

BIOF&T Technical Information

Analysis of Water Flow

Governing Equations

The mass conservation equation for isothermal water flow in an incompressible porous medium under variably saturated condition can be described by the modified form of the Richards equation [Richards, 1931; Huyakorn et al., 1984].

$$\frac{\partial}{\partial x_i} \left[K_{ij} k_{rw} \left(\frac{\partial y}{\partial x_j} + u_j \right) \right] = \left(S_w S_s + f \frac{dS_w}{dy} \right) \frac{\partial y}{\partial t} - q \quad [1]$$

where K_{ij} is the saturated hydraulic conductivity tensor, k_{rw} is the relative permeability, y is the pressure head, $x_i, x_j (i, j = 1, 2, 3)$ are the spatial coordinates, t is time, u_j is the unit vector pointing in the vertical direction upward, S_w is the water saturation, S_s is the specific storage, f is porosity, and q is the source/sink volumetric rate per unit volume of the porous medium.

The initial and boundary conditions can be expressed as

$$\begin{aligned} y(x_i, 0) &= y_0(x_i) \\ y(x_i, t) &= y_p \quad \text{on } B_1 \\ q_i n_i &= -q_n \quad \text{on } B_2 \end{aligned} \quad [2]$$

where $y_0(x_i)$ is the initial pressure head at location x_i , B_1 is the segment of the domain boundary where prescribed pressure head is equal to y_p , B_2 is the portion of the boundary where water flux equal to $-q_n$ is prescribed, n_i is the outward unit vector normal to the boundary B_2 , and the Darcy velocity, q_i is defined as

$$q_i = -K_{ij} k_{rw} \left(\frac{\partial y}{\partial x_j} + u_j \right) \quad [3]$$

If the sources and sinks are present, these are treated as point sources and sinks. The finite element mesh is usually set up such that each well coincide with a node location. The volumetric flow rate at each well is treated as the Dirac delta function and the entire discharge/recharge of the well can be assigned to the relevant nodal equation. For spatially distributed sources or sinks, the recharge and discharge rates are divided among the nodes within such areas proportional to the recharge/discharge area represented by each node. Under heterogeneous conditions due weighting should be given to the transmissivity associated with the nodes in the recharge/discharge areas.

Constitutive Relations for Flow

BIOF&T allows use of two constitutive models for relating permeability, saturation and pressure and these are 1) van Genuchten constitutive model and 2) linear constitutive model

van Genuchten model

Relationship between head, saturation, and relative permeability can be expressed as

$$\bar{S}_w = \left[1 + (\alpha y)^n \right]^{-m} \quad [4]$$

$$k_{rw} = \bar{S}_w^{0.5} \left[1 - \left(1 - \bar{S}_w \right)^{1/m} \right]^2 \quad [5]$$

where $\bar{S}_w = \frac{S_w - S_m}{1 - S_m}$ is the effective water saturation, S_m is the irreducible water saturation, α [L^{-1}] and n [-] are porous medium parameters, and $m = 1 - 1/n$.

linear constitutive model:

Water saturation, head, and relative permeability are linearly related as:

$$k_{rw} = \frac{S_w - S_m}{1 - S_m} \quad [6]$$

$$\frac{y - y_a}{y_m - y_a} = \frac{1 - S_w}{1 - S_m} \quad [7]$$

where y_a is the air entry pressure [L], and y_m is the head [L] corresponding to the irreducible water saturation S_m .

Chapter 4 of the BIOF&T document gives an overview of the approaches that are commonly used to estimate parameters in the constitutive models discussed above.

Solution Techniques

Equation [1] is approximated in three dimensional space using the Galerkin finite element method. BIOF&T allows use of rectangular 2-D/3-D prism or isoparametric quadrilateral/hexahedral elements to accurately model irregular domain and material boundaries. The influence coefficients for these elements are computed numerically in the beginning of the program execution and stored for later retrieval.

Computational cost of a typical 3-D flow and transport problem can be enormous. In BIOF&T a computationally efficient solution is obtained by discretizing the solution domain into horizontal slices. These slices are solved in sequence individually to reduce the matrix size. An iterative approach is implemented to perform solution among slices. This results in considerable calculative time saving, enabling solution of large problems on small computers.

The Newton-Raphson iterative method is used to solve the nonlinear problem. The water saturations are updated as a function of the pressure during the simulation.

Analysis of Multicomponent Transport

Governing Equations

BIOF&T models aqueous phase transport of up to five species in variably saturated porous media. The unsaturated zone and the groundwater aquifers are considered to be consisting of fractured and/or granular porous media. BIOF&T-3D allows computationally efficient uncoupled or coupled solution of the unsaturated and the saturated zones. When solution is uncoupled, the flow and transport in the unsaturated zone is modeled either in 1-D vertical direction or in 2-D planar or radial symmetric vertical sections. The flow and dissolved phase transport in the saturated zone are modeled as 2-D areal or a 3-D phenomenon. During the solution of the unsaturated zone, the temporal and spatial distribution of the contaminant effluent rates are computed. These are used to define contaminant loadings to groundwater during simulation of aqueous phase transport in the saturated zone. An option for coupled three dimensional solution of the unsaturated and saturated zones can be selected for complicated problems.

A typical subsurface transport media has five distinct regions: 1) voids filled with air, 2) mobile water located inside the larger interaggregate pores or fractures, 3) immobile water located mainly in the intra-aggregate pores or in the porous media surrounding fractures, 4) a dynamic soil region, in equilibrium with the mobile phase, and 5) a stagnant soil region where mass transfer is diffusion limited.

van Genuchten and Wierenga, 1976 expressed the general transport equation as:

$$\begin{aligned} \frac{\partial}{\partial t}(q_m C_{wm}) + \frac{\partial}{\partial t}(q_{im} C_{wim}) + \frac{\partial}{\partial t}(f r P_{wm}) + \frac{\partial}{\partial t}[(1-f)r P_{wim}] \\ = \frac{\partial}{\partial x_i} \left(q_m D_{ij} \frac{\partial C_{wm}}{\partial x_j} \right) - \frac{\partial}{\partial x_i} (q_i C_{wm}) - q_s C_{ws} \end{aligned} \quad [8]$$

where q_m and q_{im} (equal to 0.0 for unfractured porous media) are the fraction of the soil filled with mobile and immobile water respectively, C_{wm} and C_{wim} are the concentration $[ML^{-3}]$ of species w in the mobile and immobile water respectively, q_i is the Darcy velocity $[L/T]$, P_{wm} and P_{wim} are adsorbed phase concentration of species w in the mobile and immobile phase $[M/M]$ respectively, f is the fraction of the sorption sites which is in direct contact with the mobile liquid (equal to 1.0 for unfractured porous media), r is soil bulk density $[ML^{-3}]$, q_s is the volumetric flow rate of fluid injection (or withdrawal) per unit volume of the porous medium and C_{ws} is the concentration of species w in the injected fluid and D_{ij} is the hydrodynamic dispersion tensor.

Incorporating linear adsorption ($P = K_d C$), mass transfer between mobile and immobile phases, decay losses I_{wm} , and contaminant loading from a contaminant source to the mobile phase H_w , in equation [8] gives

$$\begin{aligned} \frac{\partial C_{wm}}{\partial t} (q_m + f r k_d) + \frac{\partial C_{wim}}{\partial t} [q_{im} + (1-f)r k_d] \\ = \frac{\partial}{\partial x_i} \left(q_m D_{ij} \frac{\partial C_{wm}}{\partial x_j} \right) - q_i \frac{\partial C_{wm}}{\partial x_i} - q(C_{ws} - C_{wm}) - I_{wm} + H_w \end{aligned} \quad [9]$$

$$\frac{\partial C_{wim}}{\partial t} [q_{im} + (1-f)r k_d] = c(C_{wm} - C_{wim}) - I_{wim} \quad [10]$$

Equation [10] expresses the diffusive mass exchange between the mobile and immobile phases where C is a mass transfer coefficient $[T^{-1}]$. Equation [10] is needed only when fractured media is simulated.

Estimating Decay Losses in the Mobile and Immobile Phases

Contaminants entering the soil and groundwater undergo losses through:

1) Biodegradation, and 2) Radioactive decay.

Biodegradation

The biodegradation of dissolved chemicals (mostly organic molecules) is a matter of great interest to hydrogeologists. Biodegradation can completely destroy, transform, or immobilize hydrocarbon species. Hydrocarbons are substrate for microbial growth and an energy source for biodegradation processes that can occur under aerobic or anaerobic conditions.

Aerobic Degradation

Aerobic degradation requires the presence of oxygen as an electron acceptor, substrate as an electron donor, nutrients, moisture and microbial biomass. *Bedient et al.*, 1984 show that under field conditions microbial rates of growth are high compared to the groundwater flow and, therefore, the microbial population can be assumed constant. This eliminates the need for solving an additional equation for microbial growth and transport in the soil and groundwater system. The biodegradation rate of species w in p phase ($p = m$ and im for mobile and immobile phases, respectively) has been estimated by the following two approaches

(1) instantaneous reaction is assumed between the oxygen and the body of the contaminant plume, in p phase

(2) Oxygen and the contaminant are in nonequilibrium and biodegradation losses are expressed by *Monod kinetics*

Anaerobic Biodegradation

Biodegradation in absence of oxygen occurs when microorganisms use other electron acceptors such as nitrate and sulfate. Anaerobic decomposition of species w has been described by a variation of the *Monod kinetics* expressed by *Bouwer and McCarty*, 1984

First Order Biodegradation

If the concentration C_{wp} of the species w is much smaller than the half-maximum rate concentration K_{wan} , decay losses can be expressed as a first order decay phenomenon

Radioactive Decay

When radionuclides enter the soil and groundwater system, they will undergo radioactive decay that can be expressed as a first order process

Biodegradation of Daughter Products

Many chlorinated organics undergo anaerobic transformations that produce daughter products. For example, degradation of PCE may produce TCE, DCE, VC, and CE sequence of daughter species. BIOF&T allows sequential transformation simulations either as an anaerobic or a first order process. Transport equations for each species (maximum 5) are solved where the decay (sink) of the parent species provides a source term in the daughter species equation. It is assumed that the amount of various species used in tissue building and energy production are insignificant so that the decay (sink) of the parent species is equal to the source term in the daughter species equation.

Loading from Hydrocarbon Dissolution

BIOF&T computes the loading to the groundwater H_w from dissolution of nonaqueous phase liquid (NAPL) due to the water infiltrating through the NAPL plume H_{iw} and by groundwater flowing under the NAPL plume H_{gw} as

$$H_w = H_{iw} + H_{gw} \quad [11]$$

H_{iw} is computed assuming an equilibrium between the infiltrating water and the NAPL plume and mass transfer due to the contact between the groundwater and the NAPL plume is computed using the mass transfer model of *Pfannkuch*, 1984.

Initial and Boundary Conditions

The initial and boundary conditions can be expressed as

$$C_{wm}(x_i, 0) = C_{w0} \quad [12]$$

$$C_{wm}(x_i, t) = C_{wt} \quad \text{on B1} \quad [13]$$

$$\left(q_m D_{ij} \frac{\partial C_{wm}}{\partial x_j} \right) = q_{wD} \quad \text{on B2} \quad [14]$$

$$\left(q_m D_{ij} \frac{\partial C_{wm}}{\partial x_j} \right) - q_i \frac{\partial C_{wm}}{\partial x_i} = q_{wT} \quad \text{on B3} \quad [15]$$

where C_{w0} is the initial concentration of species w at location x_i , B1 is the segment of the domain boundary where prescribed concentration is equal to C_{wt} , B2 and B3 are portions of the boundary where dispersive and total solute mass fluxes equal to q_{wD} and q_{wT} respectively are prescribed.

Solution Techniques

Equation [2] is approximated in three dimensional space using the Galerkin finite element method. BIOF&T uses 3-D prism or hexahedral elements to accurately model irregular domain and material boundaries. The elemental influence coefficients are computed numerically in the beginning of the program execution. A computationally efficient solution is obtained by discretizing the solution domain into horizontal slices. These slices are solved in sequence individually to reduce the matrix size. An iterative approach is implemented to perform solution among slices and this results in considerable reduction in the processor time enabling solution of large transport problems on small computers. The Picard iterative method is used in this formulation to solve the species transport equations in series for respective aqueous phase concentrations.