  5.0  1.0  0.5  0.0  0.0   0.0
457 12  13  9.0  1.0  0.5  3.0  0.0   0.0
419 1   13  0.0  1.0  1.0  3.0  0.0   0.0
445 0    0  5.0  1.0  1.0  0.0  0.0   0.0
458 12  13  9.0  1.0  1.0  3.0  0.0   0.0
420 1   13  0.0  1.0  1.5  3.0  0.0   0.0
446 0    0  5.0  1.0  1.5  0.0  0.0   0.0
459 12  13  9.0  1.0  1.5  3.0  0.0   0.0
421 1   13  0.0  1.0  2.0  3.0  0.0   0.0
447 0    0  5.0  1.0  2.0  0.0  0.0   0.0
460 12  13  9.0  1.0  2.0  3.0  0.0   0.0
422 1   13  0.0  1.0  2.5  3.0  0.0   0.0
448 0    0  5.0  1.0  2.5  0.0  0.0   0.0
461 12  13  9.0  1.0  2.5  3.0  0.0   0.0
423 1   13  0.0  1.0  3.0  3.0  0.0   0.0
449 0    0  5.0  1.0  3.0  0.0  0.0   0.0
462 12  13  9.0  1.0  3.0  3.0  0.0   0.0
424 1   13  0.0  1.0  3.5  3.0  0.0   0.0
450 0    0  5.0  1.0  3.5  0.0  0.0   0.0
463 12  13  9.0  1.0  3.5  3.0  0.0   0.0
425 1   13  0.0  1.0  4.0  3.0  0.0   0.0
451 0    0  5.0  1.0  4.0  0.0  0.0   0.0
464 12  13  9.0  1.0  4.0  3.0  0.0   0.0
426 1   13  0.0  1.0  4.5  3.0  0.0   0.0
452 0    0  5.0  1.0  4.5  0.0  0.0   0.0
465 12  13  9.0  1.0  4.5  3.0  0.0   0.0
427 1   13  0.0  1.0  5.0  3.0  0.0   0.0
453 0    0  5.0  1.0  5.0  0.0  0.0   0.0
466 12  13  9.0  1.0  5.0  3.0  0.0   0.0
428 1   13  0.0  1.0  5.5  3.0  0.0   0.0
454 0    0  5.0  1.0  5.5  0.0  0.0   0.0
467 12  13  9.0  1.0  5.5  3.0  0.0   0.0
```

429	1	13	0.0	1.0	6.0	3.0	0.0	0.0
455	0	0	5.0	1.0	6.0	0.0	0.0	0.0
468	12	13	9.0	1.0	6.0	3.0	0.0	0.0
625	1	13	0.0	1.5	0.0	3.0	0.0	0.0
651	0	0	5.0	1.5	0.0	0.0	0.0	0.0
664	12	13	9.0	1.5	0.0	3.0	0.0	0.0
626	1	13	0.0	1.5	0.5	3.0	0.0	0.0
652	0	0	5.0	1.5	0.5	0.0	0.0	0.0
665	12	13	9.0	1.5	0.5	3.0	0.0	0.0
627	1	13	0.0	1.5	1.0	3.0	0.0	0.0
653	0	0	5.0	1.5	1.0	0.0	0.0	0.0
666	12	13	9.0	1.5	1.0	3.0	0.0	0.0
628	1	13	0.0	1.5	1.5	3.0	0.0	0.0
654	0	0	5.0	1.5	1.5	0.0	0.0	0.0
667	12	13	9.0	1.5	1.5	3.0	0.0	0.0
629	1	13	0.0	1.5	2.0	3.0	0.0	0.0
655	0	0	5.0	1.5	2.0	0.0	0.0	0.0
668	12	13	9.0	1.5	2.0	3.0	0.0	0.0
630	1	13	0.0	1.5	2.5	3.0	0.0	0.0
656	0	0	5.0	1.5	2.5	0.0	0.0	0.0
669	12	13	9.0	1.5	2.5	3.0	0.0	0.0
631	1	13	0.0	1.5	3.0	3.0	0.0	0.0
657	0	0	5.0	1.5	3.0	0.0	0.0	0.0
670	12	13	9.0	1.5	3.0	3.0	0.0	0.0
632	1	13	0.0	1.5	3.5	3.0	0.0	0.0
658	0	0	5.0	1.5	3.5	0.0	0.0	0.0
671	12	13	9.0	1.5	3.5	3.0	0.0	0.0
633	1	13	0.0	1.5	4.0	3.0	0.0	0.0
659	0	0	5.0	1.5	4.0	0.0	0.0	0.0
672	12	13	9.0	1.5	4.0	3.0	0.0	0.0
634	1	13	0.0	1.5	4.5	3.0	0.0	0.0
660	0	0	5.0	1.5	4.5	0.0	0.0	0.0
673	12	13	9.0	1.5	4.5	3.0	0.0	0.0
635	1	13	0.0	1.5	5.0	3.0	0.0	0.0
661	0	0	5.0	1.5	5.0	0.0	0.0	0.0
674	12	13	9.0	1.5	5.0	3.0	0.0	0.0
636	1	13	0.0	1.5	5.5	3.0	0.0	0.0
662	0	0	5.0	1.5	5.5	0.0	0.0	0.0
675	12	13	9.0	1.5	5.5	3.0	0.0	0.0
637	1	13	0.0	1.5	6.0	3.0	0.0	0.0
663	0	0	5.0	1.5	6.0	0.0	0.0	0.0
676	12	13	9.0	1.5	6.0	3.0	0.0	0.0
833	1	13	0.0	2.0	0.0	3.0	0.0	0.0
859	0	0	5.0	2.0	0.0	0.0	0.0	0.0
872	12	13	9.0	2.0	0.0	3.0	0.0	0.0
834	1	13	0.0	2.0	0.5	3.0	0.0	0.0
860	0	0	5.0	2.0	0.5	0.0	0.0	0.0
873	12	13	9.0	2.0	0.5	3.0	0.0	0.0
835	1	13	0.0	2.0	1.0	3.0	0.0	0.0
861	0	0	5.0	2.0	1.0	0.0	0.0	0.0
874	12	13	9.0	2.0	1.0	3.0	0.0	0.0
836	1	13	0.0	2.0	1.5	3.0	0.0	0.0
862	0	0	5.0	2.0	1.5	0.0	0.0	0.0
875	12	13	9.0	2.0	1.5	3.0	0.0	0.0
837	1	13	0.0	2.0	2.0	3.0	0.0	0.0
863	0	0	5.0	2.0	2.0	0.0	0.0	0.0
876	12	13	9.0	2.0	2.0	3.0	0.0	0.0
838	1	13	0.0	2.0	2.5	3.0	0.0	0.0
864	0	0	5.0	2.0	2.5	0.0	0.0	0.0
877	12	13	9.0	2.0	2.5	3.0	0.0	0.0
839	1	13	0.0	2.0	3.0	3.0	0.0	0.0
865	0	0	5.0	2.0	3.0	0.0	0.0	0.0

878	12	13	9.0	2.0	3.0	3.0	0.0	0.0
840	1	13	0.0	2.0	3.5	3.0	0.0	0.0
866	0	0	5.0	2.0	3.5	0.0	0.0	0.0
879	12	13	9.0	2.0	3.5	3.0	0.0	0.0
841	1	13	0.0	2.0	4.0	3.0	0.0	0.0
867	0	0	5.0	2.0	4.0	0.0	0.0	0.0
880	12	13	9.0	2.0	4.0	3.0	0.0	0.0
842	1	13	0.0	2.0	4.5	3.0	0.0	0.0
868	0	0	5.0	2.0	4.5	0.0	0.0	0.0
881	12	13	9.0	2.0	4.5	3.0	0.0	0.0
843	1	13	0.0	2.0	5.0	3.0	0.0	0.0
869	0	0	5.0	2.0	5.0	0.0	0.0	0.0
882	12	13	9.0	2.0	5.0	3.0	0.0	0.0
844	1	13	0.0	2.0	5.5	3.0	0.0	0.0
870	0	0	5.0	2.0	5.5	0.0	0.0	0.0
883	12	13	9.0	2.0	5.5	3.0	0.0	0.0
845	1	13	0.0	2.0	6.0	3.0	0.0	0.0
871	0	0	5.0	2.0	6.0	0.0	0.0	0.0
884	12	13	9.0	2.0	6.0	3.0	0.0	0.0
1041	1	13	0.0	2.5	0.0	3.0	0.0	0.0
1067	0	0	5.0	2.5	0.0	0.0	0.0	0.0
1080	12	13	9.0	2.5	0.0	3.0	0.0	0.0
1042	1	13	0.0	2.5	0.5	3.0	0.0	0.0
1068	0	0	5.0	2.5	0.5	0.0	0.0	0.0
1081	12	13	9.0	2.5	0.5	3.0	0.0	0.0
1043	1	13	0.0	2.5	1.0	3.0	0.0	0.0
1069	0	0	5.0	2.5	1.0	0.0	0.0	0.0
1082	12	13	9.0	2.5	1.0	3.0	0.0	0.0
1044	1	13	0.0	2.5	1.5	3.0	0.0	0.0
1070	0	0	5.0	2.5	1.5	0.0	0.0	0.0
1083	12	13	9.0	2.5	1.5	3.0	0.0	0.0
1045	1	13	0.0	2.5	2.0	3.0	0.0	0.0
1071	0	0	5.0	2.5	2.0	0.0	0.0	0.0
1084	12	13	9.0	2.5	2.0	3.0	0.0	0.0
1046	1	13	0.0	2.5	2.5	3.0	0.0	0.0
1072	0	0	5.0	2.5	2.5	0.0	0.0	0.0
1085	12	13	9.0	2.5	2.5	3.0	0.0	0.0
1047	1	13	0.0	2.5	3.0	3.0	0.0	0.0
1073	0	0	5.0	2.5	3.0	0.0	0.0	0.0
1086	12	13	9.0	2.5	3.0	3.0	0.0	0.0
1048	1	13	0.0	2.5	3.5	3.0	0.0	0.0
1074	0	0	5.0	2.5	3.5	0.0	0.0	0.0
1087	12	13	9.0	2.5	3.5	3.0	0.0	0.0
1049	1	13	0.0	2.5	4.0	3.0	0.0	0.0
1075	0	0	5.0	2.5	4.0	0.0	0.0	0.0
1088	12	13	9.0	2.5	4.0	3.0	0.0	0.0
1050	1	13	0.0	2.5	4.5	3.0	0.0	0.0
1076	0	0	5.0	2.5	4.5	0.0	0.0	0.0
1089	12	13	9.0	2.5	4.5	3.0	0.0	0.0
1051	1	13	0.0	2.5	5.0	3.0	0.0	0.0
1077	0	0	5.0	2.5	5.0	0.0	0.0	0.0
1090	12	13	9.0	2.5	5.0	3.0	0.0	0.0
1052	1	13	0.0	2.5	5.5	3.0	0.0	0.0
1078	0	0	5.0	2.5	5.5	0.0	0.0	0.0
1091	12	13	9.0	2.5	5.5	3.0	0.0	0.0
1053	1	13	0.0	2.5	6.0	3.0	0.0	0.0
1079	0	0	5.0	2.5	6.0	0.0	0.0	0.0
1092	12	13	9.0	2.5	6.0	3.0	0.0	0.0
1249	1	13	0.0	3.0	0.0	3.0	0.0	0.0
1275	0	0	5.0	3.0	0.0	0.0	0.0	0.0
1288	12	13	9.0	3.0	0.0	3.0	0.0	0.0
1250	1	13	0.0	3.0	0.5	3.0	0.0	0.0

1276	0	0	5.0	3.0	0.5	0.0	0.0	0.0
1289	12	13	9.0	3.0	0.5	3.0	0.0	0.0
1251	1	13	0.0	3.0	1.0	3.0	0.0	0.0
1277	0	0	5.0	3.0	1.0	0.0	0.0	0.0
1290	12	13	9.0	3.0	1.0	3.0	0.0	0.0
1252	1	13	0.0	3.0	1.5	3.0	0.0	0.0
1278	0	0	5.0	3.0	1.5	0.0	0.0	0.0
1291	12	13	9.0	3.0	1.5	3.0	0.0	0.0
1253	1	13	0.0	3.0	2.0	3.0	0.0	0.0
1279	0	0	5.0	3.0	2.0	0.0	0.0	0.0
1292	12	13	9.0	3.0	2.0	3.0	0.0	0.0
1254	1	13	0.0	3.0	2.5	3.0	0.0	0.0
1280	0	0	5.0	3.0	2.5	0.0	0.0	0.0
1293	12	13	9.0	3.0	2.5	3.0	0.0	0.0
1255	1	13	0.0	3.0	3.0	3.0	0.0	0.0
1281	0	0	5.0	3.0	3.0	0.0	0.0	0.0
1294	12	13	9.0	3.0	3.0	3.0	0.0	0.0
1256	1	13	0.0	3.0	3.5	3.0	0.0	0.0
1282	0	0	5.0	3.0	3.5	0.0	0.0	0.0
1295	12	13	9.0	3.0	3.5	3.0	0.0	0.0
1257	1	13	0.0	3.0	4.0	3.0	0.0	0.0
1283	0	0	5.0	3.0	4.0	0.0	0.0	0.0
1296	12	13	9.0	3.0	4.0	3.0	0.0	0.0
1258	1	13	0.0	3.0	4.5	3.0	0.0	0.0
1284	0	0	5.0	3.0	4.5	0.0	0.0	0.0
1297	12	13	9.0	3.0	4.5	3.0	0.0	0.0
1259	1	13	0.0	3.0	5.0	3.0	0.0	0.0
1285	0	0	5.0	3.0	5.0	0.0	0.0	0.0
1298	12	13	9.0	3.0	5.0	3.0	0.0	0.0
1260	1	13	0.0	3.0	5.5	3.0	0.0	0.0
1286	0	0	5.0	3.0	5.5	0.0	0.0	0.0
1299	12	13	9.0	3.0	5.5	3.0	0.0	0.0
1261	1	13	0.0	3.0	6.0	3.0	0.0	0.0
1287	0	0	5.0	3.0	6.0	0.0	0.0	0.0
1300	12	13	9.0	3.0	6.0	3.0	0.0	0.0
1457	1	13	0.0	3.5	0.0	3.0	0.0	0.0
1483	0	0	5.0	3.5	0.0	0.0	0.0	0.0
1496	12	13	9.0	3.5	0.0	3.0	0.0	0.0
1458	1	13	0.0	3.5	0.5	3.0	0.0	0.0
1484	0	0	5.0	3.5	0.5	0.0	0.0	0.0
1497	12	13	9.0	3.5	0.5	3.0	0.0	0.0
1459	1	13	0.0	3.5	1.0	3.0	0.0	0.0
1485	0	0	5.0	3.5	1.0	0.0	0.0	0.0
1498	12	13	9.0	3.5	1.0	3.0	0.0	0.0
1460	1	13	0.0	3.5	1.5	3.0	0.0	0.0
1486	0	0	5.0	3.5	1.5	0.0	0.0	0.0
1499	12	13	9.0	3.5	1.5	3.0	0.0	0.0
1461	1	13	0.0	3.5	2.0	3.0	0.0	0.0
1487	0	0	5.0	3.5	2.0	0.0	0.0	0.0
1500	12	13	9.0	3.5	2.0	3.0	0.0	0.0
1462	1	13	0.0	3.5	2.5	3.0	0.0	0.0
1488	0	0	5.0	3.5	2.5	0.0	0.0	0.0
1501	12	13	9.0	3.5	2.5	3.0	0.0	0.0
1463	1	13	0.0	3.5	3.0	3.0	0.0	0.0
1489	0	0	5.0	3.5	3.0	0.0	0.0	0.0
1502	12	13	9.0	3.5	3.0	3.0	0.0	0.0
1464	1	13	0.0	3.5	3.5	3.0	0.0	0.0
1490	0	0	5.0	3.5	3.5	0.0	0.0	0.0
1503	12	13	9.0	3.5	3.5	3.0	0.0	0.0
1465	1	13	0.0	3.5	4.0	3.0	0.0	0.0
1491	0	0	5.0	3.5	4.0	0.0	0.0	0.0
1504	12	13	9.0	3.5	4.0	3.0	0.0	0.0

1466	1	13	0.0	3.5	4.5	3.0	0.0	0.0
1492	0	0	5.0	3.5	4.5	0.0	0.0	0.0
1505	12	13	9.0	3.5	4.5	3.0	0.0	0.0
1467	1	13	0.0	3.5	5.0	3.0	0.0	0.0
1493	0	0	5.0	3.5	5.0	0.0	0.0	0.0
1506	12	13	9.0	3.5	5.0	3.0	0.0	0.0
1468	1	13	0.0	3.5	5.5	3.0	0.0	0.0
1494	0	0	5.0	3.5	5.5	0.0	0.0	0.0
1507	12	13	9.0	3.5	5.5	3.0	0.0	0.0
1469	1	13	0.0	3.5	6.0	3.0	0.0	0.0
1495	0	0	5.0	3.5	6.0	0.0	0.0	0.0
1508	12	13	9.0	3.5	6.0	3.0	0.0	0.0
1665	1	13	0.0	4.0	0.0	3.0	0.0	0.0
1691	0	0	5.0	4.0	0.0	0.0	0.0	0.0
1704	12	13	9.0	4.0	0.0	3.0	0.0	0.0
1666	1	13	0.0	4.0	0.5	3.0	0.0	0.0
1692	0	0	5.0	4.0	0.5	0.0	0.0	0.0
1705	12	13	9.0	4.0	0.5	3.0	0.0	0.0
1667	1	13	0.0	4.0	1.0	3.0	0.0	0.0
1693	0	0	5.0	4.0	1.0	0.0	0.0	0.0
1706	12	13	9.0	4.0	1.0	3.0	0.0	0.0
1668	1	13	0.0	4.0	1.5	3.0	0.0	0.0
1694	0	0	5.0	4.0	1.5	0.0	0.0	0.0
1707	12	13	9.0	4.0	1.5	3.0	0.0	0.0
1669	1	13	0.0	4.0	2.0	3.0	0.0	0.0
1695	0	0	5.0	4.0	2.0	0.0	0.0	0.0
1708	12	13	9.0	4.0	2.0	3.0	0.0	0.0
1670	1	13	0.0	4.0	2.5	3.0	0.0	0.0
1696	0	0	5.0	4.0	2.5	0.0	0.0	0.0
1709	12	13	9.0	4.0	2.5	3.0	0.0	0.0
1671	1	13	0.0	4.0	3.0	3.0	0.0	0.0
1697	0	0	5.0	4.0	3.0	0.0	0.0	0.0
1710	12	13	9.0	4.0	3.0	3.0	0.0	0.0
1672	1	13	0.0	4.0	3.5	3.0	0.0	0.0
1698	0	0	5.0	4.0	3.5	0.0	0.0	0.0
1711	12	13	9.0	4.0	3.5	3.0	0.0	0.0
1673	1	13	0.0	4.0	4.0	3.0	0.0	0.0
1699	0	0	5.0	4.0	4.0	0.0	0.0	0.0
1712	12	13	9.0	4.0	4.0	3.0	0.0	0.0
1674	1	13	0.0	4.0	4.5	3.0	0.0	0.0
1700	0	0	5.0	4.0	4.5	0.0	0.0	0.0
1713	12	13	9.0	4.0	4.5	3.0	0.0	0.0
1675	1	13	0.0	4.0	5.0	3.0	0.0	0.0
1701	0	0	5.0	4.0	5.0	0.0	0.0	0.0
1714	12	13	9.0	4.0	5.0	3.0	0.0	0.0
1676	1	13	0.0	4.0	5.5	3.0	0.0	0.0
1702	0	0	5.0	4.0	5.5	0.0	0.0	0.0
1715	12	13	9.0	4.0	5.5	3.0	0.0	0.0
1677	1	13	0.0	4.0	6.0	3.0	0.0	0.0
1703	0	0	5.0	4.0	6.0	0.0	0.0	0.0
1716	12	13	9.0	4.0	6.0	3.0	0.0	0.0
1873	1	13	0.0	4.5	0.0	3.0	0.0	0.0
1899	0	0	5.0	4.5	0.0	0.0	0.0	0.0
1912	12	13	9.0	4.5	0.0	3.0	0.0	0.0
1874	1	13	0.0	4.5	0.5	3.0	0.0	0.0
1900	0	0	5.0	4.5	0.5	0.0	0.0	0.0
1913	12	13	9.0	4.5	0.5	3.0	0.0	0.0
1875	1	13	0.0	4.5	1.0	3.0	0.0	0.0
1901	0	0	5.0	4.5	1.0	0.0	0.0	0.0
1914	12	13	9.0	4.5	1.0	3.0	0.0	0.0
1876	1	13	0.0	4.5	1.5	3.0	0.0	0.0
1902	0	0	5.0	4.5	1.5	0.0	0.0	0.0

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1915 12  13  9.0  4.5  1.5  3.0  0.0   0.0
1877 1   13  0.0  4.5  2.0  3.0  0.0   0.0
1903 0    0  5.0  4.5  2.0  0.0  0.0   0.0
1916 12  13  9.0  4.5  2.0  3.0  0.0   0.0
1878 1   13  0.0  4.5  2.5  3.0  0.0   0.0
1904 0    0  5.0  4.5  2.5  0.0  0.0   0.0
1917 12  13  9.0  4.5  2.5  3.0  0.0   0.0
1879 1   13  0.0  4.5  3.0  3.0  0.0   0.0
1905 0    0  5.0  4.5  3.0  0.0  0.0   0.0
1918 12  13  9.0  4.5  3.0  3.0  0.0   0.0
1880 1   13  0.0  4.5  3.5  3.0  0.0   0.0
1906 0    0  5.0  4.5  3.5  0.0  0.0   0.0
1919 12  13  9.0  4.5  3.5  3.0  0.0   0.0
1881 1   13  0.0  4.5  4.0  3.0  0.0   0.0
1907 0    0  5.0  4.5  4.0  0.0  0.0   0.0
1920 12  13  9.0  4.5  4.0  3.0  0.0   0.0
1882 1   13  0.0  4.5  4.5  3.0  0.0   0.0
1908 0    0  5.0  4.5  4.5  0.0  0.0   0.0
1921 12  13  9.0  4.5  4.5  3.0  0.0   0.0
1883 1   13  0.0  4.5  5.0  3.0  0.0   0.0
1909 0    0  5.0  4.5  5.0  0.0  0.0   0.0
1922 12  13  9.0  4.5  5.0  3.0  0.0   0.0
1884 1   13  0.0  4.5  5.5  3.0  0.0   0.0
1910 0    0  5.0  4.5  5.5  0.0  0.0   0.0
1923 12  13  9.0  4.5  5.5  3.0  0.0   0.0
1885 1   13  0.0  4.5  6.0  3.0  0.0   0.0
1911 0    0  5.0  4.5  6.0  0.0  0.0   0.0
1924 12  13  9.0  4.5  6.0  3.0  0.0   0.0
2081 1   13  0.0  5.0  0.0  3.0  0.0   0.0
2107 0    0  5.0  5.0  0.0  0.0  0.0   0.0
2120 12  13  9.0  5.0  0.0  3.0  0.0   0.0
2082 1   13  0.0  5.0  0.5  3.0  0.0   0.0
2108 0    0  5.0  5.0  0.5  0.0  0.0   0.0
2121 12  13  9.0  5.0  0.5  3.0  0.0   0.0
2083 1   13  0.0  5.0  1.0  3.0  0.0   0.0
2109 0    0  5.0  5.0  1.0  0.0  0.0   0.0
2122 12  13  9.0  5.0  1.0  3.0  0.0   0.0
2084 1   13  0.0  5.0  1.5  3.0  0.0   0.0
2110 0    0  5.0  5.0  1.5  0.0  0.0   0.0
2123 12  13  9.0  5.0  1.5  3.0  0.0   0.0
2085 1   13  0.0  5.0  2.0  3.0  0.0   0.0
2111 0    0  5.0  5.0  2.0  0.0  0.0   0.0
2124 12  13  9.0  5.0  2.0  3.0  0.0   0.0
2086 1   13  0.0  5.0  2.5  3.0  0.0   0.0
2112 0    0  5.0  5.0  2.5  0.0  0.0   0.0
2125 12  13  9.0  5.0  2.5  3.0  0.0   0.0
2087 1   13  0.0  5.0  3.0  3.0  0.0   0.0
2113 0    0  5.0  5.0  3.0  0.0  0.0   0.0
2126 12  13  9.0  5.0  3.0  3.0  0.0   0.0
2088 1   13  0.0  5.0  3.5  3.0  0.0   0.0
2114 0    0  5.0  5.0  3.5  0.0  0.0   0.0
2127 12  13  9.0  5.0  3.5  3.0  0.0   0.0
2089 1   13  0.0  5.0  4.0  3.0  0.0   0.0
2115 0    0  5.0  5.0  4.0  0.0  0.0   0.0
2128 12  13  9.0  5.0  4.0  3.0  0.0   0.0
2090 1   13  0.0  5.0  4.5  3.0  0.0   0.0
2116 0    0  5.0  5.0  4.5  0.0  0.0   0.0
2129 12  13  9.0  5.0  4.5  3.0  0.0   0.0
2091 1   13  0.0  5.0  5.0  3.0  0.0   0.0
2117 0    0  5.0  5.0  5.0  0.0  0.0   0.0
2130 12  13  9.0  5.0  5.0  3.0  0.0   0.0
2092 1   13  0.0  5.0  5.5  3.0  0.0   0.0
```

```
2118 0    0  5.0  5.0  5.5  0.0  0.0   0.0
2131 12  13  9.0  5.0  5.5  3.0  0.0   0.0
2093 1   13  0.0  5.0  6.0  3.0  0.0   0.0
2119 0    0  5.0  5.0  6.0  0.0  0.0   0.0
2132 12  13  9.0  5.0  6.0  3.0  0.0   0.0
  0  0 0  0.0    0.0   0.0   0.0   0.0   0.0 END OF COORDINATES
===== DATA SET 8: SUBREGIONAL DATA
    11                                      NREGN
    1    10   1  208    0
    0    0    0    0    0                   END OF NNPLR(K)
    1  207    1    1    1
    0    0    0    0    0                   END OF GNLR(I,1)
    1  207    1  209    1
    0    0    0    0    0                   END OF GNLR(I,2)
    1  207    1  417    1
    0    0    0    0    0                   END OF GNLR(I,2)
    1  207    1  625    1
    0    0    0    0    0                   END OF GNLR(I,2)
    1  207    1  833    1
    0    0    0    0    0                   END OF GNLR(I,2)
    1  207    1  1041   1
    0    0    0    0    0                   END OF GNLR(I,2)
    1  207    1  1249   1
    0    0    0    0    0                   END OF GNLR(I,2)
    1  207    1  1457   1
    0    0    0    0    0                   END OF GNLR(I,2)
    1  207    1  1665   1
    0    0    0    0    0                   END OF GNLR(I,2)
    1  207    1  1873   1
    0    0    0    0    0                   END OF GNLR(I,2)
    1  207    1  2081   1
    0    0    0    0    0                   END OF GNLR(I,2)
===== DATA SET 9 : ELEMENT INCIDENCES
  1800                  NEL
    1   14   12    1   14  222  209   2    15  223  210   13
    2   14   12    2   15  223  210   3    16  224  211   13
    3   14   12    3   16  224  211   4    17  225  212   13
    4   14   12    4   17  225  212   5    18  226  213   13
    5   14   12    5   18  226  213   6    19  227  214   13
    6   14   12    6   19  227  214   7    20  228  215   13
    7   14   12    7   20  228  215   8    21  229  216   13
    8   14   12    8   21  229  216   9    22  230  217   13
    9   14   12    9   22  230  217  10    23  231  218   13
   10   14   12   10   23  231  218  11    24  232  219   13
   11   14   12   11   24  232  219  12    25  233  220   13
   12   14   12   12   25  233  220  13    26  234  221   13
  181   14   12   209 222  430  417  210  223  431  418   13
  182   14   12   210 223  431  418  211  224  432  419   13
  183   14   12   211 224  432  419  212  225  433  420   13
  184   14   12   212 225  433  420  213  226  434  421   13
  185   14   12   213 226  434  421  214  227  435  422   13
  186   14   12   214 227  435  422  215  228  436  423   13
  187   14   12   215 228  436  423  216  229  437  424   13
  188   14   12   216 229  437  424  217  230  438  425   13
  189   14   12   217 230  438  425  218  231  439  426   13
  190   14   12   218 231  439  426  219  232  440  427   13
  191   14   12   219 232  440  427  220  233  441  428   13
  192   14   12   220 233  441  428  221  234  442  429   13
  361   14   12   417 430  638  625  418  431  639  626   13
  362   14   12   418 431  639  626  419  432  640  627   13
  363   14   12   419 432  640  627  420  433  641  628   13
  364   14   12   420 433  641  628  421  434  642  629   13
```

365	14	12	421	434	642	629	422	435	643	630	13
366	14	12	422	435	643	630	423	436	644	631	13
367	14	12	423	436	644	631	424	437	645	632	13
368	14	12	424	437	645	632	425	438	646	633	13
369	14	12	425	438	646	633	426	439	647	634	13
370	14	12	426	439	647	634	427	440	648	635	13
371	14	12	427	440	648	635	428	441	649	636	13
372	14	12	428	441	649	636	429	442	650	637	13
541	14	12	625	638	846	833	626	639	847	834	13
542	14	12	626	639	847	834	627	640	848	835	13
543	14	12	627	640	848	835	628	641	849	836	13
544	14	12	628	641	849	836	629	642	850	837	13
545	14	12	629	642	850	837	630	643	851	838	13
546	14	12	630	643	851	838	631	644	852	839	13
547	14	12	631	644	852	839	632	645	853	840	13
548	14	12	632	645	853	840	633	646	854	841	13
549	14	12	633	646	854	841	634	647	855	842	13
550	14	12	634	647	855	842	635	648	856	843	13
551	14	12	635	648	856	843	636	649	857	844	13
552	14	12	636	649	857	844	637	650	858	845	13
721	14	12	833	846	1054	1041	834	847	1055	1042	13
722	14	12	834	847	1055	1042	835	848	1056	1043	13
723	14	12	835	848	1056	1043	836	849	1057	1044	13
724	14	12	836	849	1057	1044	837	850	1058	1045	13
725	14	12	837	850	1058	1045	838	851	1059	1046	13
726	14	12	838	851	1059	1046	839	852	1060	1047	13
727	14	12	839	852	1060	1047	840	853	1061	1048	13
728	14	12	840	853	1061	1048	841	854	1062	1049	13
729	14	12	841	854	1062	1049	842	855	1063	1050	13
730	14	12	842	855	1063	1050	843	856	1064	1051	13
731	14	12	843	856	1064	1051	844	857	1065	1052	13
732	14	12	844	857	1065	1052	845	858	1066	1053	13
901	14	12	1041	1054	1262	1249	1042	1055	1263	1250	13
902	14	12	1042	1055	1263	1250	1043	1056	1264	1251	13
903	14	12	1043	1056	1264	1251	1044	1057	1265	1252	13
904	14	12	1044	1057	1265	1252	1045	1058	1266	1253	13
905	14	12	1045	1058	1266	1253	1046	1059	1267	1254	13
906	14	12	1046	1059	1267	1254	1047	1060	1268	1255	13
907	14	12	1047	1060	1268	1255	1048	1061	1269	1256	13
908	14	12	1048	1061	1269	1256	1049	1062	1270	1257	13
909	14	12	1049	1062	1270	1257	1050	1063	1271	1258	13
910	14	12	1050	1063	1271	1258	1051	1064	1272	1259	13
911	14	12	1051	1064	1272	1259	1052	1065	1273	1260	13
912	14	12	1052	1065	1273	1260	1053	1066	1274	1261	13
1081	14	12	1249	1262	1470	1457	1250	1263	1471	1458	13
1082	14	12	1250	1263	1471	1458	1251	1264	1472	1459	13
1083	14	12	1251	1264	1472	1459	1252	1265	1473	1460	13
1084	14	12	1252	1265	1473	1460	1253	1266	1474	1461	13
1085	14	12	1253	1266	1474	1461	1254	1267	1475	1462	13
1086	14	12	1254	1267	1475	1462	1255	1268	1476	1463	13
1087	14	12	1255	1268	1476	1463	1256	1269	1477	1464	13
1088	14	12	1256	1269	1477	1464	1257	1270	1478	1465	13
1089	14	12	1257	1270	1478	1465	1258	1271	1479	1466	13
1090	14	12	1258	1271	1479	1466	1259	1272	1480	1467	13
1091	14	12	1259	1272	1480	1467	1260	1273	1481	1468	13
1092	14	12	1260	1273	1481	1468	1261	1274	1482	1469	13
1261	14	12	1457	1470	1678	1665	1458	1471	1679	1666	13
1262	14	12	1458	1471	1679	1666	1459	1472	1680	1667	13
1263	14	12	1459	1472	1680	1667	1460	1473	1681	1668	13
1264	14	12	1460	1473	1681	1668	1461	1474	1682	1669	13
1265	14	12	1461	1474	1682	1669	1462	1475	1683	1670	13
1266	14	12	1462	1475	1683	1670	1463	1476	1684	1671	13

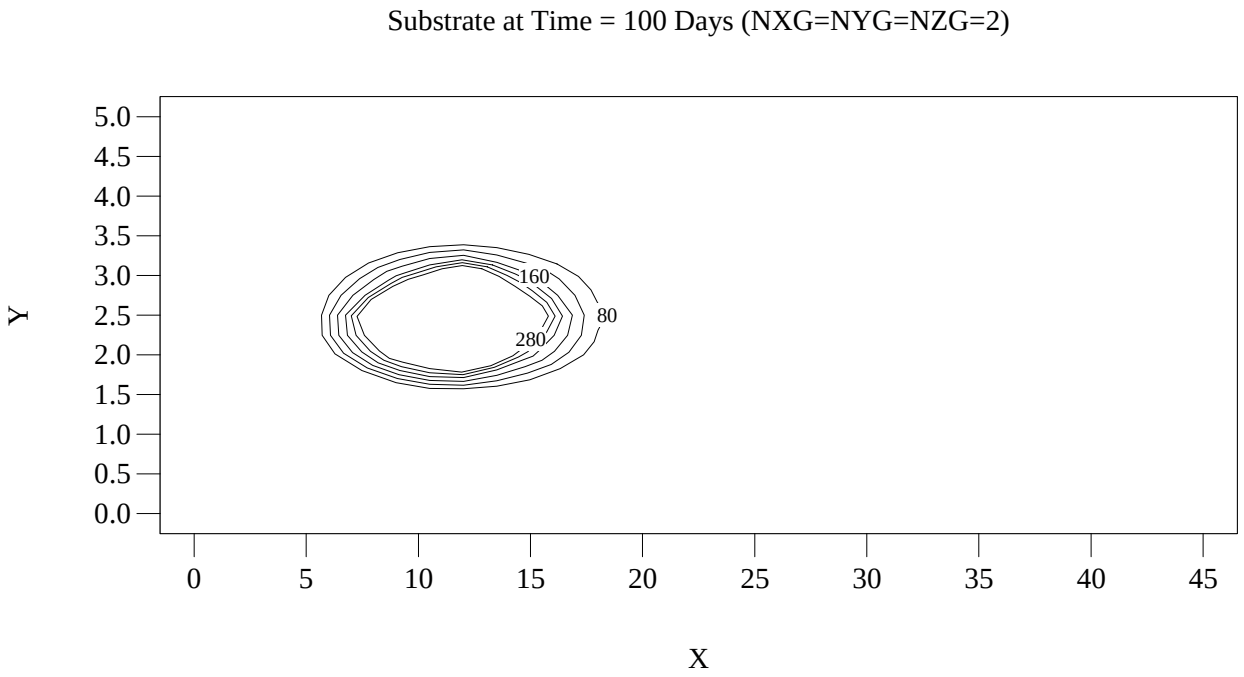
```
 1267   14   12  1463 1476 1684 1671 1464 1477 1685 1672   13
 1268   14   12  1464 1477 1685 1672 1465 1478 1686 1673   13
 1269   14   12  1465 1478 1686 1673 1466 1479 1687 1674   13
 1270   14   12  1466 1479 1687 1674 1467 1480 1688 1675   13
 1271   14   12  1467 1480 1688 1675 1468 1481 1689 1676   13
 1272   14   12  1468 1481 1689 1676 1469 1482 1690 1677   13
 1441   14   12  1665 1678 1886 1873 1666 1679 1887 1874   13
 1442   14   12  1666 1679 1887 1874 1667 1680 1888 1875   13
 1443   14   12  1667 1680 1888 1875 1668 1681 1889 1876   13
 1444   14   12  1668 1681 1889 1876 1669 1682 1890 1877   13
 1445   14   12  1669 1682 1890 1877 1670 1683 1891 1878   13
 1446   14   12  1670 1683 1891 1878 1671 1684 1892 1879   13
 1447   14   12  1671 1684 1892 1879 1672 1685 1893 1880   13
 1448   14   12  1672 1685 1893 1880 1673 1686 1894 1881   13
 1449   14   12  1673 1686 1894 1881 1674 1687 1895 1882   13
 1450   14   12  1674 1687 1895 1882 1675 1688 1896 1883   13
 1451   14   12  1675 1688 1896 1883 1676 1689 1897 1884   13
 1452   14   12  1676 1689 1897 1884 1677 1690 1898 1885   13
 1621   14   12  1873 1886 2094 2081 1874 1887 2095 2082   13
 1622   14   12  1874 1887 2095 2082 1875 1888 2096 2083   13
 1623   14   12  1875 1888 2096 2083 1876 1889 2097 2084   13
 1624   14   12  1876 1889 2097 2084 1877 1890 2098 2085   13
 1625   14   12  1877 1890 2098 2085 1878 1891 2099 2086   13
 1626   14   12  1878 1891 2099 2086 1879 1892 2100 2087   13
 1627   14   12  1879 1892 2100 2087 1880 1893 2101 2088   13
 1628   14   12  1880 1893 2101 2088 1881 1894 2102 2089   13
 1629   14   12  1881 1894 2102 2089 1882 1895 2103 2090   13
 1630   14   12  1882 1895 2103 2090 1883 1896 2104 2091   13
 1631   14   12  1883 1896 2104 2091 1884 1897 2105 2092   13
 1632   14   12  1884 1897 2105 2092 1885 1898 2106 2093   13
    0    0    0    0    0    0    0    0    0    0    0   0  END OF IE
===== DATA SET 10: MATERIAL CORRECTION
    0                                          NCM
===== DATA SET 11 : INITIAL CONDIDTIONS
 1  2287 1  2.3D-2 0.0D0  0.0D0
 0   0   0  0.0D0  0.0D0  0.0D0
 1  2287 1  0.0D0  0.0D0  0.0D0
 0   0   0  0.0D0  0.0D0  0.0D0
 1  2287 1  0.0D0  0.0D0  0.0D0
 0   0   0  0.0D0  0.0D0  0.0D0
 1  848  1  0.0D0  0.0D0  0.0D0
 850 4   1  3.0d3 0.0d0  0.0d0
 855 7   1  0.0d0  0.0d0  0.0d0
 863 4   1  3.0d3 0.0d0  0.0d0
 868 189 1  0.0d0  0.0d0  0.0d0
1058 4   1  3.0d3 0.0d0  0.0d0
1063 7   1  0.0d0  0.0d0  0.0d0
1071 4   1  3.0d3 0.0d0  0.0d0
1076 189 1  0.0d0  0.0d0  0.0d0
1266 4   1  3.0d3  0.0d0  0.0d0
1271 7   1  0.0d0  0.0d0  0.0d0
1279 4   1  3.0d3  0.0d0  0.0d0
1284 1004 1 0.0d0  0.0d0  0.0d0
 0   0   0  0.0d0  0.0d0  0.0d0
 1  848  1  3.5D3  0.0D0  0.0D0
 850 4   1  1.0d3 0.0d0  0.0d0
 855 7   1  3.5d3  0.0d0  0.0d0
 863 4   1  1.0d3 0.0d0  0.0d0
 868 189 1  3.5d3  0.0d0  0.0d0
1058 4   1  1.0d3 0.0d0  0.0d0
1063 7   1  3.5d3  0.0d0  0.0d0
1071 4   1  1.0d3 0.0d0  0.0d0
```

```
1076 189 1  3.5d3  0.0d0  0.0d0
1266 4   1  1.0d3  0.0d0  0.0d0
1271 7   1  3.5d3  0.0d0  0.0d0
1279 4   1  1.0d3  0.0d0  0.0d0
1284 1004 1 3.5d3  0.0d0  0.0d0
  0  0   0  0.0d0  0.0d0  0.0d0
  1 2287 1  0.0d0  0.0d0  0.0d0
  0  0   0  0.0d0  0.0d0  0.0d0
  1 2287 1  0.0d0  0.0d0  0.0d0
  0  0   0  0.0d0  0.0d0  0.0d0
===== DATA SET 14: ELEMENT(DISTRIBUTED) SOURCE/SINK OF TRANSPORT
    0  0  0  0                  NSELT NSPRT NSDPT KSAIT
===== DATA SET 15: POINT(WELL) SOURCE/SINK OF TRANSPORT
    0  0  0  0                  NWNPT NWPRT NWDPT KWAIT
===== DATA SET 20: VARIABLE BOUNDARY CONDITIONS OF TRANSPORT
    120  143 1  2  0            NVEST NVNPT NRPRT NRDPT KRAIT
    0.0D0  0.0D0  1.0D38  0.0D0
    1  119 1  1  0
    0  0   0  0  0
    1  119 1  1  0
    0  0   0  0  0
    1  119 1  1  0
    0  0   0  0  0
    1  119 1  1  0
    0  0   0  0  0
    1  119 1  1  0
    0  0   0  0  0
    1  119 1  1  0
    0  0   0  0  0
   1  11  1  196  404  405  197  1   1  1  1
  13  11  1  404  612  613  405  1   1  1  1
  25  11  1  612  820  821  613  1   1  1  1
  37  11  1  820 1028 1029  821  1   1  1  1
  49  11  1 1028 1236 1237 1029  1   1  1  1
  61  11  1 1236 1444 1445 1237  1   1  1  1
  73  11  1 1444 1652 1653 1445  1   1  1  1
  85  11  1 1652 1860 1861 1653  1   1  1  1
  97  11  1 1860 2068 2069 1861  1   1  1  1
 109  11  1 2068 2276 2277 2069  1   1  1  1
  0    0  0   0   0     0    0   0  0  0  0
  1  12   1  196  1
  14 12   1  404  1
  27 12   1  612  1
  40 12   1  820  1
  53 12   1 1028  1
  66 12   1 1236  1
  79 12   1 1444  1
  92 12   1 1652  1
 105 12   1 1860  1
 118 12   1 2068  1
 131 12   1 2276  1
   0  0   0    0  0
===== DATA SET 21:  DIRICHLET BOUNDARY CONDITIONS OF TRANSPORT
  143  2  2  0                  NDNPT NDPRT NDDPT KDAIT
   0.0D0  0.0D0  1.0D38  0.0D0
   0.0D0  3.5D3  1.0D38  3.5D3
   1  12  1  1   1
  14  12  1  209 1
  27  12  1  417 1
  40  12  1  625 1
```

```
  53  12  1  833 1
  66  12  1 1041 1
  79  12  1 1249 1
  92  12  1 1457 1
 105  12  1 1665 1
 118  12  1 1873 1
 131  12  1 2081 1
   0   0   0  0  0
   1  142  1  1  0
   0  0    0  0  0
   1  142  1  1  0
   0  0    0  0  0
   1  142  1  1  0
   0  0    0  0  0
   1  142  1  1  0
   0  0    0  0  0
   1  142  1  2  0
   0  0    0  0  0
   1  142  1  1  0
   0   0   0  0  0
   1  142  1  1  0
   0   0   0  0  0
===== DATA SET 22: CAUCHY BOUNDARY CONDITIONS OF TRANSPORT
   0  0   0  0  0               NCEST NCNPT NCPRT NCDPT KCAIT
===== DATA SET 23: NEUMANN BOUNDARY CONDITIONS, TRANSPORT
    0  0  0  0  0               NNEST NNNPT NNPRT NNDPT KNAIT
===== DATA SET 24 : PARAMETERS CONTROLLOING TRACKING SCHEME
  1  1  0  2  2  2  1  1  1   2  2  2   2
  1.0d-2  1.0d-2
===== DATA SET 25 : VELOCITY AND MOISTURE CONTENT
  1  2287 1  9.0D-2 0.0D0  0.0D0  0.0D0  0.0D0  0.0D0
  0   0   0  0.0D0  0.0D0  0.0D0  0.0D0  0.0D0  0.0D0
  1  1799 1  1.0D0  0.0D0
  0   0   0  0.0D0  0.0D0
    0           ====== END OF JOB ======  00000
```

Figure 4.28, Figure 4.29, and Figure 4.30 show the simulation results of substrate, oxygen, and total microbial mass distributions at 100 days and 200 days on x-y crosssection, respectively. Figure 4.31, Figure 4.32, and Figure 4.33 are the results of substrate, oxygen, and microbe at 100 days and 200 days on x-z crosssection, respectively.

(a)



(b)

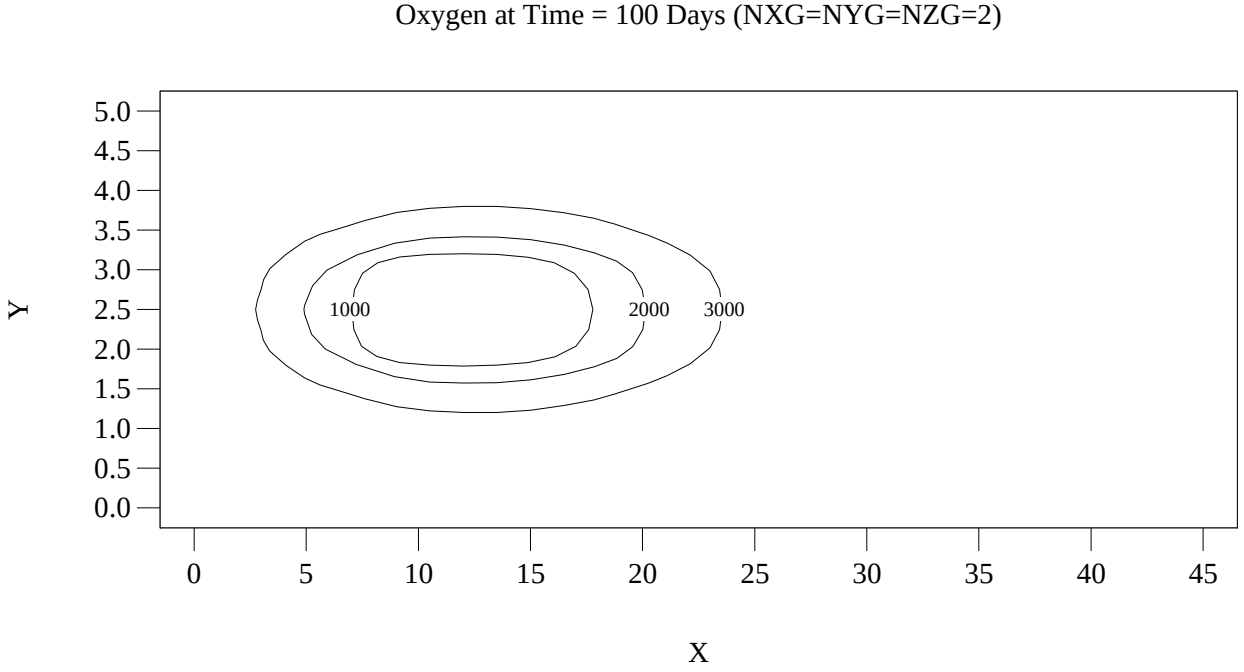
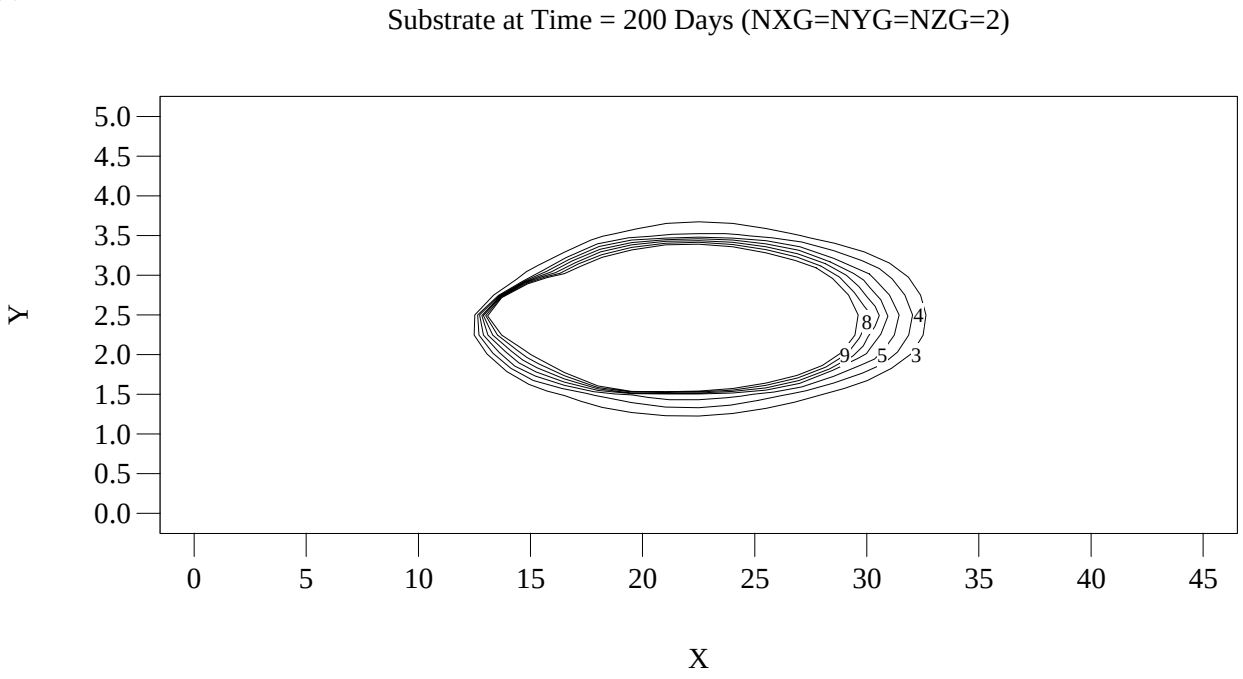


Figure 4.28 Dissolved plumes at 100 days: (a) substrate and (b) oxygen on x-y crosssection. Concentrations isolines are in micrograms per liter

(a)



(b)

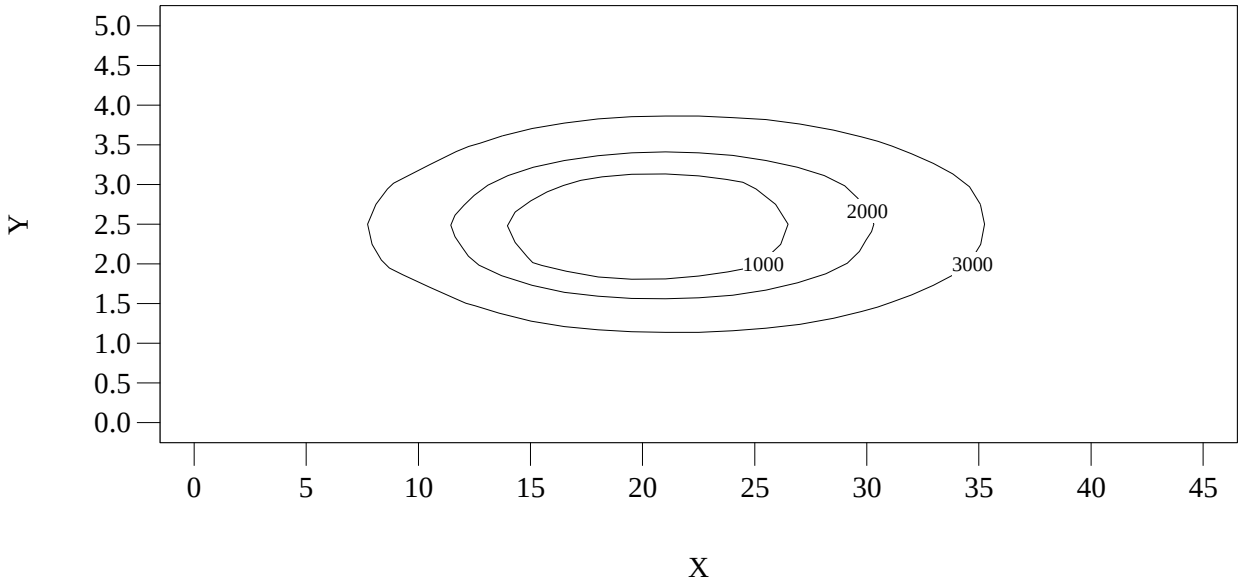
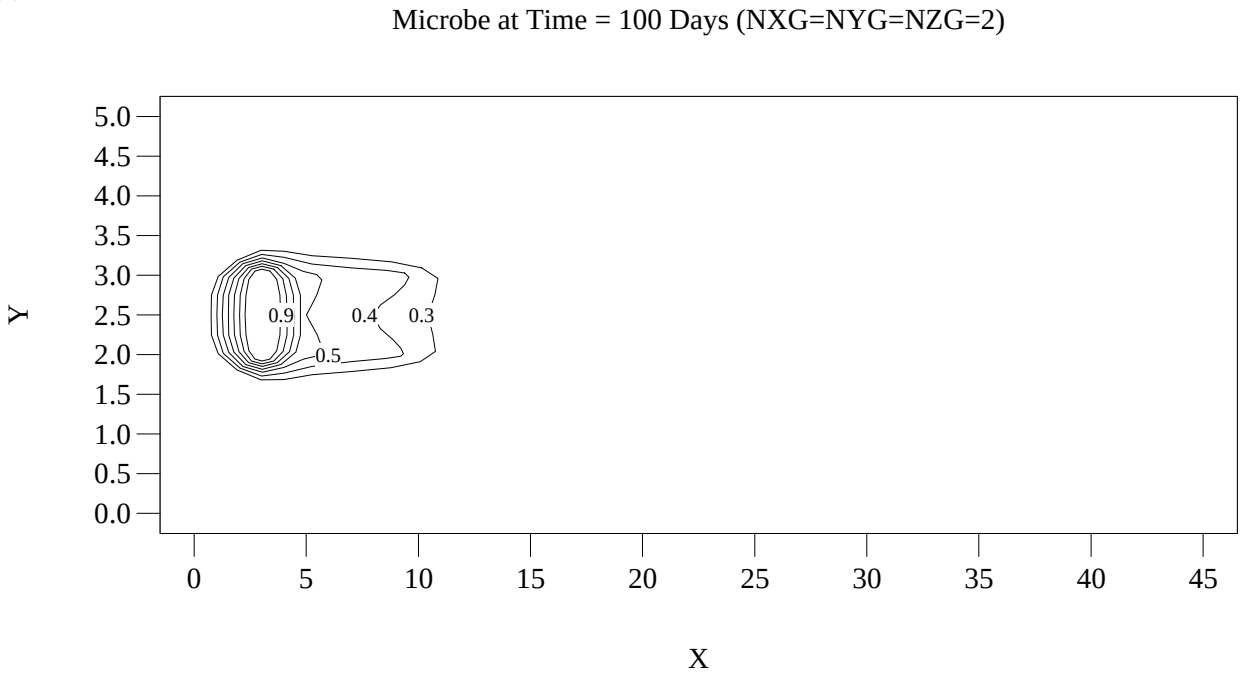


Figure 4.29 Dissolved plumes at 200 days: (a) substrate and (b) oxygen on x-y crosssection. Concentrations isolines are in micrograms per liter

(a)



(b)

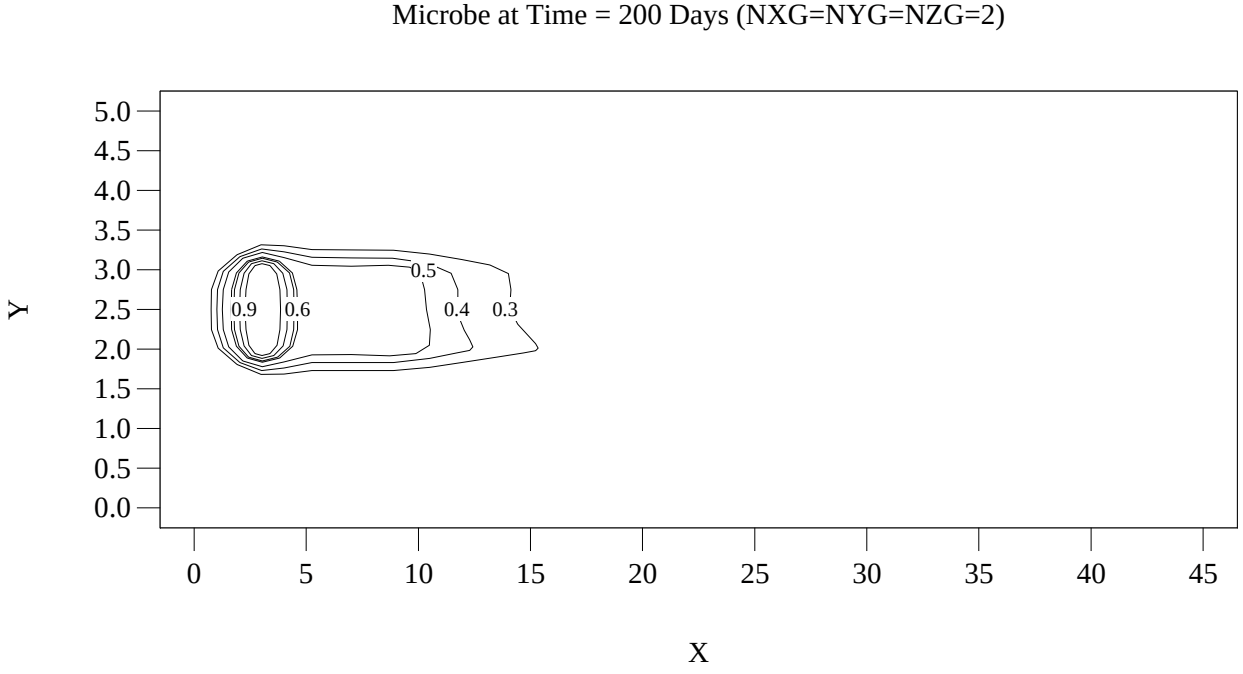
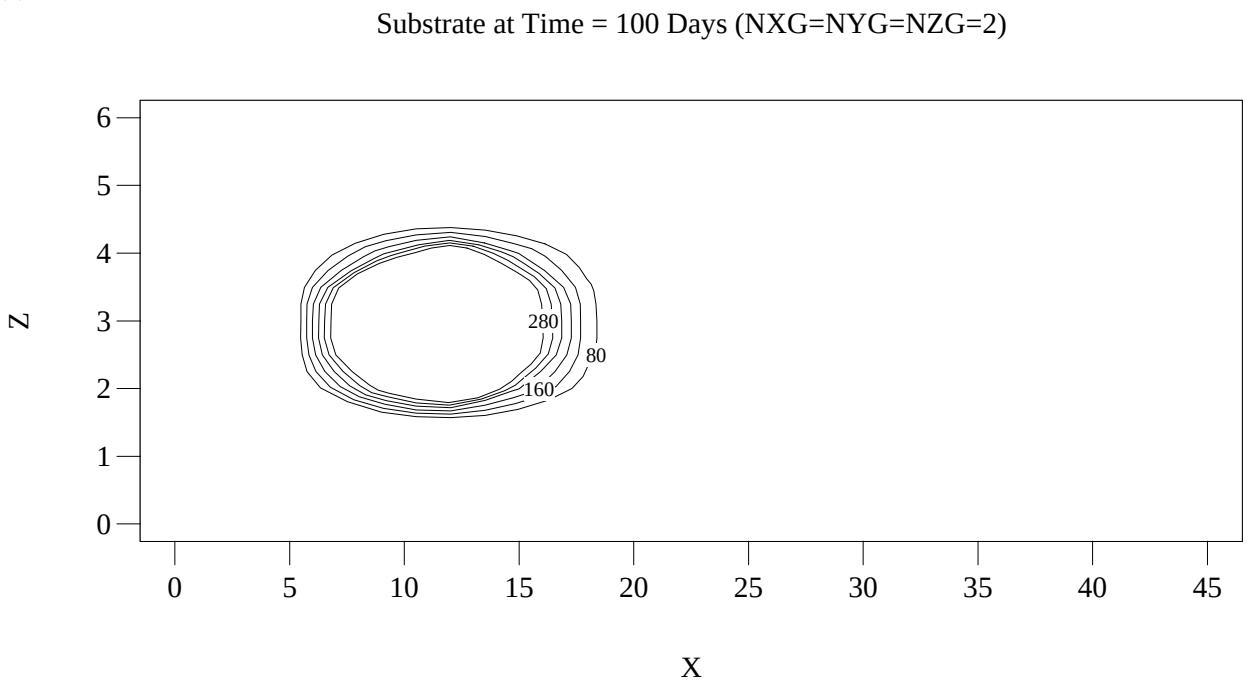


Figure 4.30 Total microbial mass distributions: (a) 100 and (b) 200 days on x-y crosssection. Concentrations isolines are in mg/liter of aquifer materials

(a)



(b)

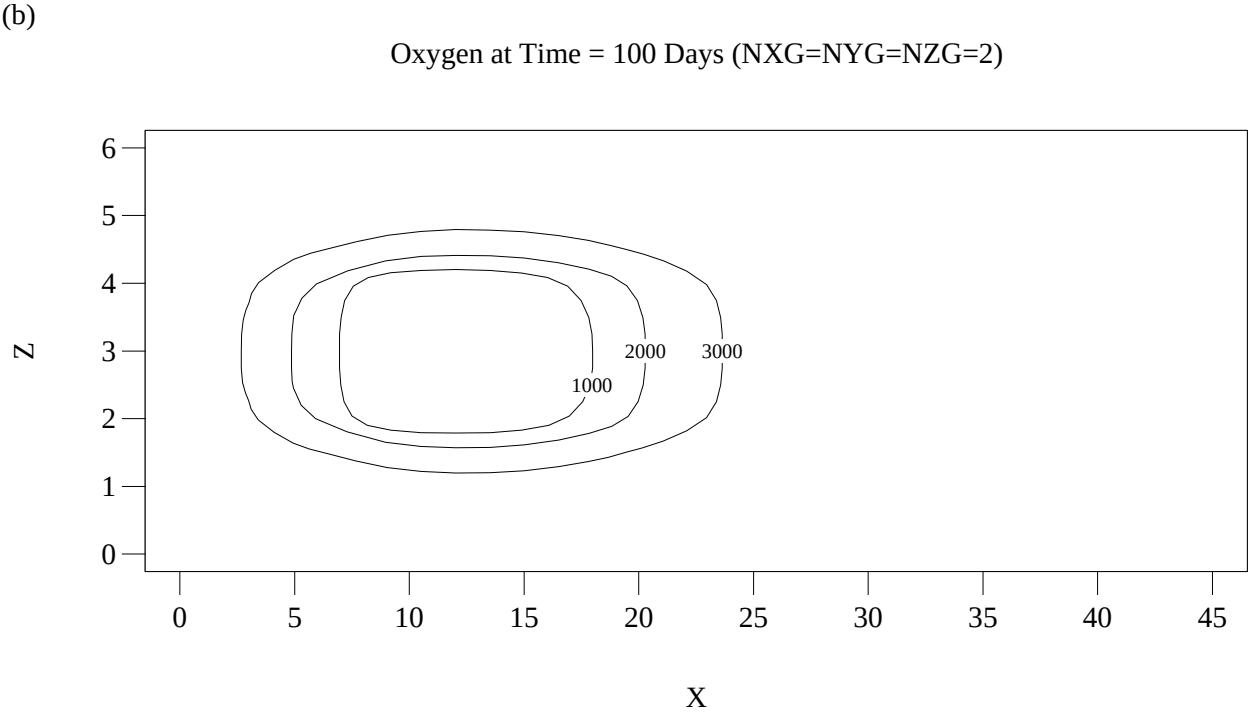
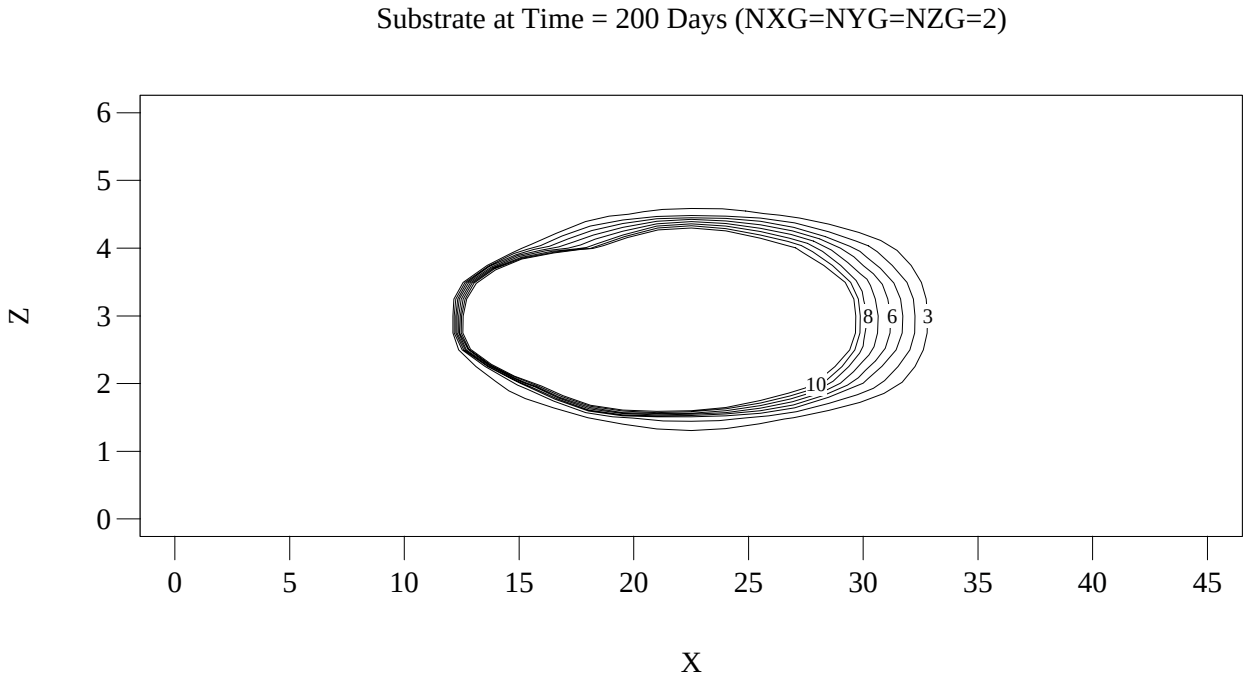


Figure 4.31 Dissolved plumes at 100 days: (a) substrate and (b) oxygen on x-z crosssection. Concentrations isolines are in micrograms per liter

(a)



(b)

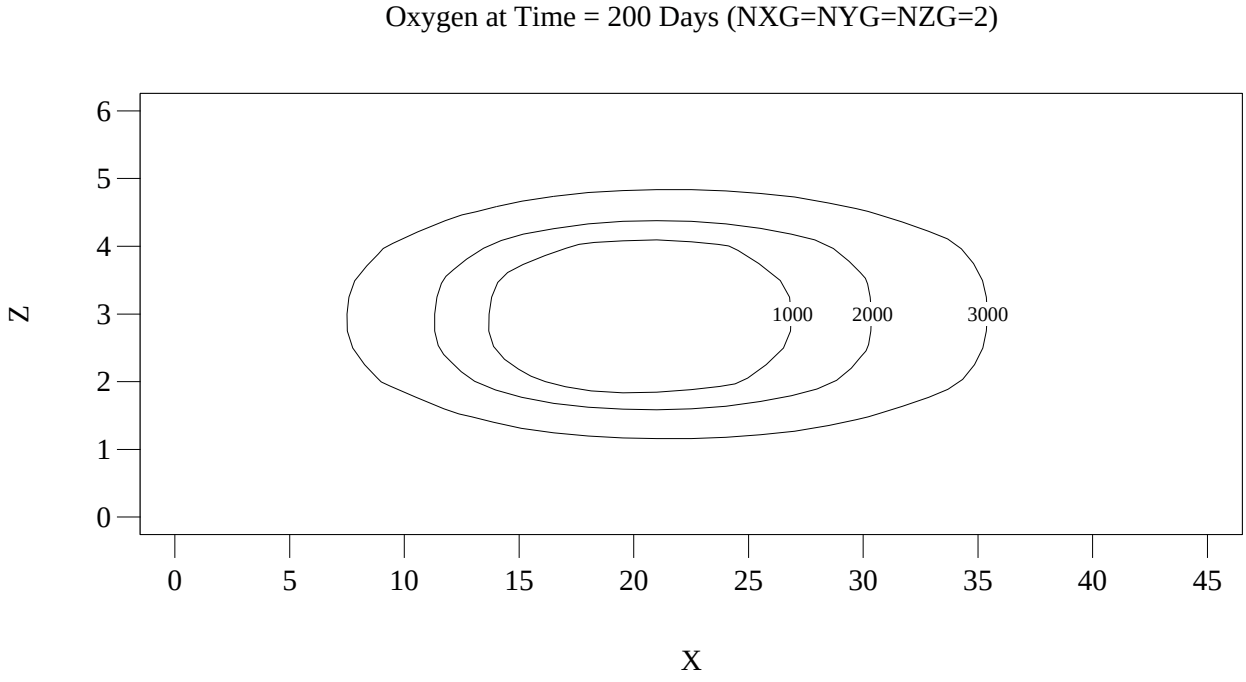
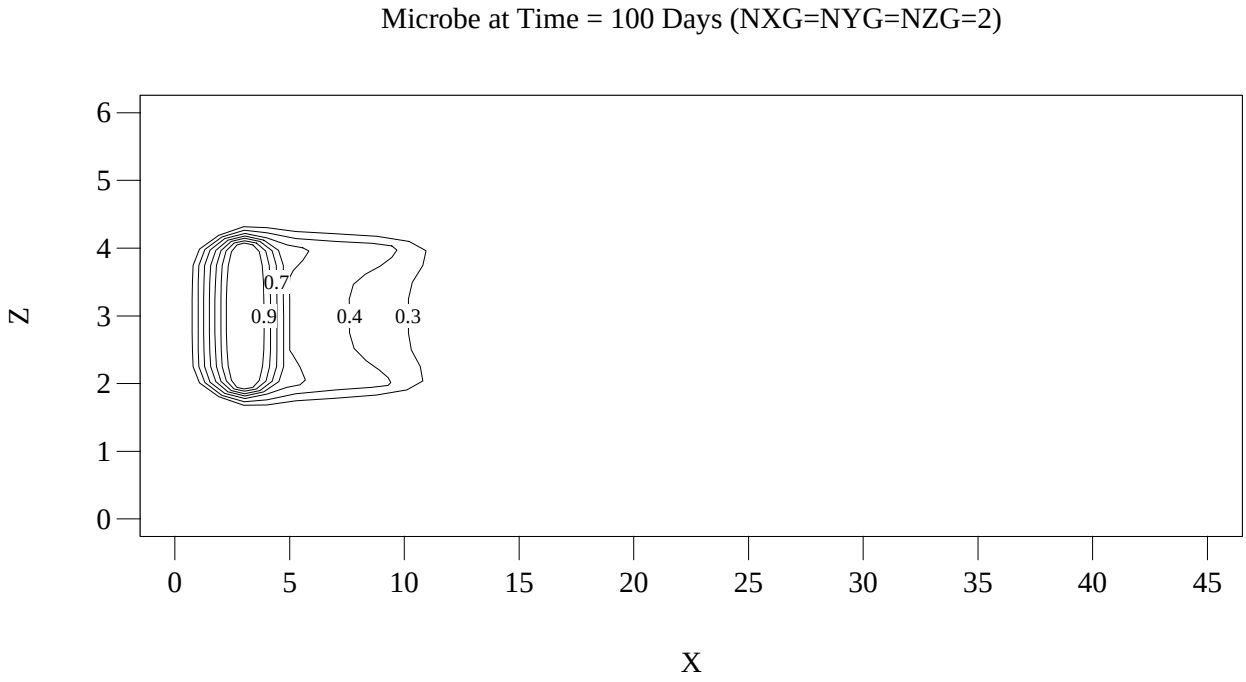


Figure 4.32 Dissolved plumes at 200 days: (a) substrate and (b) oxygen on x-z crosssection. Concentrations isolines are in micrograms per liter

(a)



(b)

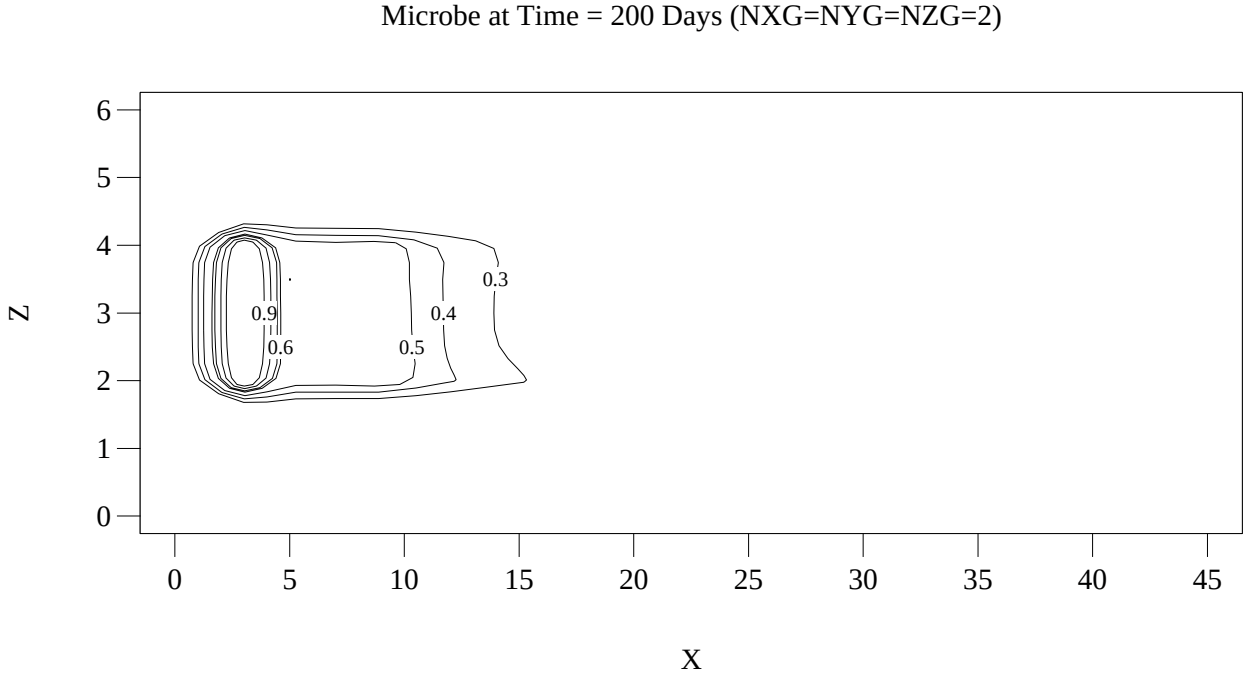


Figure 4.33 Total microbial mass distributions: (a) 100 and (b) 200 days on x-z crosssection. Concentrations isolines are in mg/liter of aquifer materials

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APPENDIX A: Data Input Guide

*** Data sets 2 through 25 must be preceded by a record ***
*** containing description of the data set ***

1. TITLE

One record with FORMAT(I5,A70) per problem. This record contains the following variables.

1. NPROB = Problem number.

2. TITLE = Title of the problem. It may contain up to 70 characters.

2. OPTION PARAMETERS

Seven lines of free-formatted data records are required for this data set.

A. Line 1:

1.1. IMOD = Integer indicating the simulation modes to be carried on. 0 = Do the initial variable computation ONLY, for both flow and transport simulations. The purpose for this mode is to verify the input data. 10 = Do the flow simulation ONLY; 1 = Do the transport simulation only; 11 = Do both flow and transport simulations.

1.2. IGEOM = Integer indicating if (1) the geometry, boundary and pointer arrays are to be printed; (2) the boundary and pointer arrays are to be computed or read via logical units. If to be computed, they should be written on logical units. If IGEOM is an even number, (1) will not be printed. If IGEOM is an odd number, (1) will be printed. If IGEOM is less than or equal to 1, boundary arrays will be computed.

1.3. IBUG = Integer indicating if the diagnostic output is desired? 0 = No, nonzero = Yes.

1.4. ICHNG = Integer control number indicating if the cyclic change of rainfall-seepage nodes is to be printed, =0, no = 1, yes.

B. Line 2:

2.1. NITFTS = Iteration numbers allowed for solving the coupled nonlinear equations for the steady-state solutions. If the steady-state simulation is for either flow or transport only, then the value of NITFTS must be set to 1.

2.2. OMEFTS = Iteration parameter for solving the coupled nonlinear equations for the steady-state solutions.

2.3. ALLOW = The allowed factor for neglecting concentrations in a convergence test.

C. Line 3:

3.1. KSSf = Flow steady-state control, 0 = steady-state solution desired, 1 = transient state or transient solutions.

3.2. KSSt = Transport steady-state control, 0 = steady-state solution desired, 1 = transient state or transient solutions.

3.3. ILUMP = Is mass lumping? 0 = no, 1 = yes.

3.4. IMID = Is mid-difference? 0 = no, 1 = yes.

3.5. IPNTSf = matrix solver indicator for flow simulation:
0 = block iteration solver,
1 = successive iteration methods,
2 = polynomial preconditioned conjugate gradient methods,
3 = incomplete Cholesky preconditioned conjugate gradient methods.

3.6. IPNTSt = matrix solver indicator for transport simulation:
0 = block iteration solver,
1 = successive iteration methods,
2 = polynomial preconditioned conjugate gradient methods,
3 = incomplete Cholesky preconditioned conjugate gradient methods.

3.7. NSTRf = No. of logical records to be read via logical unit 11 for restarting calculation.
0 = No restart.

3.8. NSTRt = No. of logical records to be read via logical unit 12 for restarting calculation.
0 = No restart.

3.9. MICONF = Index of the simulation of microbial configuration:
0 = mobile microbes
1 = immobile microbes

3.10. IQUAR = Index of using quadrature for numerical integration:
1 = Nodal quadrature for surface integration, Gaussian quadrature for element integration,
2 = Nodal quadrature for surface integration, Nodal quadrature for element integration,
3 = Gaussian quadrature for surface integration, Gaussian quadrature for element integration,
4 = Gaussian quadrature for surface integration, Nodal quadrature for element integration.

D. Line 4:

4.1. KGRAV = Gravity term control: 0 = no gravity term, 1 = with gravity term.

4.2. Wf = Time derivative weighting factor for flow simulations:
0.5 = Crank-Nicolson central,
1.0 = backward difference and/or mid-difference.

4.3. OMEf = Iteration parameter for solving the nonlinear flow equation:
0.0 - 1.0 = under-relaxation,
1.0 - 1.0 = exact relaxation,
1.0 - 2.0 = over-relaxation.

4.4. OMIf = Relaxation parameter for solving the linearized flow matrix equation pointwisely or blockwisely:
0.0 - 1.0 = under relaxation,
1.0 - 1.0 = exact relaxation,
1.0 - 2.0 = over relaxation.

4.5. CNSTKR = constraint on relative hydraulic conductivity:
0 = no constraint,
0.0001, 0.001, or 0.01 should be tried when nonconvergency occurs in solving the nonlinear flow equation.

E. Line 5:

5.1. KVIt = Velocity input control:
-1 = card input for velocity and moisture content,
1 = steady-state velocity and moisture content will be calculated from steady-state flow simulations,
2 = transient velocity and moisture content will be obtained from transient-flow simulations.

5.2. IWET = Weighting function control which is used only if the conventional FEM is employed to solve transport equations:
0 = Galerkin weighting,
1 = Upstream weighting.

5.3. IOPTIM = Optimization factor computing indicator which is used only if the conventional FEM is employed to solve transport equations:
1 = Optimization factor is to be computed,
0 = optimization factor is to be set to -1.0 or 0.0 or 1.0 depending on the velocity.

5.4. KSORP = Sorption model control:
1 = linear isotherm, the only option used in this model.

5.5. LGRN = Lagrangian approach control: 0 = no, 1 = yes.

F. Line 6:

6.1. Wt = Time derivative weighting factor for transport simulations:
0.5 = Crank-Nicolson central,

1.0 = backward difference and/or mid-difference.

6.2. WVt = Integration factor for velocity used only if the conventional FEM is employed to solve transport equations; should be between 0.0 to 1.0.

6.3. OMEt = Iteration parameter for solving the nonlinear transport equation; always used 1.0 because KSORP = 1.

6.4. OMIt = Relaxation parameter for solving the linearized transport matrix equation pointwisely or blockwisely; used only the block iteration or the pointwise solver:
0.0 - 1.0 = under relaxation,
1.0 - 1.0 = exact relaxation,
1.0 - 2.0 = over relaxation.

G. Line 7: This line is needed if and only if IPNTSf or IPNTSt is greater than 0.

7.1. IEIGEN = signal of parameter estimation for GG in the polynomial preconditioned conjugate gradient method:
zero = not requested,
non-zero = requested.

7.2. GG = the upper bound on the maximum eigenvalue of the coefficient matrix used in the polynomial preconditioned conjugate gradient method. When requested, GG is usually set to 1.0.

3. ITERATION PARAMETERS

Two subsets of free-formatted data records are required for this data set, one for flow simulations, the other for transport simulations.

A. subset 1: For flow simulations -

1.1. NITERf = Number of iterations allowed for solving the non-linear flow equation.

1.2. NCYLf = No. of cycles permitted for iterating rainfall-seepage boundary conditions per time step.

1.3. NPITERf = No. of iterations permitted for solving the linearized flow equation using block or pointwise iterative matrix solver.

1.4. TOLAf = Steady-state convergence criteria for flow simulations, (L).

1.5. TOLBf = Transient-state convergence criteria for flow simulations, (L).

B. subset 2: For transport simulations -

2.1. NITERt = Number of iterations allowed for solving the non-linear transport equation.

2.2. NPITERt = No. of iterations for block or pointwise iteration to solve the linearized transport

equation.

2.3. TOLAt = Steady-state convergence criteria for transport simulations.

2.4. TOLBt = Transient-state convergence criteria for transport simulations.

4. TIME CONTROL PARAMETERS
Five subsets of data records are required for this data set.

A. subset 1: free format

1.1. NTI = Number of time steps or time increments.

1.2. NDTCHG = No. of times to reset time-step size to initial time-step size.

B. subset 2: free format

2.1. DELT = Initial time step size, (T).

2.2. CHNG = Percentage of change in time-step size in each of the subsequent time increments, (dimensionless in decimal point).

2.3. DELMAX = Maximum value of DELT, (T).

2.4. TMAX = Maximum simulation time, (T).

C. subset 3: format = 80I1

3.1. KPR0 = Printer control for steady state and initial conditions;
0 = print nothing,
1 = print FLOW, FRATE, and TFLOW,
2 = print above (1) plus pressure head H,
3 = print above (2) plus total head,
4 = print above (3) plus moister content,
5 = print above (4) plus Darcy velocity.

3.2. KPR(I) = Printer control for the I-th (I = 1, 2, ..., NTI) time step similar to KPR0.

D. subset 4: format = 80I1

4.1. KDSK0 = Auxiliary storage control for steady state and initial condition:
0 = no storage, 1 = store on Logical Unit 11 (for flow output) or 12 (for transport output).

4.1. KDSK(I) = Auxiliary storage control for the I-th time step similar to KDSK0.

E. subset 5: free format

5.1. TDTCH(I,1) = Time when the I-th (I = 1, 2, ..., NDTCH) step-size-resetting is needed.

5.2. TDTCH(I,2) = Time-step size of the first step of the I-th (I = 1, 2, ..., NDTCH) step-size-resetting.

**** NOTE: Two ways to terminate the execution: either NTI is reached first or TMAX is reached first.

5. MATERIAL PROPERTIES

Four subsets of free-formatted data records are required for this data set.

A. subset 1:

1.1. NMAT = Number of material types.

1.2. NMPPM = No. of material properties per material. ≥ 7 for the present version.

1.3. NCC = No. of components in the system. Since the kinetic reaction model is built in the program according to Eq. (2.9) through Eq. (2.15), NCC is assigned to 7 and IRXN is set to 1 if the microbial-chemical Monod type reactions are involved. NCC can be 1 for the single component simulation and NCC is equal to 2 by using stochiometric model which results in IRXN = -1. NCC can be any value if users modify the kinetic model in the program (Subroutine ADVRX).

1.4. IRXN = the index indicating the chemical-microbial kinetic reaction type. -1 refers to stochiometric reaction; 1 indicates Monod type reaction.

The following three subdata sets (B ~ D) are needed only if IMOD = 10 or IMOD = 11.

B. subset 2: A total of NMAT records are needed per problem, one each for one material.

2.1.1. PROPf(I,1) = Saturated xx-conductivity or permeability of the medium I, (L/T or L**2).

2.1.2. PROPf(I,2) = Saturated yy-conductivity or permeability of the medium I, (L/T or L**2).

2.1.3. PROPf(I,3) = Saturated zz-conductivity or permeability of the medium I, (L/T or L**2).

2.1.4. PROPf(I,4) = Saturated xy-conductivity or permeability of the medium I, (L/T or L**2).

2.1.5. PROPf(I,5) = Saturated xz-conductivity or permeability of the medium I, (L/T or L**2).

2.1.6. PROPf(I,6) = Saturated yz-conductivity or permeability of the medium I, (L/T or L**2).

2.1.7. PROPf(I,7) = Fluid density of the medium I, (L/T or L**2).

C. subset 3: The intrinsic density for each component used in Eq. (2.2b).

A total number of NCC parameters appears in this record. NCC is the total number of components in the system.

3.1. DINTS(I) = intrinsic density (M/L**3) of the I-th component.

D. subset 4: Coefficient for calculating dynamic viscosity used in Eq. (2.2c).
A total number of NCC parameters appears in this record. NCC is the total number of components in the system.

4.1. RHOMU(I) = coefficient for calculating dynamic viscosity as a function of concentration, (L^3/M).

The following three subdata sets (E~ H) are needed only if IMOD = 1 or IMOD = 11.

Subdata sets E to G should be repeated NMAT times.

E. subset 5: A total of NMAT records are needed per problem, one each for one material.

5.1. PROPt(I,1) = Bulk density, (M/L**3) for medium I.

5.2. PROPt(I,2) = Longitudinal dispersivity, (L), for medium I.

5.3. PROPt(I,3) = Lateral dispersivity, (L), for medium I.

5.4. PROPt(I,4) = Molecular diffusion coefficient, (L**2/T), for medium I.

5.5. PROPt(I,5) = Tortuosity, (Dimensionless) for medium I.

5.6. PROPt(I,6) = Decay constant, (1/L) in medium I.

5.7. PROPt(I,7) = 0.0.

F. subset 6: A total number of NCC parameters appears in this record. NCC is the total number of components in the system.

6.1. RKD(I,J) = distribution coefficient of the J-th component in the I-th material.

G. subset 7: A total number of NCC parameters appears in this record. NCC is the total number of components in the system.

7.1. TRANC(I,J) = chemical transformation rate of the J-th component in the I-th material.

H. subset 8: MICROBE-CHEMICAL INTERACTION CONSTANTS
Eleven records of FREE-FORMATTED data are needed.

8.1. Record 1: Four parameters describing the specific growth rate of microbes (1/T) are needed in this record. If there are no microbes in this system, the following four numbers have

to be set to zeros.

(1) GRATE(1) = Maximum specific oxygen-based growth rate for microbe #1. ($\mu_o^{(1)}$ in Eqs. (2.9) ~ (2.15)).

(2) GRATE(2) = Maximum specific nitrate-based growth rate for microbe #2. ($\mu_n^{(2)}$ in Eqs. (2.9) ~ (2.15)).

(3) GRATE(3) = Maximum specific oxygen-based growth rate for microbe #3. ($\mu_o^{(3)}$ in Eqs. (2.9) ~ (2.15)).

(4) GRATE(4) = Maximum specific nitrate-based growth rate for microbe #3. ($\mu_n^{(3)}$ in Eqs. (2.9) ~ (2.15)).

8.2. Record 2 : Four yield coefficients (M/M) are needed in this record and these four values cannot be zeros.

(1) YCOEFF(1) = Yield coefficient for microbe #1 utilizing Oxygen. ($Y_o^{(1)}$ in Eqs. (2.9) & (2.12)).

(2) YCOEFF(2) = Yield coefficient for microbe #2 utilizing Nitrate. ($Y_n^{(2)}$ in Eqs. (2.9) & (2.12)).

(3) YCOEFF(3) = Yield coefficient for microbe #3 utilizing Oxygen. ($Y_o^{(3)}$ in Eqs. (2.9) & (2.12)).

(4) YCOEFF(4) = Yield coefficient for microbe #3 utilizing Nitrate. ($Y_n^{(3)}$ in Eqs. (2.9) & (2.12)).

8.3. Record 3: Four retarded substrate saturation constants (M/L^3) are needed in this record.

(1) RTARDS(1) = Retarded substrate saturation constant under aerobic conditions with respect to microbe #1. ($K_{so}^{(1)}$ in Eqs. (2.9) ~ (2.15)).

(2) RTARDS(2) = Retarded substrate saturation constant under anaerobic conditions with respect to microbe #2. ($K_{sn}^{(2)}$ in Eqs. (2.9) ~ (2.15)).

(3) RTARDS(3) = Retarded substrate saturation constant under aerobic conditions with respect to microbe #3. ($K_{so}^{(3)}$ in Eqs. (2.9) ~ (2.15)).

(4) RTARDS(4) = Retarded substrate saturation constant under anaerobic conditions with respect to microbe #3. ($K_{sn}^{(3)}$ in Eqs. (2.9) ~ (2.15)).

8.4. Record 4: Four retarded Oxygen or Nitrate saturation constants (M/L^3) are needed in this record.

(1) RTARDO(1) = Retarded Oxygen saturation constant under aerobic conditions with respect to microbe #1. ($K_o^{(1)}$ in Eqs. (2.9) ~ (2.15)).

(2) RTARDO(2) = Retarded Nitrate saturation constant under anaerobic conditions with respect to microbe #2. ($K_n^{(2)}$ in Eqs. (2.9) ~ (2.15)).

(3) RTARDO(3) = Retarded Oxygen saturation constant under aerobic conditions with respect to microbe #3. ($K_o^{(3)}$ in Eqs. (2.9) ~ (2.15)).

(4) RTARDO(4) = Retarded Nitrate saturation constant under anaerobic conditions with respect to microbe #3. ($K_n^{(3)}$ in Eqs. (2.9) ~ (2.15)).

8.5. Record 5: Four retarded nutrient saturation constants (M/L^3) are needed in this record.

(1) RTARDN(1) = Retarded nutrient saturation constant under aerobic conditions with respect to microbe #1. ($K_{po}^{(1)}$ in Eqs. (2.9) ~ (2.15)).

(2) RTARDN(2) = Retarded nutrient saturation constant under anaerobic conditions with respect to microbe #2. ($K_{pn}^{(2)}$ in Eqs. (2.9) ~ (2.15)).

(3) RTARDN(3) = Retarded nutrient saturation constant under aerobic conditions with respect to microbe #3. ($K_{po}^{(3)}$ in Eqs. (2.9) ~ (2.15)).

(4) RTARDN(4) = Retarded nutrient saturation constant under anaerobic conditions with respect to microbe #3. ($K_{pn}^{(3)}$ in Eqs. (2.9) ~ (2.15)).

8.6. Record 6: Four Oxygen-use or Nitrate-use coefficients for synthesis are needed in this record.

(1) SCOEFF(1) = Oxygen-use coefficient for synthesis by microbe #1. ($\gamma_o^{(1)}$ in Eq. (2.10)).
(2) SCOEFF(2) = Nitrate-use coefficient for synthesis by microbe #2. ($\gamma_n^{(2)}$ in Eq. (2.11)).
(3) SCOEFF(3) = Oxygen-use coefficient for synthesis by microbe #3. ($\gamma_o^{(3)}$ in Eq. (2.10)).
(4) SCOEFF(4) = Nitrate-use coefficient for synthesis by microbe #3. ($\gamma_n^{(3)}$ in Eq. (2.11)).

8.7. Record 7: Four Oxygen-use or Nitrate-use coefficients for energy are needed in this record.
(1) ECOEFF(1) = Oxygen-use coefficient for energy by microbe #1. ($\alpha_o^{(1)}$ in Eq. (2.10)).
(2) ECOEFF(2) = Nitrate-use coefficient for energy by microbe #2. ($\alpha_n^{(2)}$ in Eq. (2.11)).
(3) ECOEFF(3) = Oxygen-use coefficient for energy by microbe #3. ($\alpha_o^{(3)}$ in Eq. (2.10)).
(4) ECOEFF(4) = Nitrate-use coefficient for energy by microbe #3. ($\alpha_n^{(3)}$ in Eq. (2.11)).

8.8. Record 8: Four microbial decay coefficients (1/T) are needed in this record.
(1) DCOEFF(1) = Microbial decay coefficient of aerobic respiration of microbe #1. ($\lambda_o^{(1)}$ in Eqs. (2.13) & (2.15)).
(2) DCOEFF(2) = Microbial decay coefficient of anaerobic respiration of microbe #2. ($\lambda_n^{(2)}$ in Eqs. (2.14) & (2.15)).
(3) DCOEFF(3) = Microbial decay coefficient of aerobic respiration of microbe #3. ($\lambda_o^{(3)}$ in Eqs. (2.13) & (2.15)).
(4) DCOEFF(4) = Microbial decay coefficient of anaerobic respiration of microbe #3. ($\lambda_n^{(3)}$ in Eqs. (2.14) & (2.15)).

8.9. Record 9: Four Oxygen or Nitrate saturation constants (M/L^3) for decay are needed in this record.
(1) SATURC(1) = Oxygen-saturation constant for decay with respect to microbe #1. ($\Gamma_o^{(1)}$ in Eq. (2.10)).
(2) SATURC(2) = Nitrate-saturation constant for decay with respect to microbe #2. ($\Gamma_n^{(2)}$ in Eq. (2.11)).
(3) SATURC(3) = Oxygen-saturation constant for decay with respect to microbe #3. ($\Gamma_o^{(3)}$ in Eq. (2.10)).
(4) SATURC(4) = Nitrate-saturation constant for decay with respect to microbe #3. ($\Gamma_n^{(3)}$ in Eq. (2.11)).

8.10. Record 10: Four nutrient-use coefficients for the production are needed in this record.
(1) PCOEFF(1) = Nutrient-use coefficient for the production of microbe #1 with aerobic respiration. ($\epsilon_o^{(1)}$ in Eq. (2.12)).
(2) PCOEFF(2) = Nutrient-use coefficient for the production of microbe #2 with anaerobic respiration. ($\epsilon_n^{(2)}$ in Eq. (2.12)).
(3) PCOEFF(3) = Nutrient-use coefficient for the production of microbe #3 with aerobic respiration. ($\epsilon_o^{(3)}$ in Eq. (2.12)).
(4) PCOEFF(4) = Nutrient-use coefficient for the production of microbe #3 with anaerobic respiration. ($\epsilon_n^{(3)}$ in Eq. (2.12)).

8.11. Record 11: One variable (M/L^3) is included in this record.
(1) COFK = Inhibition coefficient. (K_c in inhibition function, $I(C_o)$)

6. SOIL PROPERTIES

Three or five subsets of free-formatted data records are required for this data set depending on the forms of the soil property functions given.

A. subset 1: Soil property control parameters

1.1. KSP = Soil property input control: 0 = analytical input, 1 = Tabular data input.

1.2. NSPPM = Number of points in tabular soil property functions or number of parameters to specify analytical soil functions per material.

1.3. KCP = Permeability input control:
0 = input saturated hydraulic conductivity,
1 = input saturated permeability.

1.4. RHO = Referenced density of water, (M/L**3).

1.5. GRAV = Acceleration of gravity, (L/T**2).

1.6. VISC = Referenced dynamic viscosity of water, (M/L/T).

B. subset 2a: Analytical soil parameters - This sub-data-set is needed if and only if KSP is 0. Two sets of records are required, one for moisture-content parameters and the other for conductivity (permeability) parameters and each set should be repeated NMAT times.

2.1. SPP(J,I,1) = Analytical moisture-content parameter J of material I, J = 1..NSPPM. NMAT sets of these parameters are required for I = 1..NMAT. That is, if SPP(J,I,1) for J = 1..NSPPM can be put on a single line, NMAT consecutive lines are needed for the sets of parameters.

2.2. SPP(J,I,2) = Analytical relative conductivity parameter J of material I. Similar input data setting is required for these parameters as for SPP(J,I,1).

C. subset 2b: Soil properties in tabular form - This sub-data-set is needed if and only if KSP is not 0. Four sets of records are needed -- for pressure, water-content, relative conductivity (or relative permeability), and water capacity, respectively.

3.1. SPP(J,I,4) = Tabular value of pressure head of the J-th point for material I. NMAT sets of these parameters are required for I = 1..NMAT. That is, if SPP(J,I,4) for J = 1..NSPPM can be put on a single line, NMAT consecutive lines are needed for the sets of parameters.

3.2. SPP(J,I,1) = Tabular value of moisture-content of the J-th point in material I. Similar input data setting is required for these parameters as for SPP(J,I,4).

3.3. SPP(J,I,2) = Tabular value of relative conductivity of the J-th point in material I. Similar input data setting is required for these parameters as for SPP(J,I,4).

3.4. SPP(J,I,3) = Tabular value of moisture-content capacity of the J-th point in material I. Similar input data setting is required for these parameters as for SPP(J,I,4).

7. NODAL COORDINATE

Two subsets of free-formatted data records are required if NSTRf = 0 and NSTRt = 0.

A. subset 1:

1.1. NNP = Number of nodes.

B. subset 2: nodal coordinates - Coordinates for NNP nodes are needed if KVI .LE. 0. Usually a total of NNP records (KVI records are required. However, if a group of subsequent nodes appear in a regular pattern, automatic generation can be made. Each record contains the following variables and is FREE-FORMATTED.

2.1. NI = Node number of the first node in the sequence.

2.2. NSEQ = NSEQ subsequent nodes will be automatically generated.

2.3. NAD = Increment of node number for each of the NSEQ subsequent nodes.

2.4. XNI = x-coordinate of node NI, (L).

2.5. YNI = y-coordinate of node NI, (L).

2.6. ZNI = z-coordinate of node NI, (L).

2.7. XAD = Increment of x-coordinate for each of the NSEQ subsequent nodes, (L).

2.8. YAD = Increment of y-coordinate for each of the NSEQ subsequent nodes, (L).

2.9. ZAD = Increment of z-coordinate for each of the NSEQ subsequent nodes, (L).

**** NOTE: A record with 9 0's must be used to signal the end of this data set.

8. SUBREGION DATA

This data set is required if either IPNTSf or IPNTSt is 0. Three subsets of free-formatted data records are required.

A. subset 1: One free format data record is needed for this sub-data-set.

1.1. NREGN = No. of subregions.

B. subset 2: No. of Nodes for each Subregion - Normally, NREGN records are required. However, if regular pattern appears, automatic generation can be made. Each record contains the 5 variables and is FREE-FORMATTED.

2.1. NK = Subregion number of the first subregion region in a sequence.

2.2. NSEQ = NSEQ subsequent subregions will have their no. of nodes automatically generated.

2.3. NKAD = Increment of NK in each of the NSEQ subsequent subregions.

2.4. NODES = No. of nodes for the subregion NK.

2.5. NOAD = Increment of NODES in each of the NSEQ subsequent subregions.

**** NOTE: A record with 5 0's must be used to end the input of this subdata set.

C. subset 3: Mapping between Global nodes and Subregion Nodes - This subdata set should be repeated NREGN times, one for each subregion. For each subregion, normally, LNNP records are needed. However, automatic generation can be made if subregional node number appears in regular pattern. Each record contains 5 variables and is FREE-FORMATTED.

3.1. LI = Local node number of the first node in a sequence.

3.2. NSEQ = NSEQ subsequent local nodes will be generated automatically.

3.3. LIAD = Increment of LI for each of the NSEQ subsequent nodes.

3.4. NI = Global node number of local node LI.

3.5. NIAD = Increment of NI for each of the NSEQ subsequent nodes.

**** NOTE: A record with 5 0's must be used to signal the end of this subdata set.

9. ELEMENT DATA

Two subsets of free-formatted data records are required for this data set.

A. subset 1:

1.1. NEL = Number of elements.

B. subset 2: Element incidence for NEL elements is needed if NSTRt = 0 and NSTRf = 0. Usually, a total of NEL records are needed. However, if a group of elements appear in a regular pattern, automatic generation is made. Each record contains the following variable and is FREE-FORMATTED.

2.1. MI = Global element number of the first element in a sequence.

2.2. NSEQ = NSEQ subsequent elements will be automatically generated.

2.3. MIAD = Increment of MI for each of the NSEQ subsequent elements.

2.4. IE(MI,1) = Global node number of the first node of element MI.

2.5. IE(MI,2) = Global node number of the second node of element MI.

2.6. IE(MI,3) = Global node number of the third node of element MI.

2.7. IE(MI,4) = Global node number of the fourth node of element MI.

2.8. IE(MI,5) = Global node number of the fifth node of element MI.

2.9. IE(MI,6) = Global node number of the sixth node of element MI.

2.10. IE(MI,7) = Global node number of the seventh node of element MI.

2.11. IE(MI,8) = Global node number of the eighth node of element MI.

2.12. IEMAD = Increment of IE(MI,1) through IE(MI,8) for each of the NSEQ elements.

**** Note: IE(MI,1) - IE(MI,8) are numbered according to the convention shown in following diagram. The first four nodes start from the front, lower, left corner and progress around the bottom element surface in a counterclockwise direction. The other four nodes begin from the front, upper, left corner and progress around the top element surface in a counterclockwise direction.

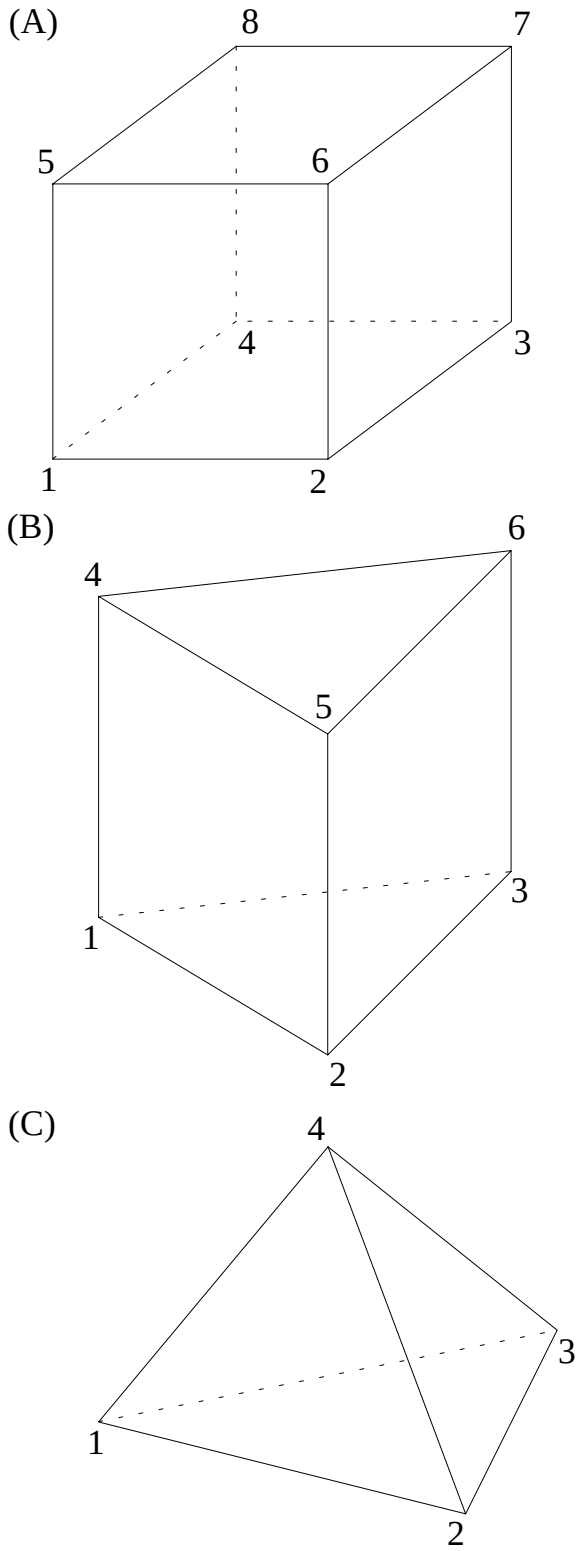

Figure A.1 Global Node Number Index of (A) a Hexahedral, (B) a Triangular Prism, and (C) a Tetrahedral Element.

10. MATERIAL TYPE CORRECTION

Two subsets of free-formatted data records are required for this data set.

A. subset 1:

1.1. NCM = Number of elements with material corrections.

B. subset 2: This set of data records is required only if NCM > 0. Normally, NCM records are required. However, if a group of elements appear in a regular pattern, automatic generation may be made. Each record contains the following variables.

2.1. MI = Global element number of the first element in the sequence.

2.2. NSEQ = NSEQ subsequent elements will be generated automatically.

2.3. MAD = Increment of element number for each of the NSEQ subsequent elements.

2.4. MITYP = Type of material correction for element MI.

2.5. MTYPAD = Increment of MITYP for each of the NSEQ subsequent elements.

**** NOTE: A line with 5 0's must be used to signal the end of this data set.

11. CARD INPUT FOR INITIAL OR PRE-INITIAL CONDITIONS

Two subsets of free-formatted data records are required for this data set, one for initial pressure head, the other for initial concentration. Generally, for each subset NNP record, one record for each node is needed. However, if a group of nodes appears in regular pattern, auto-generation is made.

A. subset 1: Initial pressure head -The first record contains one variable and each of subsequent records contains 6 variables. This subset is needed if IMOD = 10 or IMOD = 11.

1.1 IHTR = Is total head to be read as the initial condition? 0 = No, 1 = yes.

2.1. NI = Global node number of the first node in the sequence.

2.2. NSEQ = NSEQ subsequent nodes will be generated automatically.

2.3. NAD = Increment of node number for each of the NSEQ nodes.

2.4. HNI = Initial or pre-initial pressure head of node NI, (L).

2.5. HAD = Increment of initial or pre-initial head for each of the NSEQ nodes, (L).

2.6. HRD = 0.0.

**** NOTE: A line with 6 0's must be used to signal the end of this data set.

NOTE ON INITIAL CONDITIONS AND RESTARTING: The initial condition for a transient calculation may be obtained in two different ways: from card input, or steady-state calculation using time-invariant boundary conditions that are different from those for transient computation. In the latter case a card input of the pre-initial conditions is required as the zero-th order iterate of the steady-state solution.

NOTE ON STEADY-STATE INPUT: Steady-state option may be used to provide either the final state of a system under study or the initial conditions for a transient state calculation. In the former case KSSf = 0, KSSt = 0, and NTI = 0, and in the latter case KSSf = 0 or KSSt $\geq$ 0 and NTI > 0. If KSSf > 0, there will be no steady-state calculation for flow part.

B. subset 2: Initial concentration for microbe #1 - each record contains the following variables. This subset is needed if IMOD = 1 or IMOD = 11.

2.1. NI = Global node number of the first node in the sequence.

2.2. NSEQ = NSEQ subsequent nodes will be generated automatically.

2.3. NAD = Increment of node number for each of the NSEQ nodes.

2.4. CNI = Initial or pre-initial concentration of node NI, (M/L**3).

2.5. CAD = Increment of CNI for each of the NSEQ nodes, (M/L**3).

2.6. CRD = Geometrical increment of CNI for each of the NSEQ subsequent nodes.

**** NOTE: A record with 6 0's must be used to signal the end of this data set.

C. subset 3 ~ subset 8: Initial concentration for microbe #2, microbe #3, substrate, oxygen,nitrate, and nutrient, respectively. The input format is the same as subset 2.

NOTE ON INITIAL CONDITIONS: The initial condition for a transient calculation may be obtained in two different ways: from card input or steady-state calculation using time-invariant boundary conditions that are different from those for transient computation. In the latter case a card input of the pre-initial conditions is required as the zero-th order iterate of the steady-state solution.

NOTE ON STEADY-STATE INPUT: Steady-state option may be used to provide either the final state of a system under study or the initial conditions for a transient state calculation. In the former case KSSt = 0, KSSf $\geq$ and NTI = 0, and in the latter case KSSt = 0, KSSf $\geq$ and NTI > 0. If KSSt > 0, there will be no steady-state calculation for transport part.

12. ELEMENT (DISTRIBUTED) SOURCE/SINK FOR FLOW SIMULATIONS
This data set is needed if IMOD = 10 or IMOD = 11.
Four subsets of free-formatted data records are required in this data set.

A. subset 1: control parameters

1.1. NSEL = No. of source/sink elements.

1.2. NSPR = No. of source/sink profiles.

1.3. NSDP = No. of data points in each of the NSPR source/sink profiles.

1.4. KSAI = Is element-source/sink profile to be input analytically, 0 = no, 1 = yes.

B. subset 2: source/sink profiles - This group of data is needed if and only if NSEL .GT. 0. For each sub-data-record, NSDP of the data pair (TSOSF(J,I),SOSF(J,I)) are required. If this sub-data-record can be fitted in a line, NSPR lines are needed.

2.1. TSOSF(J,I) = Time of the J-th data point in the I-th profile, (T).

2.2. SOSF(1,I) = Source/sink value of the J-th data point in the I-th profile, (L**3/T/L**2/L).

C. subset 3: global source/sink element number - This group of data is needed if and only if NSEL .GT. 0. NSEL data points are required for this record.

3.1. MSEL(I) = Global element number of the I-th compressed distributed source/sink element.

D. subset 4: Source type assigned to each element - Usually one record per element. However, automatic generation can be made. For I-th (I = 1, 2, ...,) record, it contains the following.

4.1. MI = Global element number of the first element in the sequence.

4.2. NSEQ = NSEQ elements will be generated automatically.

4.3. MAD = Increment of element number for each of the NSEQ elements.

4.4. MITYP = Source type in element MI.

4.5. MTYPAD = Increment of MITYP for each of the NSEQ elements.

**** NOTE: A line with 5 0's is used to signal the end of this data set.

13. POINT (WELL) SOURCE/SINK DATA FOR FLOW SIMULATION
This data set is needed if IMOD = 10 or IMOD = 11.
Four subsets of free-formatted data records are required for this data set.

A. subset 1: control parameters

1.1. NWNP = No. of well or point source/sink nodal points.

1.2. NWPR = No. of well or point source/sink strength profiles.

1.3. NWDP = No. of data points in each of the NWPR profiles.

1.4. KWAI = Is well-source/sink profile to be input analytically, 0 = no, 1 = yes.

B. subset 2: source/sink profiles - This group of data is needed if and only if NWNP .GT. 0. For each sub-data-record, NWDP of the data pair (TWSSF(J,I),WSSF(J,I)) are required. If this sub-data-record can be fitted in a line, only NWPR lines are needed.

2.1. TWSSF(J,I) = Time of the J-th data point in the I-th profile, (T).

2.2. WSSF(J,I) = Source/sink value of the J-th data point in the I-th profile, (L**3/T/L).

C. Record 3: global source/sink nodal number - This group of data is needed if and only if NWNP .GT. 0. NWNP data points are required for this record.

3.1. NPW(I) = Global node number of the I-th compressed well source/sink node.

D. subset 4: Source type assigned to each well - Usually one record per well. However, automatic generation can be made. For I-th (I = 1, 2, ...,) record, it contains the following.

4.1. NI = Compressed well node number of the first node in the sequence.

4.2. NSEQ = NSEQ nodes will be generated automatically.

4.3. NAD = Increment of well node number for each of the NSEQ nodes.

4.4. NITYP = Source type in node NI.

4.5. NTYPAD = Increment of NITYP for each of the NSEQ nodes.

**** NOTE: A line with 5 0's is used to signal the end of this data set.

14. ELEMENT (DISTRIBUTED) SOURCE/SINK FOR TRANSPORT SIMULATIONS
This data set is needed if IMOD = 1 or IMOD = 11.

Ten subsets of free-formatted data records are required in this data set.

A. subset 1: control parameters

1.1. NSEL = No. of source/sink elements.

1.2. NSPR = No. of source profiles, should be .GE. 1.

1.3. NSDP = No. of data points in each profile, should be .GE. 2.

1.4. KSAI = Is element-source/sink profile to be input analytically? 0 = no, 1 = yes.

B. Subset 2: source/sink profile - This sub-data-set is needed if and only if NSEL .GT. 0. For each sub-data-record, NSDP of the data group (TSOSF(J,I), SOSF(J,I,1), SOSF(J,I,2)) are required. If this sub-data-record can be fitted in a line, only NSPR lines are needed.

2.1. TSOSF(J,I) = Time of J-th data point in I-th profile, (T).

2.2. SOSF(J,I,1) = Source/sink flow rate of the J-th data point in the I-th profile, (L**3/T/L**3); positive for source and negative for sink.

2.3. SOSF(J,I,2) = Source/sink concentration of the J-th data point in the I-th profile, (M/L**3).

C. subset 3: global source/sink element number. NSEL data points are required for this record.

3.1. LES(I) = Global element number of the I-th compressed distributed source/sink element.

D. subset 4: Source type assigned to each element for microbe # 1 - Usually one record per element. However, automatic generation can be made. For I-th (I = 1, 2, ...,) record, it contains the following.

4.1. MI = Global element number of the first element in the sequence.

4.2. NSEQ = NSEQ elements will be generated automatically.

4.3. MAD = Increment of element number for each of the NSEQ elements.

4.4. MITYP = Source type in element MI.

4.5. MTYPAD = Increment of MITYP for each of the NSEQ elements.

**** NOTE: A line with 5 0's is used to signal the end of this data set.

E. subset 5 ~ Subset 10: Source type assigned to each element for microbe #2, microbe #3, substrate, Oxygen, Nitrate, and nutrient. The input format is the same as subset 4.

15. POINT (WELL) SOURCE/SINK DATA FOR TRANSPORT SIMULATION
This data set is needed if IMOD = 1 or IMOD = 11.
Ten subsets of data records are required for this data set.

A. subset 1: control parameters

1.1. NWNP = No. of well or point source/sink nodes.

1.2. NWPR = No. of well or point source/sink strength profiles.

1.3. NWDP = No. of data points in each of the NWPR profiles.

1.4. KWAI = Is well-source/sink profile to be input analytically? 0 = no, 1 = yes.

B. subset 2: source/sink profiles - This group of data is needed if and only if NWNP .GT. 0. For each sub-data-record, NWDP of the data group (TWSSF(J,I), WSSF(J,I,1), WSSF(J,I,2)) are required. If this sub-data-record can be fitted in a line, only NWPR lines are needed.

2.1. TWSSF(J,I) = Time of J-th data point in I-th profile, (T).

2.2. WSSF(J,I,1) = Source/sink flow rate of the J-th data point in the I-th profile, (L**3/T/L**3); positive for source and negative for sink.

2.3. WSSF(J,I,2) = Source/sink concentration of the J-th data point in the I-th profile, (M/L**3).

C. subset 3: global source/sink element number - This group of data is needed if and only if NWNP .GT. 0. NWNP data points are required for this record.

3.1. NPW(I) = Global node number of the I-th compressed point source/sink node.

D. subset 4: Source type assigned to each well for microbe #1 - Usually one record per element. However, automatic generation can be made.

4.1. NI = Compressed point source/sink node number of the first node in a sequence.

4.2. NSEQ = NSEQ nodes will contain the source types that will be automatically generated.

4.3. NIAD = Increment of NI for each of the NSEQ nodes.

4.4. NITYP = Source type in node NI.

4.5. NTYPAD = Increment of NITYP for each of the NSEQ subsequent nodes.

**** NOTE: A record with 5 0's must be used to signal the end of this data set.

E. subset 5 ~ Subset 10: Source type assigned to each well for microbe #2, microbe #3, substrate, Oxygen, Nitrate, and nutrient. The input format is the same as subset 4.

16. RAINFALL/EVAPORATION-SEEPAGE BOUNDARY CONDITIONS
This data set is needed if IMOD = 10 or IMOD = 11.
Seven subsets of data records are required for this data set.

A. subset 1: control parameters

1.1. NVES = No. of variable boundary element sides.

1.2. NVNP = No. of variable boundary nodal points.

1.3. NVPR = No. of rainfall profiles.

1.4. NVDP = No. of rainfall data points in each of the NRPR rainfall profiles.

1.5. KVAI = Is rainfall profile to be input analytically? 0 = no, 1 = yes.

B. subset 2: boundary profiles - This subset is required only when NVES is not 0. NRPR profiles are needed. For each profile, NRDP of the data pair (TRF(J,I),RF(J,I)) are required. If these data pairs can fit in a line, only NRPR lines are needed.

2.1. TRF(J,I) = Time of the J-th data point in the I-th profile, (T).

2.2. RF(J,I) = Rainfall/evaporation rate of the J-th data point in the I-th profile, (L/T).

C. subset 3: boundary profile types assigned to each element. At most NVES records are needed. However, automatic generation can be made. For I-th (I = 1, 2, ...,) record, it contains the following variables.

3.1. MI = Compressed VB element side of the first side in the sequence.

3.2. NSEQ = NSEQ sides will be generated automatically.

3.3. MIAD = Increment of NI for each of the NSEQ sides.

3.4. MITYP = Type of rainfall/evaporation profiles assigned to side MI.

3.5. MTYPAD = Increment of MITYP for each of the NSEQ sides.

**** NOTE: A line with 5 0's is used to signal the end of this data set.

D. subset 4: Specification of Rainfall/evaporation-seepage sides. Normally, NVES records are required, one each for a variable boundary (VB) element side. However, if a group of rainfall/evaporation-seepage element sides appears in a regular pattern, automatic generation may be made. For I-th (I = 1, 2, ...,) record, it contains the following variables.

4.1. MI = Compressed VB element side number of the first element side in a sequence.

4.2. NSEQ = NSEQ subsequent VB element sides will be generated automatically.

4.3. MIAD = Increment of MI for each of the NSEQ subsequent VB element sides.

4.4. I1 = Global node number of the first node of element side MI.

4.5. I2 = Global node number of the second node of element side MI.

4.6. I3 = Global node number of the third node of element side MI.

4.7. I4 = Global node number of the fourth node of element side MI.

4.8. I1AD = Increment of I1 for each of the NSEQ subsequent VB element sides.

4.9. I2AD = Increment of I2 for each of the NSEQ subsequent VB element sides.

4.10. I3AD = Increment of I3 for each of the NSEQ subsequent VB element sides.

4.11. I4AD = Increment of I4 for each of the NSEQ subsequent VB element sides.

**** NOTE: A blank with 11 0's must be used to signal the end of this subdata set.

E. subset 5: Global Node Number of All Compressed Variable Boundary (VB) Nodes. At most, NVNP records are needed for this subset, one each for NVNP variable boundary nodes. For I-th (I = 1, 2, ...,) Record, it contains the following 5 variables.

5.1. NI = Compressed VB node number of the first node in the sequence.

5.2. NSEQ = NSEQ nodes will be generated automatically.

5.3. NIAD = Increment of NI for each of the NSEQ nodes.

5.4. NODE = Global node number of node NI.

5.5. NODEAD = Increment of NODE for each of the NSEQ nodes.

**** NOTE: A line with 5 0's is used to signal the end of this data set.

F. subset 6: Ponding Depth Allowed in Each of NVNP Variable Boundary Nodes. Normally, NVNP records are needed, one for each of the NVNP nodes. However, if a group of nodes has a regular pattern of ponding depth, automatic generation is made. For I-th (I = 1, 2, ...,) record, it contains the following variables.

6.1. NI = Compressed VB node number of the first node in a sequence.

6.2. NSEQ = NSEQ subsequent nodes will be generated automatically.

6.3. NIAD = Increment of NI for each of the NSEQ subsequent nodes.

6.4. HCONNI = Ponding depth of node NI, (L).

6.5. HCONAD = Increment of HCONNI for each of the NSEQ nodes, (L).

6.6. 0.0

**** NOTE: A line with 6 0's must be used to signal the end of this data set.

G. subset 7: Minimum Pressure Head Allowed in Each NVNP Variable Boundary Nodes. This subset is read-in similar to the above subset. For I-th (I = 1, 2, ...,) record, it contains the following variables.

7.1. NI = Compressed VB node number of the first node in a sequence.

7.2. NSEQ = NSEQ subsequent nodes will be generated automatically.

7.3. NIAD = Increment of NI for each of the NSEQ subsequent nodes.

7.4. HMINNI = Minimum pressure head allow for node NI, (L).

7.5. HMINAD = Increment of HMINNI for each of the NSEQ nodes, (L).

7.6. 0.0

**** NOTE: A line with 6 0's must be used to signal the end of this data set.

17. DIRICHLET BOUNDARY CONDITIONS FOR FLOW SIMULATION
This data set is needed if IMOD = 10 or IMOD = 11.
Four subsets of data records are required for this data set.

A. subset 1: control parameters

1.1. NDNP = No. of Dirichlet nodal points, should be .GE. 1.

1.2. NDPR = No. of total Dirichlet-head profiles, should be .GE. 1.

1.3. NDDP = No. of data points in each total head profiles, should be .GE. 1.

1.4. KDAI = Is Dirichlet boundary value profile to be input analytically? 0= no, 1= yes.

B. subset 2: Dirichlet-head profiles - This subset is required only if NDNP is not 0. NDPR of profiles are needed. For each profile, NDDP of the data pair (THDBF(J,I),HDBF(J,I)) are needed. If these data pairs can fit in a line, only NDPR lines are needed.

2.1. THDBF(J,I) = Time of the J-th data point in the I-th profile, (T).

2.2. HDBF(J,I) = Total head of the J-th data point in the I-th profile, (L).

C. subset 3: Dirichlet nodes - At most, NDNP records are needed for this subset, one each for NDNP Dirichlet boundary nodes. However, if the Dirichlet nodes appear in a regular pattern, automatic generation may be made. For I-th (I = 1, 2, ...,) Record, it contains the following 5 variables.

3.1. NI = Compressed DB node number of the first node in the sequence.

3.2. NSEQ = NSEQ nodes will be generated automatically.

3.3. NIAD = Increment of NI for each of the NSEQ nodes.

3.4. NODE = Global node number of node NI.

3.5. NODEAD = Increment of NODE for each of the NSEQ nodes.

**** NOTE: A line with 5 0's is used to signal the end of this data set.

D. subset 4: boundary profile type assign to each Dirichlet node - Normally one record per Dirichlet node; i.e., a total of NDNP records. However, if the Dirichlet nodes appear in regular pattern, automatic generation may be made. For I-th (I = 1, 2, ...,) record, it contains the following variables.

4.1. NI = Compressed Dirichlet node number of the first node in the sequence.

4.2. NSEQ = NSEQ subsequent Dirichlet nodes will be generated automatically.

4.3. NAD = Increment of NI for each of the NSEQ nodes.

4.4. NITYP = Type of total head profile for node NI and NSEQ subsequent nodes.

4.5. NTYPAD = Increment of NITYP for each of the NSEQ subsequent nodes.

**** NOTE: A line with 5 0's must be used to signal the end of this data set.

18. CAUCHY BOUNDARY CONDITIONS FOR FLOW SIMULATIONS
This data set is needed if IMOD = 10 or IMOD = 11.
Five subsets of data records are required for this data set.

A. subset 1: control parameters

1.1. NCES = No. of Cauchy boundary element sides.

1.2. NCNP = No. of Cauchy nodal points.

1.3. NCPR = No. of Cauchy-flux profiles.

1.4. NCDP = No. of data points in each of the NCPR Cauchy-flux profiles.

1.5. KCAI = Is Cauchy flux profile to be input analytically? 0 = no, 1 = yes.

B. subset 2: prescribed Cauchy-flux profiles - This set is required only if NCES is not 0. NCPR of profiles are needed. For each profile, NCDP of the data pair (TQCBF(J,I),QCBF(J,I)) are needed. If these data pairs can fit in a line, only NDPR lines are needed.

2.1. TQCBF(J,I) = Time of the J-th data point in the I-th profile, (T).

2.2. QCBF(J,I) = Normal Cauchy flux of the J-th data point in the I-th profile, (L**3/T/L**2); positive out from the region, negative into the region.

C. subset 3: type of Cauchy flux profiles assigned to each of all NCES sides. At most NCES records are needed. However, automatic generation can be made. For I-th (I = 1, 2, ...,) record, it contains the following variables.

3.1. MI = Compressed Cauchy side number of the first side in the sequence.

3.2. NSEQ = NSEQ sides will be generated automatically.

3.3. MIAD = Increment of MI for each of the NSEQ sides.

3.4. MITYP = Type of Cauchy flux profile assigned to side MI.

3.5. MTYPAD = Increment of MITYP for each of the NSEQ sides.

**** NOTE: A line with 5 0's is used to signal the end of this data set.

D. subset 4: Cauchy boundary element sides - Normally, NCES records are required, one each for a Cauchy boundary element side. However, if a group of Cauchy boundary element sides appears in a regular pattern, automatic generation may be made. For I-th (I = 1, 2, ...,) record, it contains the following variables.

4.1. MI = Compressed Cauchy element side number of the first element-side in a sequence.

4.2. NSEQ = NSEQ subsequent Cauchy element-sides will be generated automatically.

4.3. MIAD = Increment of MI for each of the NSEQ subsequent sides.

4.4. I1 = Global node number of the first node on the Cauchy element-side MI.

4.5. I2 = Global node number of the second node on the Cauchy element-side MI.

4.6. I3 = Global node number of the third node on the Cauchy element-side MI.

4.7. I4 = Global node number of the fourth node on the Cauchy element-side MI.

4.8. I1AD = Increment of I1 for each of the NSEQ subsequent element-sides.

4.9. I2AD = Increment of I2 for each of the NSEQ subsequent element-sides.

4.10. I3AD = Increment of I3 for each of the NSEQ subsequent element-sides.

4.11. I4AD = Increment of I4 for each of the NSEQ subsequent element-sides.

**** NOTE: A line with 11 0's is used to end this data set input.

E. subset 5: global node number of all compressed Cauchy nodes - Normally one record per compressed Cauchy node; i.e., a total of NCNP records. However, if the Cauchy nodes appear in a regular pattern, automatic generation may be made. For I-th (I = 1, 2, ...,) record, it contains the following variables.

5.1. NI = Compressed Cauchy node number of the first node in the sequence.

5.2. NSEQ = NSEQ subsequent Cauchy nodes will be generated automatically.

5.3. NAD = Increment of NI for each of the NSEQ nodes.

5.4. NODE = Global node number for node NI and NSEQ subsequent nodes.

5.5. NODEAD = Increment of NODE for each of the NSEQ subsequent nodes.

**** NOTE: A line with 5 0's must be used to signal the end of this sub-data set.

19. NEUMANN BOUNDARY CONDITIONS FOR FLOW SIMULATIONS
This data set is needed if IMOD = 10 or IMOD = 11.
Five subsets of data records are required for this data set.

A. subset 1: control parameters

1.1. NNES = No. of Neumann boundary element sides.

1.2. NNNP = No. of Neumann nodal points.

1.3. NNPR = No. of Neumann flux profiles.

1.4. NNDP = No. of data points in each of the NNPR Neumann-flux profiles.

1.5. KNAI = Is Neumann flux profile to be input analytically; 0 = no, 1 = yes.

B. subset 2: prescribed Neumann-flux profiles - This sub-data-set is required only if NNES is not 0. NNPR of profiles are needed. For each profile, NNDP of the data pair (TQNBF(J,I),QNBF(J,I)) are needed. If these data pairs can fit in a line, only NDPR lines are needed.

2.1. TQNBF(J,I) = Time of the J-th data point in the I-th profile, (T).

2.2. QNBF(J,I) = Normal Neumann flux of the J-th data point in the I-th profile, (L**3/T/ L**2); positive out from the region, negative into the region.

C. subset 3: type of Neumann flux profiles assigned to each of all NNES sides. At most NNES records are needed. However, automatic generation can be made. For I-th (I = 1, 2, ...,) record, it contains the following variables.

3.1. MI = Compressed Neumann side number of the first side in the sequence.

3.2. NSEQ = NSEQ sides will be generated automatically.

3.3. MIAD = Increment of MI for each of the NSEQ sides.

3.4. MITYP = Type of Neumann flux profile assigned to side MI.

3.5. MTYPAD = Increment of MITYP for each of the NSEQ sides.

**** NOTE: A line with 5 0's is used to signal the end of this data set.

D. subset 4: Neumann boundary element sides - Normally, NNES records are required, one each for a Neumann boundary element side. However, if a group of Neumann boundary element sides appears in a regular pattern, automatic generation may be made. For I-th (I = 1, 2, ...,) record, it contains the following variables.

4.1. MI = Compressed Neumann side number of the first side in sequence.

4.2. NSEQ = NSEQ subsequent Neumann sides will be generated automatically.

4.3. MIAD = Increment of MI for each of the NSEQ subsequent sides.

4.4. I1 = Global node number of the first node on the Neumann element-side MI.

4.5. I2 = Global node number of the second node on Neumann element-side MI.

4.6. I3 = Global node number of the third node on the Neumann element-side MI.

4.7. I4 = Global node number of the fourth node on the Neumann element-side MI.

4.8. I1AD = Increment of I1 for each of the NSEQ subsequent element-sides.

4.9. I2AD = Increment of I2 for each of the NSEQ subsequent element-sides.

4.10. I3AD = Increment of I3 for each of the NSEQ subsequent element-sides.

4.11. I4AD = Increment of I4 for each of the NSEQ subsequent element-sides.

**** NOTE: A line with 11 0's is used to end this data set input.

E. subset 5: global node number of all compressed Neumann nodes - Normally one record per compressed Neumann node; i.e., a total of NNNP records. However, if the Neumann nodes appear in a regular pattern, automatic generation may be made. For I-th (I = 1, 2, ...,) record, it contains the following variables.

5.1. NI = Compressed Neumann node number of the first node in the sequence.

5.2. NSEQ = NSEQ subsequent Neumann nodes will be generated automatically.

5.3. NAD = Increment of NI for each of the NSEQ nodes.

5.4. NITYP = Type of total head profile for node NI and NSEQ subsequent nodes.

5.5. NTYPAD = Increment of NITYP for each of the NSEQ subsequent nodes.

**** NOTE: A line with 5 0's must be used to signal the end of this data set.

20. RUN-IN/FLOW-OUT (VARIABLE) BOUNDARY CONDITIONS FOR TRANSPORT SIMULATIONS

This data set is needed if IMOD = 1 or IMOD = 11.
Eleven subsets of data records are required for this data set.

A. subset 1: control parameters

1.1. NVES = No. of variable boundary element sides.

1.2. NVNP = No. of variable boundary nodal points.

1.3. NVPR = No. of incoming fluid concentration profiles to be applied to variable boundary element sides.

1.4. NVDP = No. of data points in each of the NRPR profiles.

1.5. KVAI = Is incoming concentration profile to be input analytically? 0 = no, 1 = yes.

B. subset 2: variable boundary flux profile - NRPR records are needed. Each record contains NRDP data points and is FREE-FORMATTED. Each data point has 2 numbers representing the time and run-in flow-out concentrations, respectively as follows:

2.1. TCVSF(J,I) = Time of the J-th data point on the I-th run-in concentration profile, (T).

2.2. CVSF(J,I) = Concentration of the J-th data point on the I-th profile, (M/L**3).

C. subset 3: Run-in concentration type assigned to each of all NVES sides for microbe #1. Usually one record per variable element side. However, automatic generation can be made. Each record contains 5 variables and is FREE-FORMATTED.

3.1. MI = Compressed VB element side of the first side in a sequence.

3.2. NSEQ = NSEQ subsequent sides will be generated automatically.

3.3. MIAD = Increment of MI for each of NSEQ subsequent sides.

3.4. MITYP = Type of concentration profile assigned to side MI.

3.5. MTYPAD = Increment of MITYP for each of the NSEQ subsequent sides.

**** NOTE: A record with 5 0's must be used to signal the end of this data set.

D. subset 4 ~ Subset 9: Run-in concentration type assigned to each element for microbe #2, microbe #3, substrate, Oxygen, Nitrate, and nutrient. The input format is the same as subset 4.

J. subset 10: Specification of run-in boundary element sides - Normally, NVES records are required, one each for a VB element side. However, if a group of VB element sides appears in a regular pattern, automatic generation may be made. Each record contains 11 variables and is FREE-FORMATTED.

10.1. MI = Compressed VB element side number of the first side in a sequence.

10.2. NSEQ = NSEQ subsequent VB element sides will be generated automatically.

10.3. MIAD = Increment of MI for each of the NSEQ subsequent Vb element sides.

10.4. I1 = Global node number of the first node of element side MI.

10.5. I2 = Global node number of the second node of element side MI.

10.6. I3 = Global node number of the third node of element side MI.

10.7. I4 = Global node number of the fourth node of element side MI .

10.8. I1AD = Increment of I1 for each of the NSEQ subsequent element sides.

10.9. I2AD = Increment of I2 for each of the NSEQ subsequent element sides.

10.10. I3AD = Increment of I3 for each of the NSEQ subsequent element sides.

10.11. I4AD = Increment of I4 for each of the NSEQ subsequent element sides.

**** NOTE: A record with 11 0's is used to signal the end of this data set.

K. subset 11: global nodal number of all run-in flow-out boundary nodes. Usually NVNP records are needed for this subdata set. However, automatic generation can be made. Each record contains 5 variables and is FREE-FORMATTED.

11.1. NI = Compressed VB node number of the first node in a sequence.

11.2. NSEQ = NSEQ subsequent nodes will be generated automatically.

11.3. NIAD = Increment for NI for each of the NSEQ nodes.

11.4. NODE = Global nodal number of the node NI.

11.5. NODEAD = Increment of NODE for each of the NSEQ subsequent nodes.

**** NOTE: A record with 5 0's is used to signal end of this data set.

21. DIRICHLET BOUNDARY CONDITIONS FOR TRANSPORT SIMULATIONS
This data set is needed if IMOD = 1 or IMOD = 11.
Ten subsets of data records are required for this data set.

A. subset 1: control parameters

1.1. NDNP = No. of Dirichlet nodes, should be .GE. 1.

1.2. NDPR = No. of Dirichlet profiles, should be .GE. 1.

1.3. NDDP = No. of data points in each profile, should be .GE. 2.

1.4. KDAI = Is Dirichlet boundary value profile to be input analytically? 0 = no, 1 = yes.

B. subset 2: Dirichlet-concentration profiles - NDPR records are needed. Each record contains NDDP data points and is FREE-FORMATTED. Each data point has 2 numbers representing the time and Dirichlet concentrations, respectively as follows:

2.1. TCDBF(J,I) = Time of J-th data point in I-th Dirichlet-concentration profile, (T).

2.2. CDBF(J,I) = Concentration of J-th data point in I-th Dirichlet-concentration profile, (M/L**3).

C. subset 3: global node number of compressed Dirichlet nodes - Usually NDNP records are needed for this subdata set. However, automatic generation can be made. Each record contains 5 variables and is FREE-FORMATTED.

3.1. NI = Compressed Dirichlet boundary node number of the first node in a sequence.

3.2. NSEQ = NSEQ subsequent nodes will be generated automatically.

3.3. NIAD = Increment for NI for each of the NSEQ nodes.

3.4. NODE = Global nodal number of the node NI.

3.5. NODEAD = Increment of the global nodal number for each of the NSEQ subsequent nodes.

**** NOTE: A record with 5 0's is used to signal end of this data set.

D. subset 4: Dirichlet concentration types assigned to Dirichlet nodes for microbe #1. Normally one record per Dirichlet node; i.e., a total of NDNP records, is needed. However, if the

Dirichlet nodes appear in a regular pattern, automatic generation may be made. Each record contains 5 variables and is FREE-FORMATTED.

4.1. NI = Compressed Dirichlet node number of the first node in the sequence.

4.2. NSEQ = NSEQ nodes will contain the Dirichlet concentration types that will be automatically generated.

4.3. NIAD = Increment of NI for each of the NSEQ nodes.

4.4. NITYP = Dirichlet concentration type in node NI.

4.5. NTYPAD = Increment of NITYP for each of the NSEQ subsequent nodes.

**** NOTE: A record with 5 0's must be used to signal the end of this data set.

E. subset 5 ~ Subset 10: Dirichlet concentration type assigned to each node for microbe #2, microbe #3, substrate, Oxygen, Nitrate, and nutrient. The input format is the same as subset 4.

22. CAUCHY BOUNDARY CONDITIONS FOR TRANSPORT SIMULATION
This data set is needed if IMOD = 1 or IMOD = 11.
Eleven subsets of data records are required for this data set.

A. subset 1: control parameters

1.1. NCES = No. of Cauchy element sides.

1.2. NCNP = No. of Cauchy nodal points.

1.3. NCPR = No. of Cauchy-flux profiles.

1.4. NCDP = No. of data points on each Cauchy-flux profile.

1.5. KCAI = Is Cauchy flux profile to be input analytically? 0 = no, 1 = yes.

B. subset 2: Cauchy flux profiles - NCPR records are needed. Each record contains NCDP data points and is FREE-FORMATTED. Each data point has 2 numbers representing the time and Cauchy flux, respectively as follows:

2.1. TQCBF(J,I) = Time of the J-th data point in the I-th Cauchy flux profile, (T).

2.2. QCBF(J,I) = Value of Cauchy flux of the J-th data point in the I-th Cauchy-flux profile, (M/T/L**2).

C. subset 3: Cauchy flux type assigned to each of all NCES sides for microbe #1 - Usually one record per Cauchy element side. However, automatic generation can be made. Each record contains 5 variables and is FREE-FORMATTED.

3.1. MI = Compressed Cauchy boundary element side of the first side in a sequence.

3.2. NSEQ = NSEQ subsequent sides will be generated automatically.

3.3. MIAD = Increment of MI for each of NSEQ subsequent sides.

3.4. MITYP = Type of Cauchy flux profile assigned to side MI.

3.5. MTYPAD = Increment of MITYP for each of the NSEQ subsequent sides.

**** NOTE: A record with 5 0's must be used to signal the end of this data set.

D. subset 4 ~ Subset 9: Cauchy flux type assigned to each element for microbe #2, microbe #3, substrate, Oxygen, Nitrate, and nutrient. The input format is the same as subset 4.

J. Subset 10: specification of Cauchy boundary element sides -Normally, NCES records are required, one each for a Cauchy boundary element side. However, if a group of Cauchy element sides appears in a regular pattern, automatic generation may be made. Each record contains 11 variable and is FREE-FORMATTED.

10.1. MI = Compressed Cauchy boundary element side number of the first element side in a sequence.

10.2. NSEQ = NSEQ subsequent Cauchy boundary element sides will be generated automatically.

10.3. MIAD = Increment of MI for each of the NSEQ subsequent Cauchy boundary element sides.

10.4. I1 = Global node number of the first node of element side MI.

10.5. I2 = Global node number of the second node of element side MI.

10.6. I3 = Global node number of the third node of element side MI.

10.7. I4 = Global node number of the fourth node of element side MI

10.8. I1AD = Increment of I1 for each of the NSEQ subsequent element sides.

10.9. I2AD = Increment of I2 for each of the NSEQ subsequent element sides.

10.10. I3AD = Increment of I3 for each of the NSEQ subsequent element sides.

10.11. I4AD = Increment of I4 for each of the NSEQ subsequent element sides.

**** NOTE: A record with 11 0's is used to signal the end of this data set.

K. subset 11: global nodal number of all Cauchy boundary nodes - Usually NCNP records are needed for this subdata set. However, automatic generation can be made. Each record contains 5 variables and is FREE-FORMATTED.

11.1. NI = Compressed Cauchy boundary node number of the first node in a sequence.

11.2. NSEQ = NSEQ subsequent nodes will be generated automatically.

11.3. NIAD = Increment for NI for each of the NSEQ nodes.

11.4. NODE = Global nodal number of the node NI.

11.5. NODEAD = Increment of the global nodal number for each of the NSEQ subsequent nodes.

**** NOTE: A record with 5 0's is used to signal end of this data set.

23. NEUMANN BOUNDARY CONDITIONS FOR TRANSPORT SIMULATIONS
This data set is needed if IMOD = 1 or IMOD = 11.
Eleven subsets of data records are required for this data set.

A. subset 1: control parameters

1.1. NNES = No. of Neumann element sides.

1.2. NNNP = No. of Neumann nodal points.

1.3. NNPR = No. of Neumann-flux profiles.

1.4. NNDP = No. of data points on each Neumann-flux profile.

1.5. KNAI = Is Neumann flux profile to be input analytically? 0 = no, 1 = yes.

B. subset 2: Neumann flux profiles - NNPR records are needed. Each record contains NNDP data points and is FREE-FORMATTED. Each data point has 2 numbers representing the time and Neumann flux, respectively, as follows:

2.1. TQNBF(J,I) = Time of the J-th data point in the I-th Neumann flux profile, (T).

2.2. QNBF(J,I) = Value of Neumann flux of the J-th data point in the I-th Neumann-flux profile, (M/T/L**2).

C. subset 3: Neumann flux type assigned to each of all NNES sides for microbe #1 - Usually one record per Neumann element side. However, automatic generation can be made. Each record contains 5 variables and is FREE-FORMATTED.

3.1. MI = Compressed Neumann boundary element side of the first side in a sequence.

3.2. NSEQ = NSEQ subsequent sides will be generated automatically.

3.3. MIAD = Increment of MI for each of NSEQ subsequent sides.

3.4. MITYP = Type of Neumann flux profile assigned to side MI.

3.5. MTYPAD = Increment of MITYP for each of the NSEQ subsequent sides.

**** NOTE: A record with 5 0's must be used to signal the end of this data set.

D. subset 4 ~ Subset 9: Neumann flux type assigned to each element for microbe #2, microbe #3, substrate, Oxygen, Nitrate, and nutrient. The input format is the same as subset 4.

J. subset 10: specification of Neumann boundary element sides -Normally, NNES records are required, one each for a Neumann boundary element side. However, if a group of Neumann element sides appears in a regular pattern, automatic generation may be made. Each record contains 11 variables and is FREE-FORMATTED.

10.1. MI = Compressed Neumann boundary element side number of the first element side in a sequence.

10.2. NSEQ = NSEQ subsequent Neumann boundary element sides will be generated automatically.

10.3. MIAD = Increment of MI for each of the NSEQ subsequent sides.

10.4. I1 = Global node number of the first node of element side MI.

10.5. I2 = Global node number of the second node of element side MI.

10.6. I3 = Global node number of the third node of element side MI.

10.7. I4 = Global node number of the fourth node of element side MI.

10.8. I1AD = Increment of I1 for each of the NSEQ subsequent element sides.

10.9. I2AD = Increment of I2 for each of the NSEQ subsequent element sides.

10.10. I3AD = Increment of I3 for each of the NSEQ subsequent element sides.

10.11. I4AD = Increment of I4 for each of the NSEQ subsequent element sides.

**** NOTE: A record with 11 0's is used to signal the end of this data set.

K. subset 11: global nodal number of all Neumann boundary nodes - Usually NNNP records are needed for this subdata set. However, automatic generation can be made. Each record contains 5 variables and is FREE-FORMATTED.

11.1. NI = Compressed Neumann boundary node number of the first node in a sequence.

11.2. NSEQ = NSEQ subsequent nodes will be generated automatically.

11.3. NIAD = Increment for NI for each of the NSEQ nodes.

11.4. NODE = Global nodal number of the node NI.

11.5. NODEAD = Increment of the global nodal number for each of the NSEQ subsequent nodes.

**** NOTE: A record with 5 0's is used to signal end of this data set.

24. PARAMETERS CONTROLLING TRACKING SCHEME
Two subdata sets are needed if IMOD $\neq$ 10.

A. subset 1: Thirteen integers are typed by free format.

1.1. IZOOM = Is zooming needed for advection computation? 0 = No, 1 = Yes.

1.2. IDZOOM = Is zooming needed for dispersion computation? 0 = No, 1 = Yes.

1.3. IEPC = Is EPCOF scheme included? 0 = No, 1 = Yes. Note: 0 for this version.

1.4. NXA = No. of regularly refined subelements for the advection step in the X-direction in an element.

1.5. NYA = No. of regularly refined subelements for the advection step in the Y-direction in an element.

1.6. NZA = No. of regularly refined subelements for the advection step in the Z-direction in an element.

1.7. NXW = The number of subelements in each global element for element tracking in x-direction.

1.8. NYW = The number of subelements in each global element for element tracking in y-direction.

1.9. NZW = The number of subelements in each global element for element tracking in z-direction.

1.10. NXD = No. of dispersion fine subelements in each global element in X-direction.

1.11. NYD = No. of dispersion fine subelements in each global element in Y-direction.

1.12. NZD = No. of dispersion fine subelements in each global element in Z-direction.

1.13. IDETQ = Index of particle tracking pattern:
1 = Average velocity is used (more accurate);
2 = Single velocity of the starting point is used (less computation).

B. Subset 2: It reads the following 2 variables (FREE FORMAT)

2.1. ADPEPS = Error tolerance of relative concentration and nonlinear convergence criteria.

2.2. ADPARM = Error tolerance of concentration relative to maximum concentration.

25. HYDROLOGICAL VARIABLES

This data set is needed if and only if KVI .LE. 0. When KVI .LE. 0, two groups of data are needed, one group for the velocity field and the other group for the moisture content.

A. subset 1: velocity field - Usually NNP records are needed. However, if velocity appears in regular pattern, automatic generation can be made. Each record contains 9 variables and is FREE-FORMATTED.

1.1. NI = Node number of the first node in a sequence.

1.2. NSEQ = NSEQ subsequent nodes will be automatically generated.

1.3. NIAD = Increment of node number in each of the NSEQ subsequent nodes.

1.4. VXNI = x-velocity component at node NI, (L/T).

1.5. VYNI = y-velocity component at node NI, (L/T).

1.6. VZNI = z-velocity component at node NI, (L/T).

1.7. VXAD = Increment of VXNI for each of the NSEQ subsequent nodes, (L/T).

1.8. VYAD = Increment of VYNI for each of the NSEQ subsequent nodes, (L/T).

1.9. VZAD = Increment of VZNI for each of the NSEQ subsequent nodes, (L/T).

**** NOTE: A record with 9 0's is used to signal the end of this data set.

B. subset 2: moisture content field - Usually, NEL records are needed. However, if moisture content appears in regular pattern, automatic generation can be made. Each record contains 5 variables and is FREE-FORMATTED.

2.1. MI = Element number of the first element in a sequence.

2.2. NSEQ = NSEQ subsequent elements will be automatically generated.

2.3. MIAD = Increment of MI for each of NSEQ subsequent elements.

2.4. THNI = Moisture content of element NI, (Decimal point).

2.5. THNIAD = Increment of THNI for NSEQ subsequent elements, (Decimal point).

2.6. 0.0

**** NOTE: A record with 6 0's is used to signal the end of this data set.

26. END OF JOB

If another problem is to be run, then input begins again with input data set 1. If termination of the job is desired, a blank card must be inserted at the end of the data set.

APPENDIX B: Mathematical Formulation

B.1 Governing Equations for Flow

From the notion for continuity of fluid, continuity of solid, consolidation of the media, and the equation of state (Yeh, 1992), one obtains the starting equation for this derivation:

$$\nabla\cdot\left[\frac{\rho\mathbf{k}}{\mu}\cdot(\nabla p + \rho g\nabla z)\right] - \nabla\cdot(\rho n_e S\mathbf{V_s}) + \rho^* q = \frac{\partial(n_e S\rho)}{\partial t} \qquad \text{(B.1.1)}$$

where ρ is the fluid density (M/L^3), $\mathbf{k}$ is the intrinsic permeability tensor of the media (L^2), μ is the dynamic viscosity of the fluid (M/L/T), p is the fluid pressure [$(ML/T^2)/L^2$], g is the acceleration of gravity (L/T^2), z is the potential head (L), n_e is the effective porosity (L^3/L^3), S is the degree of saturation (dimensionless), $\mathbf{V}_s$ is the velocity of the deformable surface due to consolidation (L/T), ρ^* is the density of the injected fluid (M/L^3), q is the internal source/sink [$(L^3/T)/L^3$], and t is the time (T).

Expanding the right hand side of Eq.(B.1.1):

$$\frac{\partial(n_e S\rho)}{\partial t} = Sn_e\frac{\partial\rho}{\partial t} + \rho S\frac{\partial n_e}{\partial t} + n_e\rho\frac{\partial S}{\partial t} \qquad \text{(B.1.2)}$$

Expanding Eq.(B.1.2) by the chain rule:

$$\frac{\partial(n_e S\rho)}{\partial t} = Sn_e\frac{\partial\rho}{\partial p}\frac{\partial p}{\partial t} + Sn_e\frac{\partial\rho}{\partial C}\frac{\partial C}{\partial t} + \rho S\frac{\partial n_e}{\partial t} + n_e\rho\frac{\partial S}{\partial t} \qquad \text{(B.1.3)}$$

where C is chemical concentration (M/L^3). Rearranging Eq.(B.1.3), one obtains:

$$\frac{\partial(n_e S\rho)}{\partial t} = Sn_e\frac{\partial\rho}{\partial p}\frac{\partial p}{\partial t} + \rho S\frac{\partial n_e}{\partial t} + Sn_e\frac{\partial\rho}{\partial C}\frac{\partial C}{\partial t} + n_e\rho\frac{\partial S}{\partial t} \qquad \text{(B.1.4)}$$

where the first and second terms represent the storativity term, the third term is the density-concentration coupling term, and the fourth term is the unsaturated term. Substituting Eq.(B.1.4) into Eq.(B.1.1):

APPENDIX C

The determination of Maximum Control Parameters for LEZOOMPC implementation

The example shown in this section is Example 6 with 510 global nodes and 224 hexahedral elements. According to the input data file, the number of refined subelements in each global element is NXA=NXW=2, NYA=NYW=1, NZA=NZW=2 in the Lagrangian step and NXD=2, NYD=1, NZD=2 in the Eulerian step. Consider NX, NY, and NZ to represent the above values for both Lagrangian and Eulerian steps. Hence, there are NX*NY*NZ, NX*NX*NZ, and NX*NX*NX regular refined subelements in each hexahedral global element, triangular prism global element, and tetrahedral global element, respectively. The number of regular fine grids is (NX+1)*(NY+1)*(NZ+1), $\frac{1}{2}(NX+1)*(NX+2)*(NZ+1)$, and $\frac{1}{6}(NX+1)*(NX+2)*(NX+3)$ for each hexahedral, triangular prism, and tetrahedral global element, respectively. During the simulation, 54 rough elements are assumed to be zoomed. Therefore, there are 54×(NX+1)×(NY+1)×(NZ+1) regular fine grids and 54×NX×NY×NZ regular subelements in the region of interest. The assumption that 340 peak and valley points in the associated subelements are captured increases the total fine grids to 54×(NX+1)×(NY+1)×(NZ+1)+340. Because NCC components is included in the system, MXNPFGK is equal to NCC×[54×(NX+1)×(NY+1)×(NZ+1)+340)]. Then, 2200 additional subelements are assumed to be generated after tetrangulating the captured peak and valley points and MXKGLK is assigned to 54×NX×NY×NZ+2200. The working array declaration of MXNPWK and MXELWK are 18 and 4, respectively, for particle tracking computation. If there are injection/extraction wells in the region of interest, then MXNPWS=(NXA+1)×(NYA+1)×(NZA+1)=18 and MXELWS=NXA×NYA×NZA=4. For the Eulerian step, the calculation of diffusion fine grids and of refined subelements is dependent on the number of extended rough elements which can be predicted from the number of rough elements in the Lagrangian step. In total, 79 extended rough elements are assumed in this case. Because each rough element is refined by 2 (NXD) x 2 (NYD) x 1 (NZD) = 4 subelements, the total number

Appendix D: Nomenclatures

t = time (T)

x, y, z = the coordinate in the x-, y-, and z-directions in the region of interest (L)

x_b, y_b, z_b = the x, y, z on the boundary of the region of interest (L)

R = region of interest

B = boundary of the region of interest

$\mathbf{n}$ = outward unit normal vector

h = the referenced pressure head defined as $p/\rho_w g$

p = pressure (M/LT^2)

K = hydraulic conductivity tensor (L/T)

$\mathbf{K_s}$ = the saturated hydraulic conductivity tensor (L/T)

K_r = the relative hydraulic conductivity or relative permeability

z = the potential head (L)

q = flow rate of the source and/or sink (L^3/T)

θ = the moisture content

ρ = density of the fluid (M/L^3)

μ = dynamic viscosity (M/LT)

$\mathbf{K_{sw}}$ = referenced saturated hydraulic conductivity tensor (L/T)

ρ_w = referenced density of the fluid (M/L^3),

μ_w = referenced dynamic viscosity (M/LT)

ρ^* = density of the injected fluid (M/L^3)

$\mathbf{V}$ = Darcy flux (L/T)

h_i = prescribed initial pressure head (L)

h_d = prescribed Dirichlet pressure head (L)

q_n = Neumann flux (L/T)

q_c = Cauchy flux (L/T)

q_p = the throughfall of precipitation of the variable boundary (L/T)

h_p = the allowed ponding depth on variable boundary (L)

h_m = the allowed minimum pressure head (L)

q_e = the allowed maximum evaporation rate on the variable boundary, i.e., the potential evaporation (L/T)

B_d = the Dirichlet boundary

B_n = the Neumann boundary

B_c = the Cauchy boundary

B_v = the variable boundary

C_s = dissolved concentration of the substrate (M/L^3)

ρ_s = intrinsic density of substrate, (M/L^3)

C_o = dissolved concentration of oxygen (M/L^3)

ρ_o = intrinsic density of oxygen (M/L^3)

C_n = dissolved concentration of nitrate (M/L^3)

ρ_n = intrinsic density of nitrate (M/L^3)

C_p = dissolved concentration of nutrient (M/L^3)

ρ_p = intrinsic density of nutrient (M/L^3)

C_1 = dissolved concentration of microbe #1 (M/L^3)

ρ_1 = intrinsic density of microbe #1 (M/L^3)

C_2 = dissolved concentration of microbe #2 (M/L^3)

ρ_2 = intrinsic density of microbe #2 (M/L^3)

C_3 = dissolved concentration of microbe #3 (M/L^3)

ρ_3 = intrinsic density of microbe #3 (M/L^3)

β_s = viscosity effecting factor associated with substrate (L^2/T)

β_o = viscosity effecting factor associated with oxygen (L)

β_n = viscosity effecting factor associated with nitrate (L)

β_p = viscosity effecting factor associated with nutrient (L^2/T)

β_1 = viscosity effecting factor associated with microbe #1 (L^2/T)

β_2 = viscosity effecting factor associated with microbe #2 (L^2/T)

β_3 = viscosity effecting factor associated with microbe #3 (L^2/T)

ρ_b = the bulk density of the medium (M/L^3)

D = the dispersion coefficient tensor (L^2/T)

Λ_s = transformation rate constant for substrate (1/T)

Λ_o = transformation rate constant for oxygen (1/T)

Λ_p = transformation rate constant for nutrient (1/T)

Λ_n = transformation rate constant for nitrate (1/T)

Λ_1 = transformation rate constant for microbe #1 (1/T)

Λ_2 = transformation rate constant for microbe #2 (1/T)

Λ_3 = transformation rate constant for microbe #3 (1/T)

K_{ds} = distribution coefficient of substrate (L/M^3)

K_{do} = distribution coefficient of oxygen (L/M^3)

K_{dn} = distribution coefficient of nitrate (L/M^3)

K_{dp} = distribution coefficient of nutrient (L/M^3)

K_{d1} = distribution coefficient of microbe #1 (L/M^3)

K_{d2} = distribution coefficient of microbe #2 (L/M^3)

K_{d3} = distribution coefficient of microbe #3 (L/M^3)

q_{in} = source rate of water (L^3/T)

C_{sin} = concentration of substrate in the source (M/L^3)

C_{oin} = concentration of oxygen in the source (M/L^3)

C_{nin} = concentration of nitrate in the source (M/L^3)

C_{pin} = concentration of nutrient in the source (M/L^3)

C_{1in} = concentration of microbe #1 in the source (M/L^3)

C_{2in} = concentration of microbe #2 in the source (M/L^3)

C_{3in} = concentration of microbe #3 in the source (M/L^3)

$\mu_o^{(1)}$ = maximum specific oxygen-based growth rate for microbe #1 (1/T)

$\mu_n^{(2)}$ = maximum specific nitrate-based growth rate for microbe #2 (1/T)

$\mu_o^{(3)}$ = maximum specific oxygen-based growth rate for microbe #3 (1/T)

$\mu_n^{(3)}$ = maximum specific nitrate-based growth rate for microbe #3 (1/T)

$Y_o^{(1)}$ = yield coefficient for microbe #1 utilizing oxygen in mass of microbe per unit mass of substrate (M/M)

$Y_n^{(2)}$ = the yielding coefficient for microbe #2 utilizing nitrate in mass of microbe per unit mass of substrate (M/M)

$Y_o^{(3)}$ = the yielding coefficient for microbe #3 utilizing oxygen in mass of microbe per unit mass of substrate (M/M)

$Y_n^{(3)}$ = yielding coefficient for microbe #3 utilizing nitrate in mass of microbe per unit mass of substrate (M/M)

$I(C_o)$ = an inhibition function which is under the assumption that denitrifying enzyme inhibition is reversible and noncompetitive

K_c = inhibition coefficient (M/L^3)

$K_{so}^{(1)}$ = retarded substrate saturation constants under aerobic conditions with respect to microbe #1 (M/L^3)

$K_{so}^{(3)}$ = retarded substrate saturation constants under aerobic conditions with respect to microbe #3 (M/L^3)

$K_{sn}^{(2)}$ = retarded substrate saturation constants under anaerobic conditions with respect to microbe #2 (M/L^3)

$K_{sn}^{(3)}$ = retarded substrate saturation constants under anaerobic conditions with respect to microbe #3 (M/L^3)

$K_{po}^{(1)}$ = retarded nutrient saturation constants under aerobic conditions with respect to microbe #1 (M/L^3)

$K_{po}^{(3)}$ = retarded nutrient saturation constants under aerobic conditions with respect to microbe #3 (M/L^3)

$K_{pn}^{(2)}$ = retarded nutrient saturation constants under anaerobic conditions with respect to microbe #2 (M/L^3)

$K_{pn}^{(3)}$ = retarded nutrient saturation constants under anaerobic conditions with respect to microbe #3 (M/L^3)

$K_{o}^{(1)}$ = retarded oxygen saturation constants under aerobic conditions with respect to microbe #1 (M/L^3)

$K_{o}^{(3)}$ = retarded oxygen saturation constants under aerobic conditions with respect to microbe #3 (M/L^3)

$K_{n}^{(2)}$ = retarded nitrate saturation constant under anaerobic conditions with respect to microbe #2 (M/L^3)

$K_{n}^{(3)}$ = retarded nitrate saturation constant under anaerobic conditions with respect to microbe #3 (M/L^3)

$\lambda_{o}^{(1)}$ = microbial decay constant of aerobic respiration of microbe #1 (1/T)

$\lambda_{o}^{(3)}$ = microbial decay constant of aerobic respiration of microbe #3 (1/T)

$\lambda_{n}^{(2)}$ = microbial decay constant of anaerobic respiration of microbe #3 (1/T)

$\lambda_{n}^{(3)}$ = microbial decay constant of anaerobic respiration of microbe #3 (1/T)

$\gamma_{o}^{(1)}$ = oxygen-use for syntheses by microbe #1

$\gamma_{o}^{(3)}$ = oxygen-use for syntheses by microbe #3

$\gamma_{n}^{(2)}$ = nitrate-use for syntheses by microbe #2

$\gamma_{n}^{(3)}$ = nitrate-use for syntheses by microbe #3

$\alpha_{o}^{(1)}$ = oxygen-use coefficient for energy by microbe #1

$\alpha_o^{(3)}$ = oxygen-use coefficient for energy by microbe #3

$\alpha_n^{(2)}$ = nitrate-use coefficient for energy by microbe #2

$\alpha_n^{(3)}$ = nitrate-use coefficient for energy by microbe #3

$\Gamma_o^{(1)}$ = oxygen saturation constants for decay with respect to microbe #1 (M/L^3)

$\Gamma_o^{(3)}$ = oxygen saturation constants for decay with respect to microbe #3 (M/L^3)

$\Gamma_n^{(2)}$ = nitrate saturation constants for decay with respect to microbe #2 (M/L^3)

$\Gamma_n^{(3)}$ = nitrate saturation constants for decay with respect to microbe #3 (M/L^3)

$\epsilon_o^{(1)}$ = nutrient-use coefficients for the production of microbe #1 with respect to aerobic respiration

$\epsilon_o^{(3)}$ = nutrient-use coefficients for the production of microbe #3 with respect to aerobic respiration

$\epsilon_n^{(2)}$ = nutrient-use coefficients for the production of microbe #2 with respect to anaerobic respiration

$\epsilon_n^{(3)}$ = nutrient-use coefficients for the production of microbe #3 with respect to anaerobic respiration

S = material concentration in the absorbed phase (M/M)

$r_{sop}^{(1)}$ = the removal rate of substrate under aerobic respiration with respect to microbe #1 (M/M)

$r_{sop}^{(3)}$ = the removal rate of substrate under aerobic respiration with respect to microbe #3 (M/M)

$r_{snp}^{(2)}$ = the removal rate of substrate under anaerobic respiration with respect to microbe #2 (M/M)

$r_{snp}^{(3)}$ = the removal rate of substrate under anaerobic respiration with respect to microbe #3 (M/M)

$r_s^{(1)}$ = the removal rates of substrate by microbe #1

$r_s^{(2)}$ = the removal rates of substrate by microbe #2

$r_s^{(3)}$ = the removal rates of substrate by microbe #3

$r_o^{(1)}$ = oxygen utilization rate per unit of biomass, microbe #1

$r_o^{(2)}$ = oxygen utilization rate per unit of biomass, microbe #2

$r_o^{(3)}$ = oxygen utilization rate per unit of biomass, microbe #3

$r_n^{(1)}$ = nitrate utilization rate per unit of biomass, microbe #1

$r_n^{(2)}$ = nitrate utilization rate per unit of biomass, microbe #2

$r_n^{(3)}$ = nitrate utilization rate per unit of biomass, microbe #3

$r_p^{(1)}$ = nutrient utilization rate per unit of biomass, microbe #1

$r_p^{(2)}$ = nutrient utilization rate per unit of biomass, microbe #2

$r_p^{(3)}$ = nutrient utilization rate per unit of biomass, microbe #3

δ = the Kronecker delta tensor

a_T = the lateral dispersivity (L)

a_L = the longitudinal dispersivity (L)

a_m = the molecular diffusion coefficient (L^2/T)

τ = the tortuosity

C_{si} = the prescribed initial concentrations of substrate (M/L^3)

C_{oi} = the prescribed initial concentrations of oxygen (M/L^3)

C_{ni} = the prescribed initial concentrations of nitrate (M/L^3)

C_{pi} = the prescribed initial concentrations of nutrient (M/L^3)

C_{1i} = the prescribed initial concentrations of microbe #1 (M/L^3)

C_{2i} = the prescribed initial concentrations of microbe #2 (M/L^3)

C_{3i} = the prescribed initial concentrations of microbe #3 (M/L^3)

C_{sd} = the prescribed Dirichlet boundary concentrations of substrate (M/L^3)

C_{od} = the prescribed Dirichlet boundary concentrations of oxygen (M/L^3)

C_{nd} = the prescribed Dirichlet boundary concentrations of nitrate (M/L^3)

C_{pd} = the prescribed Dirichlet boundary concentrations of nutrient (M/L^3)

C_{1d} = the prescribed Dirichlet boundary concentrations of microbe #1 (M/L^3)

C_{2d} = the prescribed Dirichlet boundary concentrations of microbe #2 (M/L^3)

C_{3d} = the prescribed Dirichlet boundary concentrations of microbe #3 (M/L^3)

C_{sv} = the prescribed concentrations of substrate (M/L^3) on variable boundary

C_{ov} = the prescribed concentrations of oxygen (M/L^3) on variable boundary

C_{nv} = the prescribed concentrations of nitrate (M/L^3) on variable boundary

C_{pv} = the prescribed concentrations of nutrient (M/L^3) on variable boundary

C_{1v} = the prescribed concentrations of microbe #1 (M/L^3) on variable boundary

C_{2v} = the prescribed concentrations of microbe #2 (M/L^3) on variable boundary

C_{3v} = the prescribed concentrations of microbe #3 (M/L^3) on variable boundary

q_{sc} = the prescribed total flux of substrate through Cauchy boundary

q_{oc} = the prescribed total flux of oxygen through Cauchy boundary

q_{nc} = the prescribed total flux of nitrate through Cauchy boundary

q_{pc} = the prescribed total flux of nutrient through Cauchy boundary

q_{1c} = the prescribed total flux of microbe #1 through Cauchy boundary

q_{2c} = the prescribed total flux of microbe #2 through Cauchy boundary

q_{3c} = the prescribed total flux of microbe #3 through Cauchy boundary

q_{sn} = the prescribed gradient flux of substrate through Neumann boundary

q_{on} = the prescribed gradient flux of oxygen through Neumann boundary

q_{nn} = the prescribed gradient flux of nitrate through Neumann boundary

q_{pn} = the prescribed gradient flux of nutrient through Neumann boundary

q_{1n} = the prescribed gradient flux of microbe #1 through Neumann boundary

q_{2n} = the prescribed gradient flux of microbe #2 through Neumann boundary

q_{3n} = the prescribed gradient flux of microbe #3 through Neumann boundary

N = the total number of nodes in the region of interest

N_j = the shape function at node j

h_j = the pressure head at node j (L)

F = water capacity; $F = d\theta/dh$ (1/L)

$\{dh/dt\}$ = column vector containing the values of dh/dt (L/T)

$\{h\}$ = column vector containing the values of h (L)

$[M]$ = mass matrix

$[S]$ = stiffness matrix

$\{G\}$ = load vector resulting from the gravity force

$\{Q\}$ = load vector due to sources/sinks

$\{B\}$ = load vector by the implementation of boundary condition

R_e = the region of element e

M_e = the set of elements that have a local side α-β coinciding with the global side i-j

N_α^e = the α-th local basis function of element e

N_β^e = the β-th local basis function of element e

B_e = the element surface of the boundary segment e

N_{se} = the set of boundary segments that have a local node α coinciding with the global node i

V_x, V_y, V_z = the Darcy flux components along the x-, y-, and z-directions (L/T)

i, **j**, **k** = the unit vectors along the x-, y-, and z-directions

$\{B_c^e\}$ = boundary-element column vector for a Cauchy boundary side

$\{B_n^e\}$ = boundary-element column vector for a Neumann boundary side

$\{B_v^e\}$ = boundary-element column vector for a variable boundary side

$\{q_c^e\}$ = Cauchy boundary flux vector

$\{q_n^e\}$ = Neumann boundary flux vector

$\{q_v^e\}$ = variable boundary flux vector

N_{ne} = number of Neumann boundary element sides

N_{ce} = number of Cauchy boundary element sides

N_{ve} = number of variable boundary element sides

$f(C_1, C_2, C_3, C_s, C_o, C_n, C_p)$ = a microbial-chemical interaction function

$g(C_1, C_2, C_3, C_s, C_o, C_n, C_p)$ = a microbial growth function

$\mathbf{V_d}$ = retarded velocity (L/T)

C_j = the concentration at node j (M/L^3)

[A] = stiffness matrix associated with the velocity term

[D] = stiffness matrix associated with the dispersion term

[K] = stiffness matrix associated with the decay term, density effect, and microbial-chemical interaction

[Bv] = stiffness matrix resulting from boundary conditions

[V] = stiffness matrix associated with the convection term

V_n = normal Darcy flux with respect to the flow-in variable boundary

w = the derivative weighting factor

t_n = previous time (T)

C^n = concentration at time t_n (M/L^3)

t_{n+1} = current time (T)

C^{n+1} = concentration at time t_{n+1} (M/L^3)

$\mathbf{x}$ = position vector representing (x, y, z) (L)

$\Delta\tau$ ($\mathbf{x}$) = the transport time associated with $\mathbf{x}$

N_n = number of activated fine-grid nodes

Δt = time-step size (T)

C_j^f = the concentration at location (x_j^f, y_j^f, z_j^f) (M/L^3)

C_j^i = approximated concentration determined from finite element interpolation (M/L^3)

C_M^f = the maximum concentration of C_j^f (M/L^3)

Err_1^r, Err_2^r = the first and second relative errors

$[A^e]$ = element coefficient matrix

$\{C^e\}$ = unknown vector of concentration

$\{R^e\}$ = element load vector

of subelements is MXKGLDK = 316. There are 584 imbedded diffusion fine grids in these 79 extended rough elements. Therefore, MXADNK=MAXNPK+584. Because of the simulation of 2-D problem by using a 3-D model, 830 of MXADNK nodes are located on the global boundaries. Hence, MXNDBK should not be less than 830. In the rough region, there are 33 global element surfaces and 66 subelemental surface located on the intra-boundaries. So MXMSVK should not be less than 33 and MXLSVK must be greater than or equal to 66. The maximum number of nodes connected to each node is assumed to 35. Thus MXJBD=35.

$$\nabla\cdot\left[\frac{\rho\mathbf{k}}{\mu}\cdot(\nabla p + \rho g\nabla z)\right] + \rho^{*}q =$$

$$Sn_e\frac{\partial\rho}{\partial p}\frac{\partial p}{\partial t} + Sn_e\frac{\partial\rho}{\partial C}\frac{\partial C}{\partial t} + n_e\rho\frac{\partial S}{\partial t} \qquad \text{(B.1.5)}$$

$$+ \rho S\frac{\partial n_e}{\partial t} + S\rho\nabla\cdot n_e\mathbf{V_s} + n_e\mathbf{V_s}\cdot\nabla(S\rho)$$

Making the approximation by neglecting the second-order term:

$$n_e\mathbf{V_s}\cdot\nabla(S\rho) \dashrightarrow 0 \qquad \text{(B.1.6)}$$

one has:

$$\nabla\cdot[\frac{\rho\mathbf{k}}{\mu}\cdot(\nabla p + \rho g\nabla z)] + \rho^{*}q =$$

$$Sn_e\frac{\partial\rho}{\partial p}\frac{\partial p}{\partial t} + Sn_e\frac{\partial\rho}{\partial C}\frac{\partial C}{\partial t} + n_e\rho\frac{\partial S}{\partial t} \qquad \text{(B.1.7)}$$

$$+ \rho S\frac{\partial n_e}{\partial t} + S\rho\nabla\cdot n_e\mathbf{V_s}$$

Defining the compressibility of the fluid as:

$$\beta = \frac{1}{\rho}\frac{\partial\rho}{\partial p} \qquad \text{(B.1.8)}$$

where β is the compressibility of the fluid (LT^2/M). Also defining the moisture content as:

$$\theta = Sn_e \qquad \text{(B.1.9)}$$

where θ is the moisture content (dimensionless). One may substitute Eqs.(B.1.8) and (B.1.9) into Eq.(B.1.7) and rewrite it to obtain:

$$\nabla\cdot[\frac{\rho\mathbf{k}}{\mu}\cdot(\nabla p + \rho g\nabla z)] + \rho^{*}q = \theta\beta\rho\frac{\partial p}{\partial t} + \theta\frac{\partial\rho}{\partial C}\frac{\partial C}{\partial t} + n_e\rho\frac{\partial S}{\partial t} + \rho S\left[\frac{\partial n_e}{\partial t} + \nabla\cdot(n_e\mathbf{V_s})\right] \quad \text{(B.1.10)}$$

Remembering that the continuity statement of incompressible solids but a compressible skeleton is (Yeh, 1992):

$$\frac{\partial(1-n_e)}{\partial t} + \nabla\cdot(1-n_e)\mathbf{V_s} = 0 \quad \text{(B.1.11)}$$

Rearranging Eq.(B.1.11) in the following form:

$$\frac{\partial n_e}{\partial t} + \nabla\cdot n_e\mathbf{V_s} = \nabla\cdot\mathbf{V_s} \quad \text{(B.1.12)}$$

Substituting Eq.(B.1.12) into Eq.(B.1.10), one obtains:

$$\nabla\cdot[\frac{\rho\mathbf{k}}{\mu}\cdot(\nabla p + \rho g\nabla z)] + \rho^{*}q = \theta\beta\frac{\partial p}{\partial t} + \theta\frac{\partial\rho}{\partial C}\frac{\partial C}{\partial t} + n_e\rho\frac{\partial S}{\partial t} + \rho S\nabla\cdot\mathbf{V_s} \quad \text{(B.1.13)}$$

Recalling that the flux of solid velocity is the divergence of $\boldsymbol{V_s}$ (Yeh, 1992):

$$\nabla\cdot\mathbf{V_s} = \alpha\frac{\partial p}{\partial t} \quad \text{(B.1.14)}$$

where α is the coefficient of consolidation of the media (LT^2/M). Substituting Eq.(B.1.14) into Eq.(B.1.13) and rewriting:

$$\nabla\cdot[\frac{\rho\mathbf{k}}{\mu}\cdot(\nabla p + \rho g\nabla z] + \rho^{*}q = \rho(\theta\beta + S\alpha)\frac{\partial p}{\partial t} + \theta\frac{\partial\rho}{\partial C}\frac{\partial C}{\partial t} + n_e\rho\frac{\partial S}{\partial t} \tag{B.1.15}$$

Remembering Eq.(B.1.9) and substituting:

$$\nabla\cdot[\frac{\rho\mathbf{k}}{\mu}\cdot(\nabla p + \rho g\nabla z] + \rho^{*}q = \rho(\theta\beta + \frac{\theta}{n_e}\alpha)\frac{\partial p}{\partial t} + \theta\frac{\partial\rho}{\partial C}\frac{\partial C}{\partial t} + n_e\rho\frac{\partial S}{\partial t} \tag{B.1.16}$$

Experimental evidence has shown that the degree of saturation is a function of pressure as:

$$S = S(p) \tag{B.1.17}$$

Substitution of Eq. (B.1.17) into Eq. (B.1.18) give:

$$\nabla\cdot\left[\frac{\rho\mathbf{k}}{\mu}\cdot(\nabla p + \rho g\nabla z)\right] + \rho^{*}q = \rho(\theta\beta + \frac{\theta}{n_e}\alpha)\frac{\partial p}{\partial t} + \theta\frac{\partial\rho}{\partial C}\frac{\partial C}{\partial t} + \rho n_e\frac{dS}{dp}\frac{\partial p}{\partial t} \tag{B.1.18}$$

Next, one needs to define the reference pressure head as:

$$h = \frac{p}{\rho_w g} \tag{B.1.19}$$

where h is the reference pressure head (L) and ρ_w is the reference water density (M/L^3). Substituting Eq.(B.1.19) into Eq.(B.1.18), one obtains:

$$\nabla\cdot\left[\frac{\rho\mathbf{k}}{\mu}\cdot(\rho_w g\nabla h + \rho g\nabla z)\right] + \rho^* q = \rho(\theta\beta + \frac{\theta}{n_e}\alpha)\rho_w g\frac{\partial h}{\partial t} + \theta\frac{\partial\rho}{\partial C}\frac{\partial C}{\partial t} + \rho n_e\frac{dS}{dh}\frac{\partial h}{\partial t} \quad \text{(B.1.20)}$$

Dividing Eq.(B.1.20) by ρ_w and rearranging, one gets:

$$\nabla\cdot\left[\frac{\rho g\mathbf{k}}{\mu}\cdot\left\{\nabla h + \frac{\rho}{\rho_w}\nabla z\right\}\right] + \frac{\rho^*}{\rho_w}q = \frac{\rho}{\rho_w}(\theta g\rho_w\beta + \frac{\theta}{n_e}g\rho_w\alpha)\frac{\partial h}{\partial t} + \frac{\theta}{\rho_w}\frac{\partial\rho}{\partial C}\frac{\partial C}{\partial t} + \frac{\rho}{\rho_w}n_e\frac{dS}{dh}\frac{\partial h}{\partial t} \quad \text{(B.1.21)}$$

Defining the modified compressibilities of the media and water as

$$\alpha' = \alpha\rho_w g \quad \text{(B.1.22)}$$

$$\beta' = \beta\rho_w g \quad \text{(B.1.23)}$$

where α' is the modified compressibility of the media (1/L) and β' is the modified compressibility of the water (1/L). Substituting Eqs.(B.1.22) and (B.1.23) into Eq.(B.1.21) and rearranging:

$$\nabla\cdot\left[\frac{\rho g\mathbf{k}}{\mu}\cdot\left\{\nabla h + \frac{\rho}{\rho_w}\nabla z\right\}\right] + \frac{\rho^*}{\rho_w}q = \frac{\rho}{\rho_w}(\alpha'\frac{\theta}{n_e} + \beta'\theta + n_e\frac{dS}{dh})\frac{\partial h}{\partial t} + \frac{\theta}{\rho_w}\frac{\partial\rho}{\partial C}\frac{\partial C}{\partial t} \quad \text{(B.1.24)}$$

Defining the storage coefficient as:

$$F = \alpha'\frac{\theta}{n_e} + \beta'\theta + n_e\frac{dS}{dh} \quad \text{(B.1.25)}$$

where F is the storage coefficient. Substituting Eq.(B.1.25) into Eq.(B.1.24) and following Frind (1982) by neglecting the second term on the right hand side of Eq.(B.1.24), one gets:

$$\nabla\cdot\left[\frac{\rho g\mathbf{k}}{\mu}\cdot\left\{\nabla h+\frac{\rho}{\rho_w}\nabla z\right\}\right]+\frac{\rho^*}{\rho_w}q=\frac{\rho}{\rho_w}F\frac{\partial h}{\partial t} \tag{B.1.26}$$

Defining the relation:

$$\mathbf{K}=\frac{\rho g\mathbf{k}}{\mu} \tag{B.1.27}$$

where **K** is the hydraulic conductivity tensor. Substituting Eq.(B.1.27) into Eq.(B.1.26) and rearranging, one gets the density-dependent flow equation:

$$\frac{\rho}{\rho_w}F\frac{\partial h}{\partial t}=\nabla\cdot\left[\mathbf{K}\cdot\left\{\nabla h+\frac{\rho}{\rho_w}\nabla z\right\}\right]+\frac{\rho^*}{\rho_w}q \tag{B.1.28}$$

From the Darcy's law :

$$\mathbf{V}=-\frac{1}{\rho}\frac{\rho\mathbf{k}}{\mu}\cdot(\nabla p+\rho g\nabla z) \tag{B.1.29}$$

where **V** is the Darcy flux (L/T). Recalling Eq.(B.1.19) and substituting into Eq.(B.1.29), one obtains:

$$\mathbf{V}=-\frac{1}{\rho}\frac{\rho\mathbf{k}}{\mu}\cdot\left(\rho_w g\nabla h+\rho g\nabla z\right) \tag{B.1.30}$$

Rearranging Eq.(B.1.30):

$$\mathbf{V}=-\frac{\rho g\mathbf{k}}{\mu}\cdot\left(\frac{\rho_w}{\rho}\nabla h+\nabla z\right) \tag{B.1.31}$$

and substituting Eq.(B.1.27) into Eq.(B.1.31), one gets the Darcy flux equation for density-dependent flow in its final form:

$$\mathbf{V}=-\mathbf{K}\cdot\left(\frac{\rho_w}{\rho}\nabla h+\nabla z\right) \tag{B.1.32}$$

The density is a function of water, chemical, and microbial concentrations, C_w, C_s, C_o, C_n, C_p, C_1, C_2, and C_3, as the following form:

$$\rho = C_w + C_s + C_o + C_n + C_p + C_1 + C_2 + C_3 \tag{B.1.33}$$

Physically, the following equation, Eq. (B.1.34), is valid.

$$1 = \frac{C_w}{\rho_w} + \frac{C_s}{\rho_s} + \frac{C_o}{\rho_o} + \frac{C_n}{\rho_n} + \frac{C_p}{\rho_p} + \frac{C_1}{\rho_1} + \frac{C_2}{\rho_2} + \frac{C_3}{\rho_3} \tag{B.1.34}$$

Eq. (B.1.35) is obtained from (B.1.33) divided by ρ_w and substituting (B.1.34) into the term $\frac{\rho}{\rho_w}$.

$$\begin{aligned}
\frac{\rho}{\rho_w} &= \frac{C_w}{\rho_w} + \frac{C_s}{\rho_w} + \frac{C_o}{\rho_w} + \frac{C_n}{\rho_w} + \frac{C_p}{\rho_w} + \frac{C_1}{\rho_w} + \frac{C_2}{\rho_w} + \frac{C_3}{\rho_w} \\
&= 1 - \sum_i \frac{C_i}{\rho_i} + \frac{1}{\rho_w}\sum_i C_i \\
&= 1 - \sum_i \left(\frac{1}{\rho_i} - \frac{1}{\rho_w} \right) C_i \\
&= 1 + \sum_i \left(\frac{1}{\rho_w} - \frac{1}{\rho_i} \right) C_i
\end{aligned} \tag{B.1.35}$$

The viscosity is assumed the following form

$$\frac{\mu}{\mu_w} = 1 + \beta_1 C_s + \beta_o C_o + \beta_n C_b + \beta_p C_p + \beta_1 C_1 + \beta_2 C_2 + \beta_3 C_3 \tag{B.1.36}$$

where C is the chemical concentration (M/L^3) and β_s, β_o, β_n, β_p, β_1, β_2, and β_3 are the parameters (L^3/M) that are used to describe the concentration dependence of dynamic viscosity.

The initial conditions for the flow equations are stated as:

$$h = h_i(x,y,z) \quad \text{in} \quad R \tag{B.1.37}$$

where R is the region of interest and h_i is the prescribed initial condition for hydraulic head. The h_i can either be obtained by solving the steady-state version of Eq. (B.1.26) or alternatively by defining through field measurements.

The specification of boundary conditions is probably the most critical and complex chore in flow modeling. As explained by Yeh (1987), the boundary conditions of the region of interest can be examined from a dynamic, physical, or mathematical point of view. From a dynamic standpoint, a boundary segment can be either considered as impermeable or flow-through. On the other hand, from a physical point of view, such a segment could be classified as a soil-soil interface, soil-air interface, or soil-water interface. Lastly, from a mathematical point of view, the boundary segment can be classified as one of four types of boundary conditions, namely as (1) Dirichlet, (2) Neumann, (3) Cauchy, or (4) variable boundary conditions. In addition, a good numerical model must be able to handle these boundary conditions when they vary on the boundary and are either abruptly or gradually time-dependent.

The Dirichlet boundary condition is usually applied to soil-water interfaces, such as streams, artificial impoundments, and coastal lines, and involves prescribing the functional value on the boundary. The Neumann boundary condition, on the other hand, involves prescribing the gradient of the function on the boundary and does not occur very often in real-world problems. This condition, however, can be encountered at the base of the media where natural drainage occurs. The third type of boundary condition, the Cauchy boundary condition, involves prescribing the total normal flux due to the gradient on the boundary. Usually surface water bodies with known infiltration rates through the layers of the bottom of their sediments or liners into the subsurface media are administered this boundary condition. If there exists a soil-air interface in the region of interest, a variable boundary condition is employed. In such a case, either Dirichlet or Cauchy boundary conditions dominate, mainly depending on the potential evaporation, the conductivity of the media, and the availability of water such as rainfall (Yeh, 1987).

From the above discussion, four types of boundary conditions can be specified for the flow equations depending on the physical location of the boundaries. These boundary conditions are stated as:

Dirichlet Boundary Conditions:

$$h = h_d(x_b,y_b,z_b,t) \quad \text{on} \quad B_d \tag{B.1.38}$$

Neumann Boundary Conditions:

$$-\mathbf{n}\cdot\mathbf{K}\left(\frac{\rho_w}{\rho}\cdot\nabla h\right) = q_n(x_b,y_b,z_b,t) \quad \text{on} \quad B_n \tag{B.1.39}$$

Cauchy Boundary Conditions:

$$-\mathbf{n}\cdot\mathbf{K}\cdot\left(\frac{\rho_w}{\rho}\nabla h + \nabla z\right) = q_c(x_b,y_b,z_b,t) \quad \text{on} \quad B_c \tag{B.1.40}$$

Variable Boundary Conditions - During Precipitation Period:

$$h = h_p(x_b,y_b,z_b,t) \quad \text{on} \quad B_v \tag{B.1.41a}$$

or

$$-\mathbf{n}\cdot\mathbf{K}\cdot\left(\frac{\rho_w}{\rho}\nabla h + \nabla z\right) = q_p(x_b,y_b,z_b,t) \quad \text{on} \quad B_v \tag{B.1.41b}$$

Variable Boundary Conditions - During Non-Precipitation Period:

$$h = h_p(x_b,y_b,z_b,t) \quad \text{on} \quad B_v \tag{B.1.41c}$$

or

$$h = h_m(x_b,y_b,z_b,t) \quad \text{on} \quad B_v \tag{B.1.41d}$$

or

$$-\mathbf{n}\cdot\mathbf{K}\cdot\left(\frac{\rho_w}{\rho}\nabla h + \nabla z\right) = q_e(x_b,y_b,z_b,t) \quad \text{on} \quad B_v \tag{B.1.41e}$$

where **n** is the outward unit vector normal to the boundary; (x_b,y_b,z_b) is the spatial coordinate on the boundary;

h_d, q_n, and q_c are the Dirichlet functional value, Neumann flux, and Cauchy flux, respectively; B_d, B_n, B_c, and B_v are the Dirichlet, Neumann, Cauchy, and variable boundaries, respectively; h_p and q_p are the allowed ponding depth and the throughfall of precipitation, respectively, on the variable boundary; h_m is the allowed minimum pressure on the variable boundary; and q_e is the allowed maximum evaporation rate (= potential evaporation) on the variable boundary. Note that only one of Eqs. (B.1.41a) through (B.1.41e) is utilized at any point on the variable boundary at any time.

B.2 Governing Equations for Transport

This section derives the governing equations for chemical and microbial transport and fate in subsurface media. The assumptions, which form the basis for the transport and fate model and which hold for each one of the four chemical compounds, i.e. substrate s, nutrient p, oxygen o, and nitrate n, and of three microbial biomass, i.e., microbe #1, microbe #2, and microbe #3, are now listed.

(1) Mass transport is via advection and dispersion plus artificial sources and sinks - To simplify the notation, let C stand for C_s, C_o, C_n, C_p, C_1, C_2, and C_3. The well known transport equation is derived in (Yeh, et al., 1994) and written as

$$\theta\frac{\partial C}{\partial t} + \rho_b\frac{\partial S}{\partial t} + \nabla\cdot\mathbf{V}C = -\alpha\frac{\partial p}{\partial t}(\theta C + \rho_b S) - \frac{\partial \theta}{\partial t}C + m \qquad \text{(B.2.1)}$$

where S is the material concentration in the absorbed phase (M/M), θ is moisture content (L^3/L^3), α is the compressibility of the medium, p is the pressure, and m is the artificial source/sink (which is equal to qC_{in} for the case of sources or equal to qC for the case sinks with C_{in} being the concentration of the source).

(2) The porous medium follows the linear isotherm rule as follows.

$$S = K_d C \qquad \text{(B.2.2)}$$

where K_d is the distribution coefficient. Substituting Eq. (B.2.2) into Eq. (B.2.1), the transport

equation becomes

$$(\theta + \rho_b K_d)\frac{\partial C}{\partial t} + \nabla\cdot\mathbf{V}C = \nabla\cdot\theta\mathbf{D}\cdot\nabla C + m - \frac{\partial\theta}{\partial t}C - \alpha\frac{\partial p}{\partial t}(\theta + \rho_b K_d)C \qquad \text{(B.2.3)}$$

(3) Loss of chemicals and microbes can occur via first order irreversible loss processes, such as chemical transformations and precipitation in both the free and sorbed phases, in addition to loss via microbial degradation or growth. Then the governing equation is given as Eq. (B.2.4).

$$(\theta + \rho_b K_d)\frac{\partial C}{\partial t} + \nabla\cdot\mathbf{V}C = \nabla\cdot\theta\mathbf{D}\cdot\nabla C - \left(\alpha\frac{\partial p}{\partial t} + \Lambda\right)(\theta + \rho_b K_d)C - \frac{\partial\theta}{\partial t}C + m \qquad \text{(B.2.4)}$$

(4) To rewrite the above conservative form of the transport equation to the advective form, the governing equation is obtained as

$$(\theta + \rho_b K_d)\frac{\partial C}{\partial t} + \mathbf{V}\cdot\nabla C = \nabla\cdot\theta\mathbf{D}\cdot\nabla C - \left(\alpha\frac{\partial p}{\partial t} + \Lambda\right)(\theta + \rho_b K_d)C - \frac{\partial\theta}{\partial t}C + m - C\nabla\cdot\mathbf{V} \qquad \text{(B.2.5)}$$

The following relationship can be derived from the Darcy velocity Eq. (B.1.32)

$$-\nabla\cdot\mathbf{K}\cdot\left(\nabla h + \frac{\rho}{\rho_w}\nabla z\right) = \nabla\cdot\left(\frac{\rho}{\rho_w}\mathbf{V}\right) = \mathbf{V}\cdot\nabla\frac{\rho}{\rho_w} + \frac{\rho}{\rho_w}\nabla\cdot\mathbf{V} \qquad \text{(B.2.6)}$$

Substituting Eq. (B.2.6) into Eq. (B.1.28), one has

$$\frac{\rho}{\rho_w}\nabla\cdot\mathbf{V} = \frac{\rho^*}{\rho_w}q - \frac{\rho}{\rho_w}F\frac{\partial h}{\partial t} - \mathbf{V}\cdot\nabla\frac{\rho}{\rho_w} \qquad \text{(B.2.7)}$$

The transport governing equation is expressed as Eq. (B.2.8) after substituting Eq. (B.2.7) into Eq. (B.2.5).

$$(\theta + \rho_b K_d)\frac{\partial C}{\partial t} + \mathbf{V}\cdot\nabla C = \nabla\cdot\theta\mathbf{D}\cdot\nabla C$$
$$- \left(\alpha\frac{\partial p}{\partial t} + \Lambda\right)(\theta + \rho_b K_d)C + m - \frac{\rho^*}{\rho}qC + (F - \frac{\partial\theta}{\partial t})\frac{\partial h}{\partial t}C + (\frac{\rho_w}{\rho})\mathbf{V}\cdot\nabla(\frac{\rho}{\rho_w})C \quad \text{(B.2.8)}$$

(5) Microbiological processes are modeled using process laws described by Molz et al. [1986] and Widdowson et al. [1988], who constructed biodegradation models using the carbon assimilation and oxidation assumptions of Herbert [1958]. The model developed here includes three microbial populations, namely C_1, C_2, and C_3. The utilization rate laws adapted from Benefield and Molz [1984] are

$$r_{sop}^{(1)} = \frac{\mu_o^{(1)}}{Y_o^{(1)}}\left[\frac{C_s}{K_{so}^{(1)} + C_s}\right]\left[\frac{C_o}{K_o^{(1)} + C_o}\right]\left[\frac{C_p}{K_{po}^{(1)} + C_p}\right] \quad \text{(B.2.9)}$$

$$r_{snp}^{(2)} = \frac{\mu_n^{(2)}}{Y_n^{(2)}}\left[\frac{C_s}{K_{sn}^{(2)} + C_s}\right]\left[\frac{C_n}{K_n^{(2)} + C_n}\right]\left[\frac{C_p}{K_{pn}^{(2)} + C_p}\right] \quad \text{(B.2.10)}$$

$$r_{sop}^{(3)} = \frac{\mu_o^{(3)}}{Y_o^{(3)}}\left[\frac{C_s}{K_{so}^{(3)} + C_s}\right]\left[\frac{C_o}{K_o^{(3)} + C_o}\right]\left[\frac{C_p}{K_{po}^{(3)} + C_p}\right] \quad \text{(B.2.11)}$$

$$r_{snp}^{(3)} = \frac{\mu_n^{(3)}}{Y_n^{(3)}}\left[\frac{C_s}{K_{sn}^{(3)} + C_s}\right]\left[\frac{C_n}{K_n^{(3)} + C_n}\right]\left[\frac{C_p}{K_{pn}^{(3)} + C_p}\right]I(C_o) \quad \text{(B.2.12)}$$

$$r_s^{(1)} = r_{sop}^{(1)}, \quad r_s^{(2)} = r_{snp}^{(2)}, \quad r_s^{(3)} = r_{sop}^{(3)} + r_{snp}^{(3)} \quad \text{(B.2.13)}$$

where $r_{sop}^{(1)}$, $r_{sop}^{(3)}$, $r_{snp}^{(2)}$, and $r_{snp}^{(3)}$ (M/M) represent the removal rate of substrate under aerobic or anaerobic conditions with respect to microbes #1, #2, or #3.

The growth of three microbial populations adapted from Widdowson et al. [1988] are

$$\left(\frac{\partial C_1}{\partial t}\right)_{\text{microbe activity}} = \left[Y_o^{(1)} r_{sop}^{(1)} - \lambda_o^{(1)}\right] C_1 \qquad \text{(B.2.14)}$$

$$\left(\frac{\partial C_2}{\partial t}\right)_{\text{microbe activity}} = \left[Y_n^{(2)} r_{snp}^{(2)} - \lambda_n^{(2)}\right] C_2 \qquad \text{(B.2.15)}$$

$$\left(\frac{\partial C_3}{\partial t}\right)_{\text{microbe activity}} = \left[\left(Y_o^{(3)} r_{sop}^{(3)} - \lambda_o^{(3)}\right) + \left(Y_n^{(3)} r_{snp}^{(3)} - \lambda_n^{(3)}\right) I(C_o)\right] C_3 \qquad \text{(B.2.16)}$$

(6) Expressions for the respective electron acceptor utilization rates are based on the assumptions that (i) utilization resulting from the energy requirement for gross heterotrophic biomass production is proportional to substrate utilization, and (ii) requirement for energy of maintenance follows a Monod-type response with respect to the particular species. Thus the oxygen utilization rate per unit of biomass (specific rate) is expressed as

$$r_o^{(1)} = \gamma_o^{(1)} Y_o^{(1)} r_{sop}^{(1)} + \alpha_o^{(1)} \lambda_o^{(1)} \left[\frac{C_o}{\Gamma_o^{(1)} + C_o}\right] \qquad \text{(B.2.17)}$$

$$r_o^{(3)} = \gamma_o^{(3)} Y_o^{(3)} r_{sop}^{(3)} + \alpha_o^{(3)} \lambda_o^{(3)} \left[\frac{C_o}{\Gamma_o^{(3)} + C_o}\right] \qquad \text{(B.2.18)}$$

Likewise, the expression for the specific rate of nitrate utilization is given by

$$r_n^{(2)} = \gamma_n^{(2)} Y_n^{(2)} r_{snp}^{(2)} + \alpha_n^{(2)} \lambda_n^{(2)} \left[\frac{C_n}{\Gamma_n^{(2)} + C_n}\right] \qquad \text{(B.2.19)}$$

$$r_n^{(3)} = \gamma_n^{(3)} Y_n^{(3)} r_{snp}^{(3)} + \alpha_n^{(3)} \lambda_n^{(3)} \left[\frac{C_n}{\Gamma_n^{(3)} + C_n}\right] I_o(C_o) \qquad \text{(B.2.20)}$$

The specific rate of nutrient removal for the synthesis of heterotrophic biomass is assumed proportional to the specific rate of the substrate utilization rate and is expressed by

$$r_p^{(1)} = \epsilon_o^{(1)} r_{sop}^{(1)}, \quad r_p^{(2)} = \epsilon_n^{(2)} r_{snp}^{(2)}, \quad r_p^{(3)} = \epsilon_o^{(3)} r_{sop}^{(3)} + \epsilon_n^{(3)} r_{snp}^{(3)} \tag{B.2.21}$$

After coupling the biodegradation and microbial growth, the governing equations of fate and transport of chemicals and microbes are expressed as the following:

$$\begin{aligned}
&(\theta + \rho_b K_{ds}) \frac{\partial C_s}{\partial t} + \mathbf{V} \cdot \nabla C_s = \nabla \cdot \theta \mathbf{D} \cdot \nabla C_s \\
&- \left(\alpha \frac{\partial p}{\partial t} + \Lambda_s \right) (\theta + \rho_b K_{ds}) C_s + m_s - \frac{\rho^*}{\rho} q C_s + (F - \frac{\partial \theta}{\partial t}) \frac{\partial h}{\partial t} C_s + (\frac{\rho_w}{\rho}) \mathbf{V} \cdot \nabla (\frac{\rho}{\rho_w}) C_s \\
&- (\theta + \rho_b K_{d1}) r_s^{(1)} C_1 - (\theta + \rho_b K_{d2}) r_s^{(2)} C_2 - (\theta + \rho_b K_{d3}) r_s^{(3)} C_3 = \nabla \cdot \theta \mathbf{D} \cdot \nabla C_s \\
&- \left(\alpha \frac{\partial p}{\partial t} + \Lambda_s \right) (\theta + \rho_b K_{ds}) C_s + m_s - \frac{\rho^*}{\rho} q C_s + (F - \frac{\partial \theta}{\partial t}) \frac{\partial h}{\partial t} C_s + (\frac{\rho_w}{\rho}) \mathbf{V} \cdot \nabla (\frac{\rho}{\rho_w}) C_s \\
&- \left[(\theta + \rho_b K_{d1}) C_1 \right] \left\{ \frac{\mu_o^{(1)}}{Y_o^{(1)}} \left[\frac{C_s}{K_{so}^{(1)} + C_s} \right] \left[\frac{C_o}{K_o^{(1)} + C_o} \right] \left[\frac{C_p}{K_{po}^{(1)} + C_p} \right] \right\} \\
&- \left[(\theta + \rho_b K_{d2}) C_2 \right] \left\{ \frac{\mu_n^{(2)}}{Y_n^{(2)}} \left[\frac{C_s}{K_{sn}^{(2)} + C_s} \right] \left[\frac{C_n}{K_n^{(2)} + C_n} \right] \left[\frac{C_p}{K_{pn}^{(2)} + C_p} \right] \right\} \\
&- \left[(\theta + \rho_b K_{d3}) C_3 \right] \left\{ \begin{array}{l} \frac{\mu_o^{(3)}}{Y_o^{(3)}} \left[\frac{C_s}{K_{so}^{(3)} + C_s} \right] \left[\frac{C_o}{K_o^{(3)} + C_o} \right] \left[\frac{C_p}{K_{po}^{(3)} + C_p} \right] \\ + \frac{\mu_n^{(3)}}{Y_n^{(3)}} \left[\frac{C_s}{K_{sn}^{(3)} + C_s} \right] \left[\frac{C_n}{K_n^{(3)} + C_n} \right] \left[\frac{C_p}{K_{pn}^{(3)} + C_p} \right] I(C_o) \end{array} \right\}
\end{aligned} \tag{B.2.22}$$

$$(\theta + \rho_b K_{do})\frac{\partial C_o}{\partial t} + \mathbf{V}\cdot\nabla C_o = \nabla\cdot\theta\mathbf{D}\cdot\nabla C_o$$

$$-\left(\alpha\frac{\partial p}{\partial t} + \Lambda_o\right)(\theta + \rho_b K_{do})C_o + m_o - \frac{\rho^*}{\rho}qC_o + (F - \frac{\partial\theta}{\partial t})\frac{\partial h}{\partial t}C_o + (\frac{\rho_w}{\rho})\mathbf{V}\cdot\nabla(\frac{\rho}{\rho_w})C_o$$

$$-(\theta + \rho_b K_{d1})r_o^{(1)}C_1 - (\theta + \rho_b K_{d3})r_o^{(3)}C_3 = \nabla\cdot\theta\mathbf{D}\cdot\nabla C_o$$

$$-\left(\alpha\frac{\partial p}{\partial t} + \Lambda_o\right)(\theta + \rho_b K_{do})C_o + m_o - \frac{\rho^*}{\rho}qC_o + (F - \frac{\partial\theta}{\partial t})\frac{\partial h}{\partial t}C_o + (\frac{\rho_w}{\rho})\mathbf{V}\cdot\nabla(\frac{\rho}{\rho_w})C_o$$

$$-\left[(\theta + \rho_b K_{d1})C_1\right]\left\{\gamma_o^{(1)}\mu_o^{(1)}\left[\frac{C_s}{K_{so}^{(1)} + C_s}\right]\left[\frac{C_o}{K_o^{(1)} + C_o}\right]\left[\frac{C_p}{K_{po}^{(1)} + C_p}\right] + \alpha_o^{(1)}\lambda_o^{(1)}\left[\frac{C_o}{\Gamma_o^{(1)} + C_o}\right]\right\}$$

$$-\left[(\theta + \rho_b K_{d3})C_3\right]\left\{\gamma_o^{(3)}\mu_o^{(3)}\left[\frac{C_s}{K_{so}^{(3)} + C_s}\right]\left[\frac{C_o}{K_o^{(3)} + C_o}\right]\left[\frac{C_p}{K_{po}^{(3)} + C_p}\right] + \alpha_o^{(3)}\lambda_o^{(3)}\left[\frac{C_o}{\Gamma_o^{(3)} + C_o}\right]\right\} \qquad \text{(B.2.23)}$$

$$(\theta + \rho_b K_{dn})\frac{\partial C_n}{\partial t} + \mathbf{V}\cdot\nabla C_n = \nabla\cdot\theta\mathbf{D}\cdot\nabla C_n$$

$$-\left(\alpha\frac{\partial p}{\partial t} + \Lambda_n\right)(\theta + \rho_b K_{dn})C_n + m_n - \frac{\rho^*}{\rho}qC_n + (F - \frac{\partial\theta}{\partial t})\frac{\partial h}{\partial t}C_n + (\frac{\rho_w}{\rho})\mathbf{V}\cdot\nabla(\frac{\rho}{\rho_w})C_n$$

$$-(\theta + \rho_b K_{d2})r_n^{(2)}C_2 - (\theta + \rho_b K_{d3})r_n^{(3)}C_3 = \nabla\cdot\theta\mathbf{D}\cdot\nabla C_n$$

$$-\left(\alpha\frac{\partial p}{\partial t} + \Lambda_n\right)(\theta + \rho_b K_{dn})C_n + m_n - \frac{\rho^*}{\rho}qC_n + (F - \frac{\partial\theta}{\partial t})\frac{\partial h}{\partial t}C_n + (\frac{\rho_w}{\rho})\mathbf{V}\cdot\nabla(\frac{\rho}{\rho_w})C_n$$

$$-\left[(\theta + \rho_b K_{d2})C_2\right]\left\{\gamma_n^{(2)}\mu_n^{(2)}\left[\frac{C_s}{K_{sn}^{(2)} + C_s}\right]\left[\frac{C_n}{K_n^{(2)} + C_n}\right]\left[\frac{C_p}{K_{pn}^{(2)} + C_p}\right] + \alpha_n^{(2)}\lambda_n^{(2)}\left[\frac{C_n}{\Gamma_n^{(2)} + C_n}\right]\right\}$$

$$-\left[(\theta + \rho_b K_{d3})C_3\right]\left\{\gamma_n^{(3)}\mu_n^{(3)}\left[\frac{C_s}{K_{sn}^{(3)} + C_s}\right]\left[\frac{C_n}{K_n^{(3)} + C_n}\right]\left[\frac{C_p}{K_{pn}^{(3)} + C_p}\right] + \alpha_n^{(3)}\lambda_n^{(3)}\left[\frac{C_n}{\Gamma_n^{(3)} + C_n}\right]\right\} \qquad \text{(B.2.24)}$$

$$(\theta + \rho_b K_{dp})\frac{\partial C_p}{\partial t} + \mathbf{V}\cdot\nabla C_p = \nabla\cdot\theta\mathbf{D}\cdot\nabla C_p$$

$$-\left(\alpha\frac{\partial p}{\partial t} + \Lambda_p\right)(\theta + \rho_b K_{dp})C_p + m_p - \frac{\rho^*}{\rho}qC_p + (F - \frac{\partial\theta}{\partial t})\frac{\partial h}{\partial t}C_p + (\frac{\rho_w}{\rho})\mathbf{V}\cdot\nabla(\frac{\rho}{\rho_w})C_p$$

$$-(\theta + \rho_b K_{d1})r_p^{(1)}C_1 - (\theta + \rho_b K_{d2})r_p^{(2)}C_2 - (\theta + \rho_b K_{d3})r_p^{(3)}C_3 = \nabla\cdot\theta\mathbf{D}\cdot\nabla C_p$$

$$-\left(\alpha\frac{\partial p}{\partial t} + \Lambda_p\right)(\theta + \rho_b K_{dp})C_p + m_p - \frac{\rho^*}{\rho}qC_p + (F - \frac{\partial\theta}{\partial t})\frac{\partial h}{\partial t}C_p + (\frac{\rho_w}{\rho})\mathbf{V}\cdot\nabla(\frac{\rho}{\rho_w})C_p$$

$$-\left[(\theta + \rho_b K_{d1})C_1\right]\left\{\epsilon_o^{(1)}\frac{\mu_o^{(1)}}{Y_o^{(1)}}\left[\frac{C_s}{K_{so}^{(1)} + C_s}\right]\left[\frac{C_o}{K_o^{(1)} + C_o}\right]\left[\frac{C_p}{K_{po}^{(1)} + C_p}\right]\right\} \qquad \text{(B.2.25)}$$

$$-\left[(\theta + \rho_b K_{d2})C_2\right]\left\{\epsilon_n^{(2)}\frac{\mu_n^{(2)}}{Y_n^{(2)}}\left[\frac{C_s}{K_{sn}^{(2)} + C_s}\right]\left[\frac{C_n}{K_n^{(2)} + C_n}\right]\left[\frac{C_p}{K_{pn}^{(2)} + C_p}\right]\right\}$$

$$-\left[(\theta + \rho_b K_{d3})C_3\right]\left\{\begin{array}{l}\epsilon_o^{(3)}\frac{\mu_o^{(3)}}{Y_o^{(3)}}\left[\frac{C_s}{K_{so}^{(3)} + C_s}\right]\left[\frac{C_o}{K_o^{(3)} + C_o}\right]\left[\frac{C_p}{K_{po}^{(3)} + C_p}\right] \\ + \epsilon_n^{(3)}\frac{\mu_n^{(3)}}{Y_n^{(3)}}\left[\frac{C_s}{K_{sn}^{(3)} + C_s}\right]\left[\frac{C_n}{K_n^{(3)} + C_n}\right]\left[\frac{C_p}{K_{pn}^{(3)} + C_p}\right]I(C_o)\end{array}\right\}$$

$$(\theta + \rho_b K_{d1})\frac{\partial C_1}{\partial t} + \mathbf{V}\cdot\nabla C_1 = \nabla\cdot\theta\mathbf{D}\cdot\nabla C_1$$

$$-\left(\alpha\frac{\partial p}{\partial t}+\Lambda_1\right)(\theta+\rho_b K_{d1})C_1 + m_1 - \frac{\rho^*}{\rho}qC_1 + (F-\frac{\partial\theta}{\partial t})\frac{\partial h}{\partial t}C_1 + (\frac{\rho_w}{\rho})\mathbf{V}\cdot\nabla(\frac{\rho}{\rho_w})C_1$$

$$+\left(\theta + \rho_b K_{d1}\right)\left(\frac{\partial C_1}{\partial t}\right)_{\textit{microbial activity}} = \nabla\cdot\theta\mathbf{D}\cdot\nabla C_1 \qquad \text{(B.2.26)}$$

$$-\left(\alpha\frac{\partial p}{\partial t}+\Lambda_1\right)(\theta+\rho_b K_{d1})C_1 + m_1 - \frac{\rho^*}{\rho}qC_1 + (F-\frac{\partial\theta}{\partial t})\frac{\partial h}{\partial t}C_1 + (\frac{\rho_w}{\rho})\mathbf{V}\cdot\nabla(\frac{\rho}{\rho_w})C_1$$

$$+\left(\theta + \rho_b K_{d1}\right)C_1\left\{u_o^{(1)}\left[\frac{C_s}{K_{so}^{(1)}+C_s}\right]\left[\frac{C_o}{K_o^{(1)}+C_o}\right]\left[\frac{C_p}{K_{po}^{(1)}+C_p}\right] - \lambda_o^{(1)}\right\}$$

$$(\theta + \rho_b K_{d2})\frac{\partial C_2}{\partial t} + \mathbf{V}\cdot\nabla C_2 = \nabla\cdot\theta\mathbf{D}\cdot\nabla C_2$$

$$-\left(\alpha\frac{\partial p}{\partial t}+\Lambda_2\right)(\theta+\rho_b K_{d2})C_2 + m_2 - \frac{\rho^*}{\rho}qC_2 + (F-\frac{\partial\theta}{\partial t})\frac{\partial h}{\partial t}C_2 + (\frac{\rho_w}{\rho})\mathbf{V}\cdot\nabla(\frac{\rho}{\rho_w})C_2$$

$$+\left(\theta + \rho_b K_{d2}\right)\left(\frac{\partial C_2}{\partial t}\right)_{\textit{microbial activity}} = \nabla\cdot\theta\mathbf{D}\cdot\nabla C_2 \qquad \text{(B.2.27)}$$

$$-\left(\alpha\frac{\partial p}{\partial t}+\Lambda_2\right)(\theta+\rho_b K_{d2})C_2 + m_2 - \frac{\rho^*}{\rho}qC_2 + (F-\frac{\partial\theta}{\partial t})\frac{\partial h}{\partial t}C_2 + (\frac{\rho_w}{\rho})\mathbf{V}\cdot\nabla(\frac{\rho}{\rho_w})C_2$$

$$+\left(\theta + \rho_b K_{d2}\right)C_2\left\{u_n^{(2)}\left[\frac{C_s}{K_{sn}^{(2)}+C_s}\right]\left[\frac{C_n}{K_n^{(2)}+C_n}\right]\left[\frac{C_p}{K_{pn}^{(2)}+C_p}\right] - \lambda_n^{(2)}\right\}$$

$$
\begin{aligned}
&(\theta + \rho_b K_{d3})\frac{\partial C_3}{\partial t} + \mathbf{V}\cdot\nabla C_3 \;=\; \nabla\cdot\theta\mathbf{D}\cdot\nabla C_3 \\
&-\left(\alpha\frac{\partial p}{\partial t}+\Lambda_3\right)(\theta+\rho_b K_{d3})C_3 \;+\; m_3 - \frac{\rho^*}{\rho}qC_3 + (F - \frac{\partial\theta}{\partial t})\frac{\partial h}{\partial t}C_3 + (\frac{\rho_w}{\rho})\mathbf{V}\cdot\nabla(\frac{\rho}{\rho_w})C_3 \\
&+\left(\theta + \rho_b K_{d3}\right)\left(\frac{\partial C_3}{\partial t}\right)_{\textit{microbial activity}} \;=\; \nabla\cdot\theta\mathbf{D}\cdot\nabla C_3 \\
&-\left(\alpha\frac{\partial p}{\partial t}+\Lambda_3\right)(\theta+\rho_b K_{d3})C_3 \;+\; m_3 - \frac{\rho^*}{\rho}qC_3 + (F - \frac{\partial\theta}{\partial t})\frac{\partial h}{\partial t}C_3 + (\frac{\rho_w}{\rho})\mathbf{V}\cdot\nabla(\frac{\rho}{\rho_w})C_3 \\
&+\left(\theta + \rho_b K_{d3}\right)C_3\left\{\begin{array}{c}
\mu_o^{(3)}\left[\frac{C_s}{K_{so}^{(3)}+C_s}\right]\left[\frac{C_o}{K_o^{(3)}+C_o}\right]\left[\frac{C_p}{K_{po}^{(3)}+C_p}\right] - \lambda_o^{(3)} \\
+\mu_n^{(3)}\left[\frac{C_s}{K_{sn}^{(3)}+C_s}\right]\left[\frac{C_n}{K_n^{(3)}+C_n}\right]\left[\frac{C_p}{K_{pn}^{(3)}+C_p}\right]I(C_o) - \lambda_n^{(3)}I(C_o)
\end{array}\right\}
\end{aligned}
\qquad \text{(B.2.28)}
$$

The specification of boundary conditions is a difficult and intricate task in transport modeling. From the dynamic point of view, a boundary segment may be classified as either flow-through or impervious. From the physical point of view, it is a soil-air interface, or soil-soil interface, or soil-water interface. From the mathematical point of view, it may be treated as a Dirichlet boundary on which the total analytical concentration is prescribed, Neumann boundary on which the flux due to the gradient of total analytical concentration is known, or Cauchy boundary on which the total flux is given. An even more difficult mathematical boundary is the variable conditions on which the boundary conditions are not known a priori but are themselves the solution to be sought. In other words, on the mathematically variable boundary, either Neumann or Cauchy conditions may prevail and change with time. Which condition prevails at a particular time can be determined only in the cyclic processes of solving the governing equations (Freeze 1972a, 1972b; Yeh and Ward 1980; Yeh and Ward, 1981).

B.3 Simplification

The governing equations derived in Appendix B represents the density-dependent flow and the fate and transport of microbes and chemicals in slightly deformable media as characterized by the modified compressibilities, α' and β'. In the development of 3DFATMIC, it is assumed that the media are non-deformable, i.e, $\alpha' = 0$ and $\beta' = 0$. As a result of this simplification, one has

$$F - \frac{\partial \theta}{\partial t} = 0 \tag{B.3.1}$$

To remove this restriction, it is as simple as making apple pie. Finally, it should be noted that the terms associated with source/sinks can be reduced to source terms only. It is obvious that

$$\begin{aligned} m - \frac{\rho^*}{\rho} qC &= q_{in} C_{in} - \frac{\rho^*}{\rho} qC \quad \text{for a source} \\ m - \frac{\rho^*}{\rho} qC &= q_{in} C_{in} \quad \text{for a sink} \end{aligned} \tag{B.3.2}$$

because for a source $m = q_{in} C_{in}$ and for a sink $m = qC$ and $\rho^* = \rho$. The governing equations used in Chapter 2 were obtained from the corresponding equations in this appendix using Eqs. (B.3.1) and (B.3.2) and setting $\alpha = 0$.