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Project Summary

User's Manuals for Two-(2DFATMIC) and Three-(3DFATMIC) Dimensional Subsurface Flow, Fate and Transport of Microbes and Chemicals Models

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Two new computer models were developed for the simulation of Subsurface Flow, FAte and Transport of MIcrobes and Chemicals Model using a Lagrangian-Eulerian adapted zooming and peak capturing algorithm. 2DFATMIC is a two-dimensional model, and 3DFATMIC is a three-dimensional model. The two models are 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 in each program. The input data 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 outputs include the spatial distribution of pressure head, total head, moisture content, Darcy velocity component, concentrations, and material fluxes at any desired time step. For each model, 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.

Each 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 the mesh Courant number is limited only by the accuracy requirement of the Eulerian step. Since these models also include 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 the diffusion step, the more accuracy at the Eulerian step. To sum up, the larger the time-step size used, the better the solution that can be obtained with respect to advective transport. 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.

This Project Summary was developed by EPA's National Risk Management Research Laboratory's Subsurface Protection and Remediation Division, Ada, OK, to announce key findings of

the research project that is fully documented in a separate report of the same title (see Project Report ordering information at back).

Introduction

The two new models (2DFATMIC and 3DFATMIC: 2-Dimensional and 3-Dimensional Subsurface Flow, FAte and Transport of MIcrobes and Chemicals) 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 a ground-water environment. The two models are identical in terms of their background theories and capabilities except for the model dimensionality. For both models, the Galerkin finite element method is used to discretize the Richards' equation for the flow module, and for the transport module, the hybrid Lagrangian-Eulerian approach with an adapted zooming and capturing algorithm is used to discretize the transport equation. This approach can completely eliminate spurious oscillation, numerical dispersion, and peak clipping due to advective 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 the time steps is the requirement of accuracy with respect to dispersive transport, which does not pose severe restrictions.

The special features of the models are their flexibility and versatility in modeling as wide a range of problems as possible. The models 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 for 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 for treating the mass matrix - consistent and lumping; (9) three options (exact relaxation, under- and over- relaxation) for estimating the nonlinear matrix; (10) automatic time-step size reset when boundary conditions or sources/sinks change abruptly; (11) two options, Galerkin weighting or upstream weighting, for the advection term in the transport module; (12) two options for the Lagrangian numerical scheme in the transport module, enabling and disabling adapted zooming scheme; (13) two options for solving the Eulerian step including the enabling and disabling of diffusion zooming; (14) mass balance checking over the entire region for every time step; and, (15) modification of the program if different conditions are used.

Description of Models

Mathematical Statement of 2DFATMIC and 3DFATMIC

2DFATMIC and 3DFATMIC are 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, which describe the flow of a variable-density fluid, are basically the Richards' equation.

Governing Flow Equation

$$\frac{\rho}{\rho_w}\frac{d\theta}{dh}\frac{\partial h}{\partial h} = \nabla\left[\mathbf{K}_s K_r \cdot \left(\nabla h + \frac{\rho}{\rho_w}\nabla z\right)\right] + \frac{\rho^*}{\rho_w} q \quad \left(\text{or } -\frac{\rho}{\rho_w} q\right) \tag{1}$$

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

$$\mathbf{K}_s = \mathbf{K}_{sw}\frac{(\rho/\rho_w)}{(\mu/\mu_w)} \tag{2}$$

where h is the referenced pressure head defined as $p/\rho_w g$ in which p is pressure (M/LT^2), $\mathbf{K}_s$ 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), 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 Darcy velocity is calculated as follows.

$$\mathbf{v} = -\mathbf{K}_s K_r \cdot \left(\frac{\rho_w}{\rho}\nabla h + \nabla z\right) \tag{3}$$

To solve the governing flow equation, the prescribed initial conditions and boundary conditions are required. In terms of initial conditions, the model can take input initial values or obtain initial values by simulating a steady state version of the system under consideration. In terms of boundary conditions, the model can handle: (1) the prescribed transient concentration over Dirichlet nodes; (2) time dependent fluxes over Neumann nodes; (3) time dependent total fluxes over Cauchy nodes; and (4) 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 (see the original reports for full description).

Governing Equations for Transport

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. Transport of the substrate, oxygen, nitrate and nutrient in the bulk pore fluid is expressed by advection-dispersion equations that are coupled sink terms that account for biodegradation. The biodegradation is modeled with the modified Monod kinetics. The transport equations for the three microbes can be derived based on mass-balance of microbes. The equation for substrate transport is presented here (for complete list of equations, see the original reports).

$$\begin{aligned}
&(\theta+\rho_b K_{ds})\frac{\partial C_s}{\partial t} + \mathbf{v}\cdot\nabla C_s = \nabla\cdot\theta\mathbf{D}\cdot\nabla C_s - \Lambda_s \\
&(\theta+\rho_b K_{ds})C_s + q_{in}C_{sin} + \left(\frac{\rho_w}{\rho}v\cdot\nabla\left(\frac{\rho}{\rho_w}\right) - \frac{\rho^*}{\rho}q_{in}\right)C_s \\
&-\left[(\theta+\rho_b K_{d1})C_1\right] \\
&\left\{\frac{\mu_o^{(1)}}{Y_o^{(1)}}\left[\frac{C_s}{K_{so}^{(1)}+C_s}\right]\left[\frac{C_o}{K_o^{(1)}+C_o}\right]\left[\frac{C_p}{K_{po}^{(1)}+C_p}\right]\right\} \\
&-\left[(\theta+\rho_b K_{d2})C_2\right] \\
&\left\{\frac{\mu_n^{(2)}}{Y_n^{(2)}}\left[\frac{C_s}{K_{sn}^{(2)}+C_s}\right]\left[\frac{C_n}{K_n^{(2)}+C_n}\right]\left[\frac{C_p}{K_{pn}^{(2)}+C_p}\right]\right\} \\
&-\left[(\theta+\rho_b K_{d3})C_3\right] \\
&\left\{\frac{\mu_o^{(3)}}{Y_o^{(3)}}\left[\frac{C_s}{K_{so}^{(3)}+C_s}\right]\left[\frac{C_o}{K_o^{(3)}+C_o}\right]\left[\frac{C_p}{K_{po}^{(3)}+C_p}\right] + \frac{\mu_n^{(3)}}{Y_n^{(3)}}\left[\frac{C_s}{K_{sn}^{(3)}+C_s}\right]\left[\frac{C_n}{K_n^{(3)}+C_n}\right]\left[\frac{C_p}{K_{pn}^{(3)}+C_p}\right]I(C_o)\right\}
\end{aligned} \tag{4}$$

where θ is the moisture content, ρ_b is the bulk density of the medium (M/L^3), t is time (T), **V** is the discharge (L/T), ∇ is the del operator, **D** is the dispersion coefficient tensor (L^2/T), where Λ_s, is the transformation rate constants, K_{ds}, K_{d1}, K_{d2}, K_{d3} are the distribution coefficient of the dissolved substrate, microbe No. 1, microbe No. 2 and microbe No. 3, q_{in} is the source rate of water, C_{sin} is the source concentration of substrate, and C_s, C_o, C_n, C_p, are the dissolved concentrations of substrate, oxygen, nitrogen and nutrient. $I(C_0) = [1 + C_0/K_c]^{-1}$ is an inhibition function which is under the assumption that denitrifying enzyme inhibition is reversible and noncompetitive, where K_c is 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 No. 1, the maximum specific nitrate-based growth rate for microbe No. 2, the maximum specific oxygen-based growth rate for microbe No. 3, and the maximum specific nitrate-based growth rate for microbe No. 3 (1/T), respectively; $Y_o^{(1)}$, $Y_n^{(2)}$, $Y_o^{(3)}$, and $Y_n^{(3)}$ are the yield coefficient for microbe No. 1 utilizing oxygen, the yielding coefficient for microbe No. 2 utilizing nitrate, the yielding coefficient for microbe No. 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 microbes No. 1 and No. 3, respectively, the retarded substrate saturation constants under anaerobic conditions with respect to microbes No. 2 and No. 3, respectively, the retarded nutrient saturation constants under aerobic conditions with respect to microbes No. 1 and No. 3, respectively, and the retarded nutrient saturation constants under anaerobic conditions with respect to microbes No. 2 and No. 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 microbes No. 1 and No. 3, respectively, and the retarded nitrate saturation constant under anaerobic conditions with respect to microbes No. 2 and No. 3 (M/L^3), respectively.

The dispersion coefficient tensor **D** in Eq. (4) is given by

$$\theta \mathbf{D} = a_T |\mathbf{v}| \delta + (a_L - a_T) \mathbf{vv}/|\mathbf{v}| + \theta a_m \tau \delta \qquad (5)$$

where $|\mathbf{V}|$ is the magnitude of **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. To solve the transport equations, appropriate type initial and boundary conditions (Dirichlet, Neumann, Cauchy, and Variable Boundary Conditions: see the main report for detail) are required.

Numerical Approximation

For the flow module, the Galerkin finite element method is used to discretize the Richards' equation which governs the flow in variably saturated media. For the transport module, the hybrid Lagrangian-Eulerian approach with an adapted zooming and peak capturing algorithm (LEZOOMPC) is used to discretize the transport equation. Basically, LEZOOMPC is a modified method of the zoomable hidden fine-mesh approach (LEZOOM) and exact peak capturing and oscillation-free scheme (EPCOF) to solve advection-dispersion transport equations. The detailed algorithm of the LEZOOMPC can be found elsewhere. This approach can completely eliminate spurious oscillation, numerical dispersion, and peak clipping due to advective 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 the time steps is the requirement of accuracy with respect to dispersive transport which does not pose severe restrictions.

Figure 1 is the basic conceptual structure for solving transport by 2DFATMIC and 3DFATMIC. It contains two main steps, Lagrangian and a Eulerian step. Readers are referred to the main reports for detailed discussion. 2DFATMIC consists of a MAIN program and 77 subroutines whereas 3DFATMIC consists of a MAIN program and 120 subroutines. The MAIN is utilized to specify the sizes of all arrays. The functions of these subroutines are described in the main reports.

Sample Problems

To verify the two models, several hypothetical sample problems are presented in each report. In the 2DFATMIC user's manual, three illustrative examples were presented. The first one is a one-dimensional flow problem through a soil column. The second one is a one-dimensional transport problem through a soil column. The third one is two-dimensional coupled flow and transport with biodegradation. In the 3DFATMIC manual, eight illustrative examples are presented. The first three examples, originally designed for 3DFEMWATER, are flow only problems. The fourth and fifth examples, originally designed for 3DLEWASTE, are 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. In this project summary, two example problems are introduced; one from 2DFATMIC and another one from 3DFATMIC program.

Two-Dimensional Coupled Flow and Multicomponent Transport Problem for 2DFATMIC program

This example is presented in the 2DFATMIC user's manual as problem number 3. The example aquifer used for this example is 1.4 meters long in the X direction, 1.6 meters thick in the Z direction, and is shown in Figure 2. This aquifer has 8 different materials, one injection well, and one extraction well. The initial condition of the flow field is obtained by simulating a steady state flow field without sources and sinks. Then the flow field and concentration distribution are updated at each time step.

There are two types of microbes included in the system, say microbe No. 1 and microbe No. 3 with 1.77×10^{-4} Kg/m³ initially. The initial concentrations of the chemicals are 5×10^{-3} Kg/m³ of substrate, 5×10^{-3} Kg/m³ of oxygen, 5×10^{-3} Kg/m³ of nitrate, and 3×10^{-3} Kg/m³ of nutrient. The daily injection and withdrawal rates of water are 3.75×10^{-3} and 3.75×10^{-3} m³, respectively. The total hydraulic head is 1.0 m at the upstream boundary AB and 0.0 m at the downstream

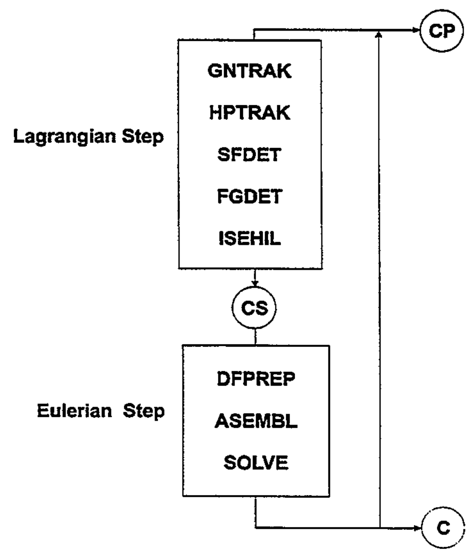


Figure 1. The basic structure for coding transport part of 2DFATMIC and 3DFATMIC.

boundary CD (Figure 2). For transport simulation, a variable boundary condition is implemented at the downstream boundary CD (Figure 2.) and 1.77×10^{-4} Kg/m^3 of microbe No. 1, 1.77×10^{-4} Kg/m^3 of microbe No. 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 flows through the upstream boundary. Because microbe No. 2 does not exist in this environment, the initial and boundary conditions for this component are set to zero in this simulation. This problem is set up for a 4 day simulation.

For numerical simulation the region is divided into 14 x 16 = 224 square elements of size = 0.1 by 0.1, and 15 x 17 = 255 nodes. A time-step size of 0.05 is used and an 80 time-step simulation is made.

Simulation Results

To execute this problem, the maximum control-integers in the MAIN program of 2DFATMIC must be modified as specified in the manual. Input parameters used in this example are shown in tabular format in the manual. The electronic files containing the model input and output of this example are attached in the main report. The results of velocity fields simulated at t = 2 days and 4 days are shown in Figure 3.

Figure 4 contains the simulation results of the transport and fate of microbes 1 and 3 at t = 2 days (see the main report for other chemicals).

Three-Dimensional Multicomponent Transport in a Uniform Flow Field for 3DFATMIC

This example is presented in the 3DFATMIC user's manual to demonstrate 3-D multicomponent transport behavior. The kinetic and microbial parameters for the simulation are shown in the 3DFATMIC manual. 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 5). The initial condition is comprised of a patch with dimensions 2mx1mx2m (Figure 5), 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 microbe No. 1 is 0.23 mg/L and the retardation factor associated with microbes is 1000. The boundary conditions and physical parameters are shown in Figure 6. Although the nitrate, nutrient, microbe No. 2 and microbe No. 3 must be included in the

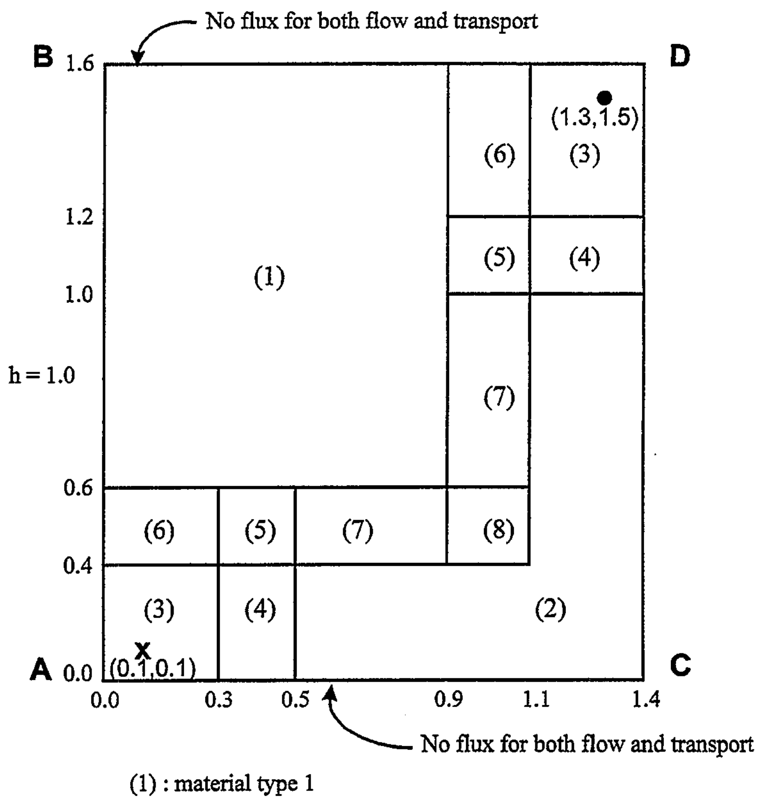


Figure 2. *The region of example problem with 8 different material properties.*

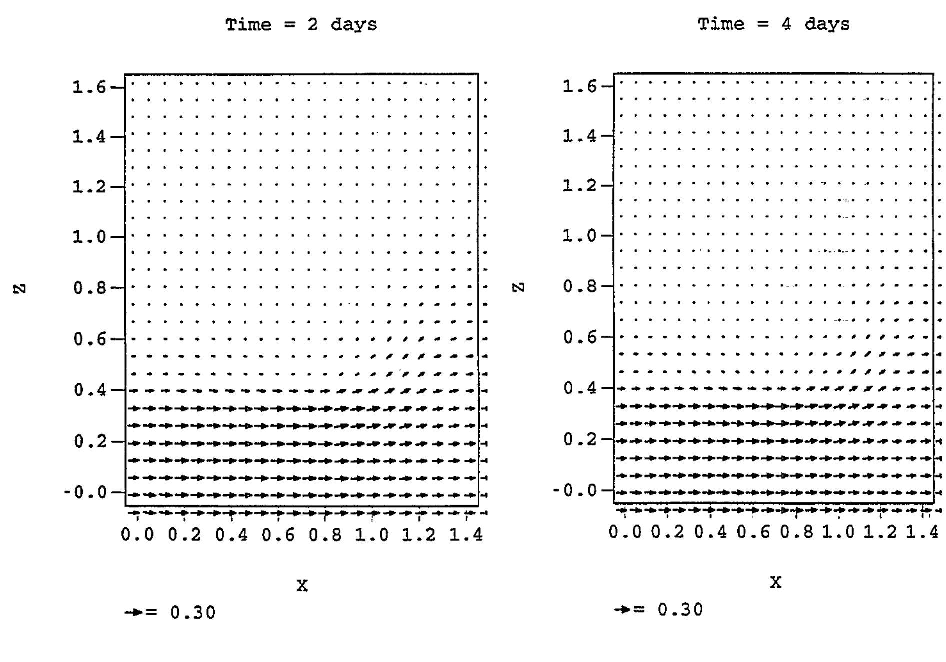


Figure 3. *The flow field at (a) t = 2 days and (b) t = 4 days.*

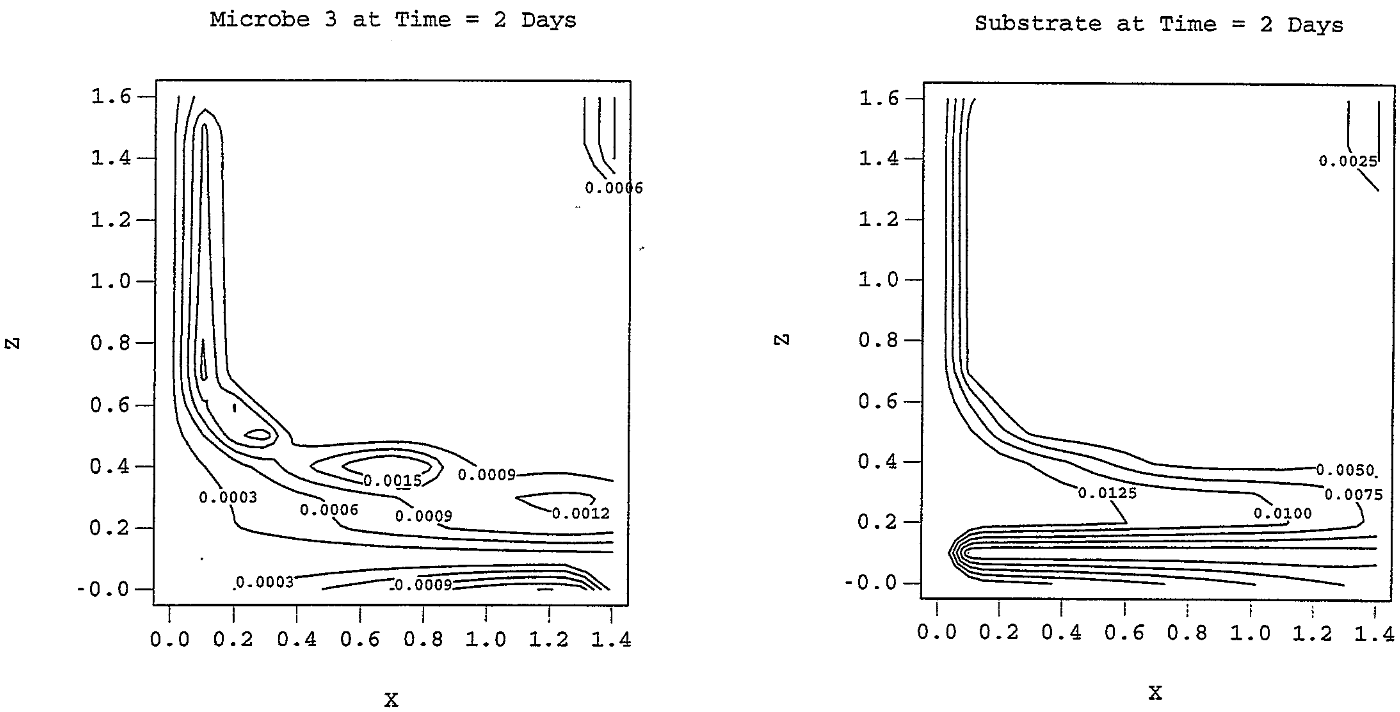


Figure 4. *Simulation results of microbes 1 and 3 at t = 2 days.*

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.

Simulation Results

To execute this problem, the maximum control-integers in MAIN program of 3DFATMIC must be modified as specified in the manual. Input parameters used in this example are shown in tabular format in the manual. The electronic files containing the model input and output of this example are attached in the main report. Figure 7 shows the simulation results of total microbial mass distributions at 200 days on an x-y cross-section.

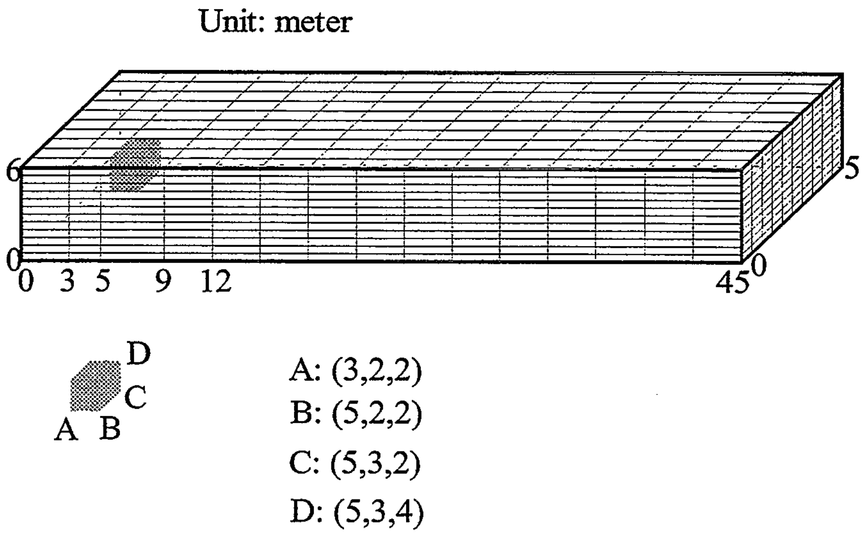


Figure 5. *The region of interest.*

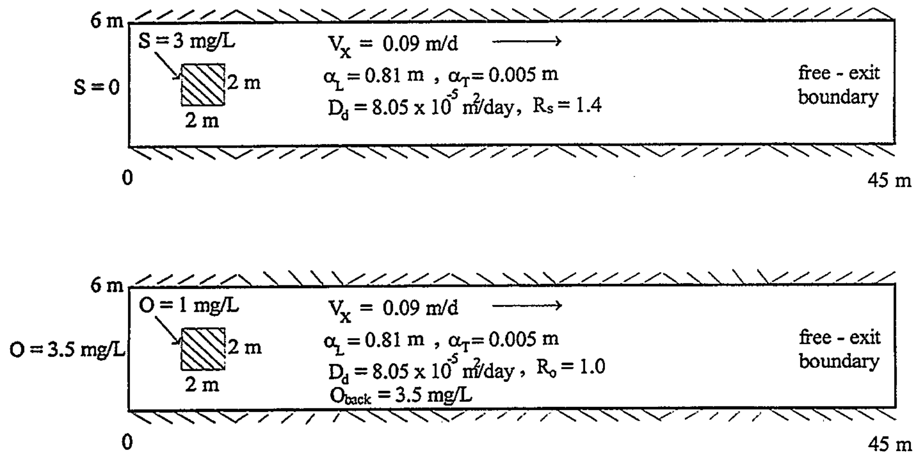
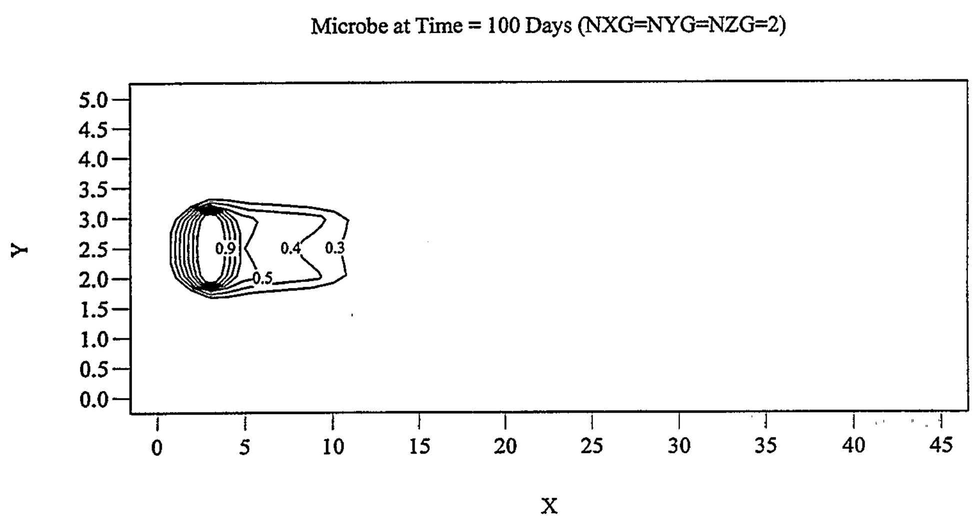


Figure 6. *The x-z cross-section of region of interest and the associated physical parameters.*



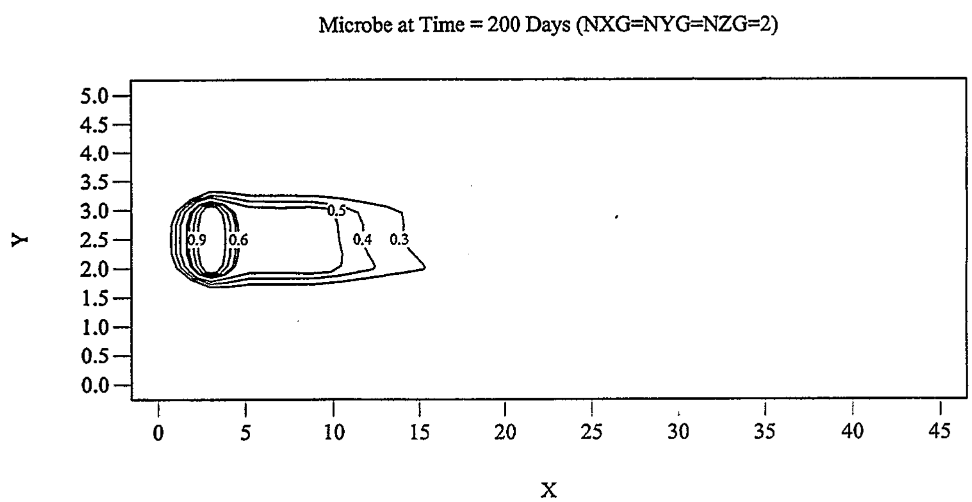


Figure 7. *Total microbial mass distributions at t = 100 and t = 200 days on an x-y cross-section. Concentration isolines are in mg/liter of aquifer materials.*

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The complete report, entitled "2DFATMIC, Two-Dimensional Subsurface Flow, Fate and Transport of Microbes and Chemicals Model, User's Manual, Version 1.0" (Order No. PB97-205637; Cost $31.00, subject to change) and "3DFATMIC, Three-Dimensional Subsurface Flow, Fate and Transport of Microbes and Chemicals Model, User's Manual, Version 1.0" (Order No. PB97-205413; Cost $44.00, subject to change) will be available only from:

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