completely unsaturated, or partially unsaturated or partially saturated subsurface media. It also computes and predicts the spatial-temporal distribution of microbes and multi-chemical components. The media may consist of as many types of soils and geologic units as desired with different material properties. Each soil type may be isotropic or anisotropic. The processes governing the distribution of chemical and microbe concentration and temperature include (1) reversible sorption, (2) microbe-chemical interaction, and (3) hydrological transport by flow advection/convection, dispersion/diffusion, and effect of unsaturation.

Method: The generalized Richards' equation and Darcy's law governing pressure distribution and water flow in saturated-unsaturated media are simulated with the Galerkin finite element method subject to appropriate initial and four types of boundary conditions. The equations (a set of PDEs) of transport and fate of chemicals and microbes are derived based on the principle of conservation of mass and the hypothesis of Monad kinetics. The coupled set of PDEs simulated with either the conventional finite element methods or the hybrid Lagrangian-Eulerian finite element method with the adaptive local grid refinement and peak capturing scheme subject to appropriate initial and four types of boundary conditions. Hexahedral elements, triangular prism, and tetrahedral elements are used to facilitate the discretization of the region of interest.

Input: (1) Geometry in terms of nodes and elements, and boundaries in terms of nodes and segments; (2) soil properties including (a) saturated hydraulic conductivities or permeabilities; (b) compressibility of water and the media, respectively; (c) bulk density; (d) three soil characteristic curves for each type of soil or geologic unit which are the retention curve, relative conductivity vs head curve, and water capacity curve; (e) effect porosity; and (f) dispersivities, and effective molecular diffusion coefficient for each soil type or geologic unit; (3) initial distribution of pressure head over the region of interest; (4) net precipitation, allowed ponding depth, potential evaporation, and allowed minimum pressure head in the soil; (5) prescribed pressure head on Dirichlet boundaries, (6) prescribed fluxes of chemicals and heat on Cauchy and/or Neumann boundaries; (7) artificial withdrawals or injections of water, (8) number of chemical components as well as microbes and microbe-chemical interaction parameters such as specific yields, utilization coefficients, saturation constants, etc; (9) artificial source/sink of water and all chemical components, heat, and microbes; (10) prescribed concentrations of all chemical components and microbes as well as temperature on Dirichlet boundaries: (11) prescribed fluxes of all chemical components and heat on variable boundaries; and (12) initial distribution of all chemical component and microbe concentrations and temperature. All inputs in items 4 through 11 can be time-dependent or constant with time.

Output: (1) pressure head, total head, moisture content, and flow velocity over two-dimensional grid at any desired time; (2) water fluxes through all types of boundaries and amount of water accumulated in the media at any desired time; (3) distribution of chemical concentrations, microbes, and temperature over a three-dimensional grid at any desired time; and (4) amount of chemical and heat fluxes through all boundary segments.

Summary of 3DFATMIC

3DFATMIC is a 3-Dimensional Subsurface Flow and FAte and Transport of MIcrobes and Chemicals Model. It can be used to investigate saturated-unsaturated flow alone, contaminant transport alone, sequential flow and transport, or coupled flow and the fate and transport of microbes and chemicals in subsurface environment. Typical applications of 3DFATMIC are problems involving the bioremediation.

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, which describes the flow of variable-density fluid, are basically the Richards' equation .

Governing Flow Equation

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

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

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

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

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

$$\frac{\mu}{\mu_w} = 1 + \beta_s C_s + \beta_o C_o + \beta_n C_n + \beta_p C_p + \beta_1 C_1 + \beta_2 C_2 + \beta_3 C_3 \tag{2c}$$

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.

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

Initial Conditions for Flow Equation

$$h = h_i(x,y,z) \qquad \text{in } R \tag{4}$$

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.(1).

Boundary Conditions for Flow Equation

Dirichlet Conditions:

$$h = h_d(x_b, y_b, z_b, t) \qquad \text{on } B_d \tag{5}$$

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) :

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

Variable Conditions - During Precipitation Period:

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

or

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

Variable Conditions - During Non-precipitation period:

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

or

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

or

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

where (x_b, y_b, z_b) is the spatial coordinate on the boundary; $\mathbf{n}$ 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 boundary, 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.

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)

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

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

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

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

(2.9)

5

$$
\begin{aligned}
&(\theta+\rho_b K_{do})\frac{\partial C_o}{\partial t} + \mathbf{V}\cdot\nabla C_o = \nabla\cdot\theta\mathbf{D}\cdot\nabla C_o - \Lambda_o(\theta+\rho_b K_{do})C_o + q_{in}C_{oin} + \left(\frac{\rho_w}{\rho}\mathbf{V}\cdot\nabla\left(\frac{\rho}{\rho_w}\right) - \frac{\rho^*}{\rho}q_{in}\right)C_o \\
&\quad (1) \qquad (2) \qquad (3) \qquad (4) \qquad (5) \qquad (6) \\
&-\left[(\theta+\rho_b K_{d1})C_1\right]\left\{\gamma_o^{(1)}\mu_o^{(1)}\left[\frac{C_s}{K_{so}^{(1)}+C_s}\right]\left[\frac{C_o}{K_o^{(1)}+C_o}\right]\left[\frac{C_p}{K_{po}^{(1)}+C_p}\right] + \alpha_o^{(1)}\lambda_o^{(1)}\left[\frac{C_o}{\Gamma_o^{(1)}+C_o}\right]\right\} \\
&\quad (7) \qquad (8) \\
&-\left[(\theta+\rho_b K_{d3})C_3\right]\left\{\gamma_o^{(3)}\mu_o^{(3)}\left[\frac{C_s}{K_{so}^{(3)}+C_s}\right]\left[\frac{C_o}{K_o^{(3)}+C_o}\right]\left[\frac{C_p}{K_{po}^{(3)}+C_p}\right] + \alpha_o^{(3)}\lambda_o^{(3)}\left[\frac{C_o}{\Gamma_o^{(3)}+C_o}\right]\right\} \\
&\quad (9) \qquad (10)
\end{aligned}
\tag{2.10}
$$

$$
\begin{aligned}
&(\theta+\rho_b K_{dn})\frac{\partial C_n}{\partial t} + \mathbf{V}\cdot\nabla C_n = \nabla\cdot\theta\mathbf{D}\cdot\nabla C_n - \Lambda_n(\theta+\rho_b K_{dn})C_n + q_{in}C_{nin} + \left(\frac{\rho_w}{\rho}\mathbf{V}\cdot\nabla\left(\frac{\rho}{\rho_w}\right) - \frac{\rho^*}{\rho}q_{in}\right)C_n \\
&\quad (1) \qquad (2) \qquad (3) \qquad (4) \qquad (5) \qquad (6) \\
&-\left[(\theta+\rho_b K_{d2})C_2\right]\left\{\gamma_n^{(2)}\mu_n^{(2)}\left[\frac{C_s}{K_{sn}^{(2)}+C_s}\right]\left[\frac{C_n}{K_n^{(2)}+C_n}\right]\left[\frac{C_p}{K_{pn}^{(2)}+C_p}\right] + \alpha_n^{(2)}\lambda_n^{(2)}\left[\frac{C_n}{\Gamma_n^{(2)}+C_n}\right]\right\} \\
&\quad (7) \qquad (8) \\
&-\left[(\theta+\rho_b K_{d3})C_3\right]\left\{\gamma_n^{(3)}\mu_n^{(3)}\left[\frac{C_s}{K_{sn}^{(3)}+C_s}\right]\left[\frac{C_n}{K_n^{(3)}+C_n}\right]\left[\frac{C_p}{K_{pn}^{(3)}+C_p}\right] + \alpha_n^{(3)}\lambda_n^{(3)}\left[\frac{C_n}{\Gamma_n^{(3)}+C_n}\right]\right\} \\
&\quad (9) \qquad (10)
\end{aligned}
\tag{2.11}
$$

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

(1) (2) (3) (4) (5) (6)

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

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

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

(2.12)

The transport equations for the three microbes are

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

(1) (2) (3) (4) (5) (6)

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

(2.13)

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

(1) (2) (3) (4) (5) (6)

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

(2.14)

(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)

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 rate under aerobic condition of microbe #1, aerobic 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 rate 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 rate 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 $|\mathbf{V}|$ is the magnitude of $\mathbf{V}$, 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. $\mathcal{I}(C_o) = \left[1 + \frac{C_o}{K_c}\right]^{-1}$ 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, #3, the retarded substrate saturation constants under anaerobic conditions with respect to microbe #2, #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 $\varepsilon_o^{(1)}$, $\varepsilon_o^{(3)}$, $\varepsilon_n^{(2)}$, and $\varepsilon_n^{(3)}$ 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

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

Prescribed Concentration (Dirichlet) Boundary Conditions

$$
\left.\begin{array}{l}
C_s = C_{sd}(x_b, y_b, z_b, t) \\
C_o = C_{od}(x_b, y_b, z_b, t) \\
C_n = C_{nd}(x_b, y_b, z_b, t) \\
C_p = C_{pd}(x_b, y_b, z_b, t) \\
C_1 = C_{1d}(x_b, y_b, z_b, t) \\
C_2 = C_{2d}(x_b, y_b, z_b, t) \\
C_3 = C_{3d}(x_b, y_b, z_b, t)
\end{array}\right. \quad on\ B_d \tag{2.18}
$$

<u>Variable Boundary Conditions</u>

$$
\left.\begin{array}{l}
\mathbf{n}\cdot(\mathbf{V}C_s - \theta\mathbf{D}\cdot\nabla C_s) = \mathbf{n}\cdot\mathbf{V}C_{sv}(x_b, y_b, z_b, t) \\
\mathbf{n}\cdot(\mathbf{V}C_o - \theta\mathbf{D}\cdot\nabla C_o) = \mathbf{n}\cdot\mathbf{V}C_{ov}(x_b, y_b, z_b, t) \\
\mathbf{n}\cdot(\mathbf{V}C_n - \theta\mathbf{D}\cdot\nabla C_n) = \mathbf{n}\cdot\mathbf{V}C_{nv}(x_b, y_b, z_b, t) \\
\mathbf{n}\cdot(\mathbf{V}C_p - \theta\mathbf{D}\cdot\nabla C_p) = \mathbf{n}\cdot\mathbf{V}C_{pv}(x_b, y_b, z_b, t) \\
\mathbf{n}\cdot(\mathbf{V}C_1 - \theta\mathbf{D}\cdot\nabla C_1) = \mathbf{n}\cdot\mathbf{V}C_{1v}(x_b, y_b, z_b, t) \\
\mathbf{n}\cdot(\mathbf{V}C_2 - \theta\mathbf{D}\cdot\nabla C_2) = \mathbf{n}\cdot\mathbf{V}C_{2v}(x_b, y_b, z_b, t) \\
\mathbf{n}\cdot(\mathbf{V}C_3 - \theta\mathbf{D}\cdot\nabla C_3) = \mathbf{n}\cdot\mathbf{V}C_{3v}(x_b, y_b, z_b, t)
\end{array}\right. \quad if\ \boldsymbol{n}\cdot\mathbf{V} \le 0 \tag{2.19a}
$$

$$
\left.\begin{array}{l}
\mathbf{n}\cdot(-\theta\mathbf{D}\cdot\nabla C_s) = 0 \\
\mathbf{n}\cdot(-\theta\mathbf{D}\cdot\nabla C_p) = 0 \\
\mathbf{n}\cdot(-\theta\mathbf{D}\cdot\nabla C_n) = 0 \\
\mathbf{n}\cdot(-\theta\mathbf{D}\cdot\nabla C_p) = 0 \\
\mathbf{n}\cdot(-\theta\mathbf{D}\cdot\nabla C_1) = 0 \\
\mathbf{n}\cdot(-\theta\mathbf{D}\cdot\nabla C_2) = 0 \\
\mathbf{n}\cdot(-\theta\mathbf{D}\cdot\nabla C_3) = 0
\end{array}\right. \quad if\ \boldsymbol{n}\cdot\mathbf{V} > 0 \tag{2.19b}
$$

<u>Cauchy Boundary Conditions</u>

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

<u>Neumann Boundary Conditions</u>

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

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.

For the flow module, 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 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, and (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.