

# 3DFEMFAT

**Purpose:** To simulate transient and/or steady state density-dependent flow field and transient and/or steady state distribution of a contaminant in a three-dimensional domain of subsurface media.

**Scope:** This program computes and predicts the distribution of pressure head, moisture content, flow velocity, and total head over a three-dimensional plane in either completely saturated, or completely unsaturated, or partially unsaturated or partially saturated subsurface media. It also computes and predicts the spatial-temporal distribution of contaminants. 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 contaminant include (1) reversible sorption and (2) 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 transport equation is derived based on the principle of conservation of mass. The contaminant transport equation is 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. Mixed hexahedral elements, triangular prisms, 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 contaminants on Cauchy and/or Neumann boundaries; (7) artificial withdrawals or injections of water; (8) adsorption constants; (9) artificial source/sink of water and contaminants; (10) prescribed concentrations of contaminants on Dirichlet boundaries; (11) prescribed fluxes of contaminants on variable boundaries; and (12) initial distribution of contaminants. 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 contaminants over a three-dimensional grid at any desired time; and (4) amount of contaminants through all boundary segments.

### ***Pre & Postprocessing***

A preprocessor (for grid generation) and postprocessor (for visualization) using GMS is included. However, the GMS FEMWATER Module is required to run these.

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## Summary of 3DFEMFAT

3DFEMFAT is a 3-Dimensional Finite Element Model of density dependent Flow And Transport through Saturated-Unsaturated Media. The model is designed for generic application. It could be applied to simulate saturated-unsaturated flow alone, contaminant transport of any chemical alone, the sequential flow and contaminant transport, or the coupled flow and contaminant transport. Typical applications are to infiltration, well-head protection, agriculture pesticides, sanitary landfill, radionuclide disposal sites, hazardous waste disposal sites, density induced flow and transport, salt intrusion, etc.

3DFEMFAT 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 are basically the modified Richards equation.

### Governing Flow Equation

$$\frac{\rho}{\rho_o} \frac{d\theta}{dh} \frac{\partial h}{\partial t} = \nabla \cdot \left[ \mathbf{K} \cdot \left( \nabla h + \frac{\rho}{\rho_o} \nabla z \right) \right] + \frac{\rho^*}{\rho_o} q \quad (1)$$

where  $h$  is the pressure head,  $t$  is time,  $\mathbf{K}$  is the hydraulic conductivity tensor,  $z$  is the potential head,  $q$  is the source and/or sink,  $\rho$  is the water density at chemical concentration  $C$ ,  $\rho_o$  is the referenced water density at zero chemical concentration,  $\rho^*$  is the density of either the injection fluid or the withdrawn water, and  $\theta$  is the moisture content. The hydraulic conductivity  $\mathbf{K}$  is given by

$$\mathbf{K} = \frac{\rho g}{\mu} \mathbf{k} = \frac{(\rho/\rho_o) \rho_o g}{(\mu/\mu_o) \mu_o} \mathbf{k}_s \mathbf{k}_r = \frac{\rho/\rho_o}{\mu/\mu_o} \mathbf{K}_s \mathbf{k}_r \quad (2a)$$

where  $\mu$  is the dynamic viscosity of water at chemical concentration  $C$ ;  $\mu_o$  is the referenced dynamic viscosity at zero chemical concentration;  $\mathbf{k}$  is the permeability tensor;  $\mathbf{k}_s$  is the saturated permeability tensor;  $\mathbf{k}_r$  is the relative permeability or relative hydraulic conductivity;  $\mathbf{K}_s$  is the referenced saturated

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hydraulic conductivity tensor. The referenced value is usually taken at zero chemical concentration. The density and dynamic viscosity of water are functions of chemical concentration and are assumed to take the following form

$$\frac{\rho}{\rho_0} = a_1 + a_2 C + a_3 C^2 + a_4 C^3 \quad (2b)$$

and

$$\frac{\mu}{\mu_0} = a_5 + a_6 C + a_7 C^2 + a_8 C^3 \quad (2c)$$

where  $a_1, a_2, \dots, a_8$  are the parameters used to define concentration dependence of water density and viscosity and  $C$  is the chemical concentration.

The Darcy velocity is calculated as follows

$$\mathbf{V} = -\mathbf{K} \cdot \left[ \frac{\rho_0}{\rho} \nabla h + \nabla z \right] \quad (3)$$

#### Initial Conditions For Flow Equation

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

where  $R$  is the region of interest and  $h_i$  is the prescribed initial condition, which can be obtained by either field measurements or by solving the steady state version of Eq. (1).

#### Boundary Conditions For Flow Equations

**Dirichlet Conditions:**

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

**Neumann Conditions:**

$$-\mathbf{n} \cdot \mathbf{K} \cdot \frac{\rho_0}{\rho} \nabla h = q_n(x_b, y_b, z_b, t) \quad \text{on } B_n, \quad (6)$$

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Cauchy Conditions:

$$-\mathbf{n} \cdot \mathbf{K} \cdot \left[ \frac{\rho_o}{\rho} \nabla h + \nabla z \right] = q_c(x_b, y_b, z_b, t) \quad \text{on } B_c, \quad (7)$$

Variable Conditions - During Precipitation Period:

$$h = h_p(x_b, y_b, z_b, t) \quad \text{on } B_v \quad (8a)$$

or

$$-\mathbf{n} \cdot \mathbf{K} \cdot \left[ \frac{\rho_o}{\rho} \nabla h + \nabla z \right] = q_p(x_b, y_b, z_b, t) \quad \text{on } B_v, \quad (8b)$$

Variable Conditions - During Nonprecipitation Period:

$$h = h_p(x_b, y_b, z_b, t) \quad \text{on } B_v, \quad (8c)$$

or

$$h = h_m(x_b, y_b, z_b, t) \quad \text{on } B_v, \quad (8d)$$

or

$$-\mathbf{n} \cdot \mathbf{K} \cdot \left[ \frac{\rho_o}{\rho} \nabla h + \nabla z \right] = q_e(x_b, y_b, z_b, t) \quad \text{on } B_v, \quad (8e)$$

River Boundary Conditions:

$$-\mathbf{n} \cdot \mathbf{K} \cdot \left[ \frac{\rho_o}{\rho} \nabla h + \nabla z \right] = -\frac{K_R}{b_R} (h_R - h) \quad \text{on } B_r \quad (9)$$

where  $\mathbf{n}$  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,  $K_R$  is the hydraulic conductivity of

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the river bottom sediment layer,  $b_R$  is the thickness of the river bottom sediment layer, and  $h_R$  is the depth of the river bottom measured from the river surface.

The major processes of transport included in 3DFEMFAT are advection, dispersion/diffusion, adsorption, decay, and source/sink.

### Governing Equations for Transport

$$\theta \frac{\partial C}{\partial t} + \rho_b \frac{\partial S}{\partial t} + \mathbf{V} \cdot \nabla C = \nabla \cdot (\theta \mathbf{D} \cdot \nabla C) - \lambda(\theta C + \rho_b S) + QC_{in} - \left[ \frac{\rho^*}{\rho} Q - \frac{\rho_o}{\rho} \mathbf{V} \cdot \nabla \left( \frac{\rho}{\rho_o} \right) \right] C \quad (10)$$

$$S = K_d C \quad \text{for linear isotherm} \quad (11a)$$

$$S = \frac{S_{max} KC}{1 + KC} \quad \text{for Langmuir isotherm} \quad (11b)$$

$$S = KC^n \quad \text{for Freundlich isotherm} \quad (11c)$$

where  $\theta$  is the moisture concentration,  $\rho_b$  is the bulk density of the medium ( $M/L^3$ ),  $C$  is the material concentration in aqueous phase ( $M/L^3$ ),  $S$  is the material concentration in adsorbed phase ( $M/M$ ),  $t$  is time,  $\mathbf{V}$  is the discharge,  $\nabla$  is the del operator,  $\mathbf{D}$  is the dispersion coefficient tensor,  $\lambda$  is the decay constant,  $Q$  is the source rate of water,  $C_{in}$  is the material concentration in the source,  $K_d$  is the distribution coefficient,  $S_{max}$  is the maximum concentration allowed in the medium in the Langmuir nonlinear isotherm,  $n$  is the power index in the Freundlich nonlinear isotherm, and  $K$  is the coefficient in the Langmuir or Freundlich nonlinear isotherm. The dispersion coefficient tensor  $\mathbf{D}$  is given by

$$\theta \mathbf{D} = a_T |\mathbf{V}| \delta + (a_L - a_T) \mathbf{V} \mathbf{V} / |\mathbf{V}| + \theta a_m \tau \delta \quad (12)$$

where  $|\mathbf{V}|$  is the magnitude of  $\mathbf{V}$ ,  $\delta$  is the Kronecker delta tensor,  $a_T$  is lateral dispersivity,  $a_L$  is the longitudinal dispersivity,  $a_m$  is the molecular diffusion coefficient, and  $\tau$  is the tortuosity.

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Initial Conditions for Transport

$$C=C_i(x,y,z) \text{ in } R \quad (13)$$

Prescribed Concentration (Dirichlet) Boundary Conditions

$$C=C_d(x_b,y_b,z_b,t) \text{ on } B_d \quad (14)$$

Variable Boundary Conditions

$$\mathbf{n} \cdot (\nabla C - \theta \mathbf{D} \cdot \nabla C) = \mathbf{n} \cdot \nabla C_v(x_b,y_b,z_b,t) \text{ if } \mathbf{n} \cdot \mathbf{V} \leq 0 \quad (15a)$$

$$\mathbf{n} \cdot (-\theta \mathbf{D} \cdot \nabla C) = 0 \text{ if } \mathbf{n} \cdot \mathbf{V} > 0 \quad (15b)$$

Cauchy Boundary Conditions

$$\mathbf{n} \cdot (\nabla C - \theta \mathbf{D} \cdot \nabla C) = q_c(x_b,y_b,z_b,t) \text{ on } B_c \quad (16)$$

Neumann Boundary Conditions

$$\mathbf{n} \cdot (-\theta \mathbf{D} \cdot \nabla C) = q_n(x_b,y_b,z_b,t) \text{ on } B_n \quad (17)$$

where  $C_i$  is initial concentration;  $R$  is the region of interest;  $(x_b, y_b, z_b)$  is the spatial coordinate on the boundary;  $\mathbf{n}$  is an outward unit vector normal to the boundary;  $C_d$  and  $C_v$  are the prescribed concentration on the Dirichlet boundary and the specified concentration of water through the variable boundary, respectively;  $B_d$  and  $B_v$  are the Dirichlet and variable boundaries respectively;  $q_c$  and  $q_n$  are the prescribed total flux and gradient flux through the Cauchy and Neumann boundaries  $B_c$  and  $B_n$ , respectively.

Since the hybrid Lagrangian-Eulerian approach is used to simulate Eq. (10), it is written in the Lagrangian-Eulerian form as

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$$(\theta + \rho_b \frac{dS}{dC}) \frac{D_{V_d} C}{Dt} = \nabla \cdot (\theta \mathbf{D} \cdot \nabla C) - \lambda(\theta C + \rho_b S) + QC_m - \left[ \frac{\rho^*}{\rho} Q - \frac{\rho_o}{\rho} \mathbf{V} \cdot \nabla \left[ \frac{\rho}{\rho_o} \right] \right] C \quad (18a)$$

$$\mathbf{V}_d = \frac{\mathbf{V}}{\theta + \rho_b K_d} \quad \text{for Linear isotherm model} \quad (18b)$$

$$\theta \frac{D_{V_r} C}{Dt} + \rho_b \frac{dS}{dC} \frac{\partial C}{\partial t} = \nabla \cdot (\theta \mathbf{D} \cdot \nabla C) - \lambda(\theta C + \rho_b S) + QC_m - \left[ \frac{\rho^*}{\rho} Q - \frac{\rho_o}{\rho} \mathbf{V} \cdot \nabla \left[ \frac{\rho}{\rho_o} \right] \right] C \quad (19a)$$

$$\mathbf{V}_r = \frac{\mathbf{V}}{\theta} \quad \text{for Freundlich and Langumir models} \quad (19b)$$

where  $\mathbf{V}_d$  and  $\mathbf{V}_r$  are the retarded and fluid pore velocities, respectively; and  $\frac{D_{V_d}(\cdot)}{Dt}$  and  $\frac{D_{V_r}(\cdot)}{Dt}$  denote

the material derivative of  $(\cdot)$  with respect to time using the retarded and fluid pore velocities, respectively.

The flow equation Eq. (1) subject to initial and boundary conditions Eqs. (5) through (9) is solved with the Galerkin finite element method. The transport equations Eq. (18) or (19) subject to initial and boundary conditions Eqs. (13) through (17) are solved either with the hybrid Lagrangian-Eulerian finite element methods or the conventional finite element methods.

3DFEMFAT consists of a flow module and a transport module. In comparison to conventional finite element (including both Galerkin and upstream finite elements) or finite difference (including both central and upwind finite differences) models, the transport module of 3DFEMFAT offers several advantages: (1) it completely eliminates numerical oscillation due to advection terms, (2) it can be applied to mesh Peclet number ranging from 0 to infinity (conventional finite element or finite difference models typically impose unduly severe restriction on the mesh Peclet number), (3) it can use very large time step size to greatly reduce numerical dispersion (in fact, the larger the time step, the better the solution with respect to advection transport; the size of time step size is only limited by the accuracy requirement with

respect to diffusion/dispersion transport, which is normally not a very severe restriction), and (4) the hybrid Lagrangian-Eulerian finite element approach is always superior to and will never be worse than its corresponding upstream finite element method. Because of these advantages, 3DFEMFAT is ideal for simulating density dependent flow and advection-dominant transport.

Input to the program includes the control indices, properties of the media either in tabular or analytical form, the geometry in the form of elements and nodes, and boundary and initial conditions either in tabular or analytical form. Principal output includes the spatial distribution of pressure head, total head, moisture content, Darcy velocity components, concentration, and material fluxes at any desired time step. Fluxes through various types of boundaries are output. In addition, diagnostic variables, such as the number of non-convergent nodes and residuals may be printed if desired for debugging purposes.

The special features of 3DFEMFAT are its flexibility and versatility in modeling a range of real-world problems. The model is designed to: (1) treat heterogeneous and anisotropic media consisting of as many geologic formations as desired, (2) consider both distributed and point sources/sinks that are spatially and temporally dependent, (3) accept the prescribed initial conditions or obtain them by simulating a steady state version of the system under consideration, (4) deal with transient Dirichlet boundary conditions, (5) handle time-dependent fluxes due to the gradient of pressure head or concentration varying along the Neumann boundary, (6) treat time-dependent total fluxes distributed over the Cauchy boundary, (7) consider river boundary conditions or the mixed-type boundary conditions, (8) automatically determine 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, (9) include the off-diagonal hydraulic conductivity components in the Richards equation for dealing with cases when the coordinate system does not coincide with the principal directions of the hydraulic conductivity tensor, (10) give three options for estimating the nonlinear matrix, (11) include four options (successive subregion block iterations, successive point iterations, polynomial preconditioned

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conjugate gradient methods, and incomplete Cholesky preconditioned conjugate gradient methods) for solving the linearized matrix equations, (12) provide two options of treating the mass matrix - consistent and lumping, (13) provide three adsorption models in the transport module - linear isotherm and nonlinear Langmuir and Freundlich isotherms, (14) employ hexahedral elements, triangular prism, tetrahedral elements, or the mixtures of these three types of elements to facilitate the discretization of the region of interest, (15) automatically reset time step size when boundary conditions or source/sinks change abruptly, and (16) check the mass balance computation over the entire region for every time step.