

# A three-dimensional multiphase flow model for assessing NAPL contamination in porous and fractured media, 1. Formulation

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## Abstract

A three-dimensional, three-phase numerical model is presented for simulating the movement of non-aqueous-phase liquids (NAPL's) through porous and fractured media. The model is designed for practical application to a wide variety of contamination and remediation scenarios involving light or dense NAPL's in heterogeneous subsurface systems. The model formulation is first derived for three-phase flow of water, NAPL and air (or vapor) in porous media. The formulation is then extended to handle fractured systems using the dual-porosity and discrete-fracture modeling approaches. The model accommodates a wide variety of boundary conditions, including withdrawal and injection well conditions which are treated rigorously using fully implicit schemes. The three-phase formulation collapses to its simpler forms when air-phase dynamics are neglected, capillary effects are neglected, or two-phase air-liquid, liquid-liquid systems with one or two active phases are considered. A Galerkin procedure with upstream weighting of fluid mobilities, storage matrix lumping, and fully implicit treatment of nonlinear coefficients and well conditions is used. A variety of nodal connectivity schemes leading to finite-difference, finite-element and hybrid spatial approximations in three dimensions are incorporated in the formulation. Selection of primary variables and evaluation of the terms of the Jacobian matrix for the Newton-Raphson linearized equations is discussed. The various nodal lattice options, and their significance to the computational time and memory requirements with regards to the block-Orthomin<sup>©</sup> solution scheme are noted. Aggressive time-stepping schemes and under-relaxation formulas implemented in the code further alleviate the computational burden.

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## 1. Introduction

The widespread contamination of natural subsurface systems by petroleum hydrocarbons and immiscible industrial chemicals poses serious environmental and health

hazards worldwide. Understanding the behavior and quantifying the migration and fate of these non-aqueous-phase liquids (NAPL's) in the subsurface is crucial in mitigating or remediating the pollution problem and in managing the groundwater resources. The simultaneous movement of water, NAPL and air (or vapor) can be mathematically represented by the multiphase mass-balance equations, introduced by the petroleum industry in the early 1960's (Collins, 1961) to evaluate oil recovery techniques. The mathematical models that evolved range in complexity from two- and three-phase to compositional simulators with complex boundary and well conditions to assess secondary and tertiary recovery processes. A review of these equations, the various levels of detail required for certain investigations, and the degrees of simplifications achieved by making practical working assumptions are provided by Panday and Corapcioglu (1989).

The multiphase flow equations have been adopted by several researchers, for evaluating NAPL contamination and remediations scenarios. A wide range of formulations have been presented that vary in complexity of the simulated physical process and dimensionality. Saturated-zone, two-phase models have been presented by Huyakorn and Pinder (1978), Schwille (1981), and Hochmuth and Sunada (1985). Three-phase models for assessing saturated–unsaturated zone contamination by NAPL have been presented by Faust et al. (1989), Kaluarachchi and Parker (1989) and Forsyth (1991), and models that include interphase mass transfer have been reported by Abriola and Pinder (1985), Corapcioglu and Baehr (1987), Panday (1989), Forsyth and Shao (1991), and Falta et al. (1992). Since investigations of NAPL contamination behavior are recent and limited (Schiegg and Schwille, 1991), most of these models make use of the three-phase relative permeability and capillary retention relations developed for oil reservoirs. It still needs to be determined which relation (if any) best represents the various aquifer materials. The flow models of Faust (1985), Kaluarachchi and Parker (1989), and Forsyth (1991) simplify the problem by treating the air phase as passive, thus solving only the water and NAPL mass-balance equations to reduce the computational effort. However, air-phase dynamics could become significant in certain situations involving, for example, air venting or sparging activities. The model of Panday (1989) is a vertical one-dimensional (1-D) compositional model which includes non-isothermal effects and the effects of freezing and thawing on the flow and transport of contaminants. Their model is practical to use only in the unsaturated zone where the 1-D vertical flow and transport assumptions are usually valid. The model of Forsyth and Shao (1991) is a comprehensive compositional simulator in which all phases are active with contaminant partitioning between phases. The numerical formulations are robust and efficient but the model always carries the extra computational burden of the compositional calculations and variable switching. Finally, none of these models consider fracture flow.

Modeling the flow of multiple fluid phases in fractured media using the dual-porosity approach has been discussed by Bear and Braester (1972), and Braester (1972). Torsaeter et al. (1987), and Kazemi and Gilman (1993) summarized the recent advances in quantifying and modeling multiphase flow in fractured media. Properties were evaluated for a water-wet chalk reservoir for imbibition oil recovery

processes, and porosity was noted to be the best correlating parameter. The model results were most sensitive to the capillary pressure relationships, and the geometric factors for the matrix blocks of the dual-porosity medium. Braester (1972) and Coats (1989) presented formulations that include permeabilities of the porous matrix in assessing the flow of the fluids. Coats (1989) described finite-difference schemes used to obtain stable, efficient and accurate solutions. Wu and Pruess (1988) presented a dual-porosity integrated finite-difference model that further subdivides the porous matrix block domain. Coats (1989) observed little need for such subdivision, considering the other error sources and calibration matching performed in reservoir simulators. Huyakorn et al. (1983) provided a scheme for reducing the computational requirement of finite-element matrix discretization in dual-porosity simulators. Discrete-fracture systems have been detailed by Gilman and Kazemi (1983), and L.K. Thomas et al. (1983). However, such studies are limited due to the difficulties in characterizing the geometry and multiphase flow processes in individual fractures.

This paper presents the flow formulation and numerical solution techniques of a comprehensive model for simulating the subsurface migration of NAPL contaminants. The three-dimensional (3-D), three-phase formulation for simultaneous flow of water, NAPL and vapor in a porous medium is first derived. The general formulation can readily degenerate to simpler forms when certain assumptions pertaining to the dynamics of certain phases are introduced. This flexibility is necessary for speeding up simulations of simpler problems, or for quick pilot studies of complex systems. Robust and efficient discretization and nonlinear solution schemes, and practical boundary and well conditions are included in the formulation which render the model applicable to a wide variety of field situations. The numerical schemes are further extended to accommodate fracture flow using the dual-porosity and the discrete-fracture conceptual approaches. A comprehensive robust and efficient model enables practical application for site studies on minicomputers and workstations, from preliminary investigations, calibration and sensitivity analyses, to predictive simulations and remedial investigations.

## 2. Porous medium flow formulation

### 2.1. Governing and supplementary equations

Consider a general situation of isothermal flow of water (w), NAPL (n) and vapor or gas (g) through a porous medium. The governing equations may be written in the form (Corapcioglu and Baehr, 1987):

$$\frac{\partial}{\partial x_i} \left[ k_{ij} \tau_\ell \frac{\partial \Phi_\ell}{\partial x_j} \right] = \frac{\partial}{\partial t} (\phi \rho_\ell S_\ell) - \dot{M}_\ell, \quad \ell = w, n, g \quad (1)$$

where  $x_i$  ( $i = 1, 2, 3$ ) are Cartesian coordinates;  $t$  is time;  $k_{ij}$  is the intrinsic permeability tensor;  $\tau_\ell$  is the mobility of the  $\ell$  phase ( $\tau_\ell = k_{r\ell} \rho_\ell / \mu_\ell$ , in which  $k_{r\ell}$  = relative permeability,  $\rho_\ell$  = fluid density, and  $\mu_\ell$  = dynamic viscosity);  $\Phi_\ell$  is the fluid potential

defined such that its gradient  $\nabla\Phi_\ell = \nabla p_\ell + \gamma_\ell \nabla z$ , in which  $p_\ell =$  phase pressure,  $g =$  gravitational acceleration,  $\gamma_\ell$  is  $\rho_\ell g$  and corresponds to the specific weight of phase  $\ell$ , and  $z =$  elevation above the datum plane;  $\phi$  is the medium porosity;  $S_\ell$  is saturation of the  $\ell$  phase; and  $M_\ell$  is the rate of mass injection or withdrawal of fluid phase  $\ell$  per unit volume of the porous medium.

The flow equations (1) need to be supplemented by the following constitutive relations (Forsyth, 1991):

$$S_w + S_n + S_g = 1 \quad (2)$$

$$p_g = p_n + \alpha p_{cgn}(S_g) + (1 - \alpha)[p_{cgw}(S_w) - p_{cnw}(S_w = 1)] \quad (3)$$

$$p_n = p_w + \alpha p_{cnw}(S_w) + (1 - \alpha)p_{cnw}(S_w = 1) \quad (4)$$

$$p_{cgw} = p_{cgw}(S_w) \quad (5a)$$

$$p_{cnw} = p_{cnw}(S_w) \quad (5b)$$

$$p_{cgn} = p_{cgn}(S_g) \quad (5c)$$

$$k_{rw} = k_{rw}(S_w) \quad (6a)$$

$$k_{rn} = k_{rn}(S_w, S_g) \quad (6b)$$

$$k_{rg} = k_{rg}(S_g) \quad (6c)$$

where  $p_{cgw}$ ,  $p_{cnw}$  and  $p_{cgn}$  are capillary pressure functions for the three fluid pairs (gas–water), (NAPL–water) and (gas–NAPL), respectively; and  $\alpha$  is the fluid interface transition parameter defined as  $\alpha = \min(1, S_n/S_n^*)$  with  $S_n^*$  being the NAPL threshold saturation above which air–water interfaces cease to exist within all pores of a representative elementary volume (REV).

As recently pointed out by Forsyth (1991), this definition of  $\alpha$  (instead of  $\alpha = 1$ ) ensures that  $p_g - p_w = p_{cgw}$  (and not  $p_g - p_w = p_{cgn} + p_{cnw}$ ) when  $S_n$  is zero in a zone where NAPL is absent and only water and gas (air) coexist. In addition, it models the transition of an REV from only air–water interfaces to only air–oil–water interfaces linearly, due to lack of characterization of interface transition behavior in various soils. However, the critical saturation  $S_n^*$  is usually assumed to be small, and hence the effect of the linear assumption is also small. This transition is required, however, to avoid mis-representing the state of pristine portions of the domain.

To provide flexibility, relative permeability and capillary pressure data may be provided in functional or tabular forms. Note that the assumption of non-hysteretic constitutive relations are invoked. With the functional option, the Brooks and Corey (1966) or the van Genuchten (1980) extended relative permeability functions for the three-phase fluid system are used. Capillary pressure functions adopted correspond to the scaled functions presented by Lenhard and Parker (1987). With the tabular option, the NAPL relative permeability may be calculated using the first or second method of Stone (1970, 1973). We recognize that additional research is needed to

ascertain which of the various methods for calculating the three-phase relative permeabilities is the most reliable for groundwater contamination scenarios.

In addition to the above constitutive relations, the equations of state are needed to determine the fluid densities and medium porosity as functions of pressures. These supplementary equations are given as follows:

$$\rho_w = \rho_w^0 [1 + \beta_w (p_w - p_{\text{atm}})] \quad (7a)$$

$$\rho_n = \rho_n^0 [1 + \beta_n (p_n - p_{\text{atm}})] \quad (7b)$$

$$\rho_g = \beta_g p_g = \rho_g^0 p_g / p_{\text{atm}} \quad (7c)$$

$$\phi = \phi^0 [1 + \beta_s (\bar{p} - p_{\text{atm}})] \quad (7d)$$

where  $\rho_\ell^0$  ( $\ell = w, n, g$ ) are the densities of water and NAPL at reference pressure ( $p_{\text{atm}}$ );  $\beta_\ell$  ( $\ell = w, n, g$ ) are the fluid compressibilities;  $\phi^0$  is the referenced porosity;  $\beta_s$  is the soil matrix compressibility; and  $\bar{p}$  is a weighted average of  $p_\ell$  ( $\ell = w, n, g$ ). Note for an ideal gas  $\beta_g = M_g / RT$ , where  $M_g$  is the gas molecular weight,  $R$  is the universal gas constant, and  $T$  is absolute temperature. The compressibilities of the liquid phases are small compared to the gas-phase compressibility, and may be neglected in the formulation.

## 2.2. Discretization

The 3-D flow domain is discretized using a grid consisting of hexahedral brick elements. The governing equations (1) are approximated using the Galerkin procedure with modifications to incorporate upstream weighting of phase mobilities and storage matrix lumping. Time integration is performed using a fully implicit finite-difference scheme. This leads to a system of nonlinear algebraic equations of the form:

$$[A_{IJ}^\ell \Phi_{\ell J}]^{t+\Delta t} + \frac{B_{II}}{\Delta t} [(\phi \rho_\ell S_\ell)_I^{t+\Delta t} - (\phi \rho_\ell S_\ell)_I^t] - \dot{M}_{\ell I}^{t+\Delta t} = 0,$$

$$\ell = w, n, g; \quad I = 1, 2, \dots, n \quad (8)$$

where  $I$  and  $J$  are nodal subscripts ranging from 1 to  $n$  with  $n$  being the number nodes in the grid; superscript  $t + \Delta t$  denotes the current time;  $\Delta t$  is the time increment;  $A_{IJ}^\ell$  and  $B_{II}$  are the fluid transmissivity and diagonalized storage coefficient matrices, respectively; and  $M_{\ell I}$  is the integrated nodal flux. Note that for the sake of convenience, the indicial summation notation has been adopted.

$$A_{IJ}^\ell \Phi_{\ell J} \equiv \sum_J A_{IJ}^\ell \Phi_{\ell J} \quad (9)$$

Eq. 8 can be written at the element level. For linear rectangular brick elements with nodal subscripts  $I$  and  $J$  ranging from 1 to 8, the element matrices can be readily evaluated without the spatial numerical integration using the influence coefficient

technique (Huyakorn et al., 1986) based on counterclockwise node numbering convention. Further, the previous influence coefficient algorithm designed to generate only the standard Galerkin 27-point finite-element nodal connectivities has been enhanced. With the new upstream Galerkin scheme, the transmissivity matrix is more efficiently evaluated by using the following formula:

$$A_{IJ}^{\ell} \Phi_{IJ} = \sum_{J \in \eta_I} \tau_{IJ}^{\ell} \gamma_{IJ} (\Phi_{II} - \Phi_{IJ}) \quad (10)$$

where  $\eta_I$  is the set of connecting neighboring nodes of  $I$  such that  $A_{IJ}^{\ell}$  is non-zero;  $\tau_{IJ}^{\ell}$  is the upstream value of the  $\ell$ -phase mobility for the discrete flow between nodes  $I$  and  $J$ ; and  $\gamma_{IJ}$  the transmissivity coefficient for the flow between nodes  $I$  and  $J$ .

Assuming that the principal components of the permeability tensor  $k_{ij}$  correspond to  $k_{xx}$ ,  $k_{yy}$  and  $k_{zz}$ , the  $\gamma_{IJ}$  coefficients can be calculated from:

$$\gamma_{IJ} = T_{xx} A_{IJ}^x + T_{yy} A_{IJ}^y + T_{zz} A_{IJ}^z \quad (11)$$

where

$$T_{xx} = \left( \frac{mH}{2L} \right) k_{xx} \quad (12a)$$

$$T_{yy} = \left( \frac{LH}{2m} \right) k_{yy} \quad (12b)$$

$$T_{zz} = \left( \frac{Lm}{2H} \right) k_{zz} \quad (12c)$$

with  $L$ ,  $m$  and  $H$  being the element dimensions in the  $x$ -,  $y$ - and  $z$ -directions, respectively; and  $A_{IJ}^x$ ,  $A_{IJ}^y$  and  $A_{IJ}^z$  are the influence coefficients. In the case where an orthogonal curvilinear grid is used,  $L$ ,  $m$  and  $H$  become the average dimensions of the distorted element, along the local axes  $x'$ ,  $y'$  and  $z'$ , respectively.

The influence coefficients have been determined such that the global discretized flow equations at node  $I$  correspond to 27-point finite-element approximation, 7-point finite-difference approximation, or 11-point hybrid (combined finite-element/finite-difference) approximation. Negative transmissivity conditions, which may be encountered with the finite-element approximations, are eliminated using a procedure similar to that of Coats and Modine (1983).

The diagonalized storage matrix element  $B_{II}$  is given by:

$$B_{II} = LmH/8 \quad (13)$$

The upstream 3-D spatial discretization scheme described above is intended to supersede the popular early upstream 2-D weighted residual (UWR) finite-element scheme based on the asymmetric weighting functions given by Huyakorn and Pinder (1978). The major shortcoming of such a finite-element scheme is that it is prone to numerical difficulties due to the existence of negative transmissivity terms in the discretized equations for certain combinations of element aspect and material anisotropy ratios. This condition arises for rectangular prism elements due to a reduction of

the transmissivity terms from the principal axes to provide the diagonal flux term in the influence coefficient matrices, and hence, is not alleviated by upstream weighting. The adverse impact of negative transmissivity conditions on two-dimensional (2-D) numerical results has been demonstrated by Forsyth (1991) for selected cases simulated using triangular elements. In some instances, where the negative transmissivity effects are dominant, the converged numerical solutions are grossly inaccurate or physically impossible as is shown by an example in the companion paper (Panday et al., 1994 in this issue).

### 2.3. Nonlinear treatment by Newton–Raphson procedure

The nonlinearity of Eq. 8 is handled using a residual-based, Newton–Raphson iterative technique. To obtain optimal behavior of the numerical solution in terms of convergence and mass balance, the primary variables must be carefully selected. For the three-phase flow situation, we select  $p_g$ ,  $S_n$  and  $S_g$  as the primary variables. The rationale for the mixed selection of one pressure and two saturations is the fact that the resulting model formulation is superior to formulations that utilize pressures or water height-equivalent pressure heads as the primary variables. The latter may be prone to serious mass-balance errors and nonlinear convergence difficulties when applied to severely nonlinear field problems. The mixed formulation used in our proposed multiphase model yields converged numerical results with negligible mass-balance error (on the order of  $\leq \pm 0.01\%$ ).

A brief description of the Newton–Raphson scheme used in the present model is given below [see Huyakorn and Pinder (1983) for further details]. Let  $R_I^\ell$  ( $\ell = w, n, g$ ) denotes the residual left-hand side of Eq. 8, which can be expressed in the form:

$$R_I^\ell(p_{gI}, S_{nI}, S_{gI}) = 0 \quad \text{for} \quad I = 1, 2, \dots, n \quad (14)$$

Application of the Newton–Raphson procedure to Eq. 14 yields:

$$\frac{\partial R_I^\ell}{\partial p_{gJ}} \Delta p_{gJ} + \frac{\partial R_I^\ell}{\partial S_{nJ}} \Delta S_{nJ} + \frac{\partial R_I^\ell}{\partial S_{gJ}} \Delta S_{gJ} = -(R_I^\ell)^k \quad (15)$$

where  $k$  is the iteration level and, for each primary variable  $\chi$  ( $\chi = p_g, S_n$  or  $S_g$ ), the increment value is defined as  $\Delta\chi = \chi^{k+1} - \chi^k$ .

Using the indicial notation and performing algebraic manipulation, a highly efficient scheme for a term-by-term evaluation of the Jacobian matrix can be derived. The elements of the resulting Jacobian matrix are obtained as follows:

$$\frac{\partial R_I^w}{\partial p_{gJ}} = A_{IJ}^w + \frac{B_{II}^*}{\Delta t} [\beta_{Tw} \rho_w S_{wI}] \delta_{IJ} \quad (16a)$$

$$\frac{\partial R_I^n}{\partial p_{gJ}} = A_{IJ}^n + \frac{B_{II}^*}{\Delta t} [\beta_{Tn} \rho_n S_{nI}] \delta_{IJ} \quad (16b)$$

$$\frac{\partial R_I^g}{\partial p_{gJ}} = (1 + \beta_{gJ} Z_J) A_{IJ}^g + \frac{B_{II}^*}{\Delta t} [\beta_g S_{gI} + \beta_s (\rho_g S_g)_I] \delta_{IJ} \quad (16c)$$

$$\frac{\partial R_I^w}{\partial S_{nJ}} = \Phi_{wL} \frac{\partial A_{IL}^w}{\partial S_{nJ}} - A_{IL}^w \frac{\partial \bar{p}_{cgwL}}{\partial S_{nJ}} - \frac{B_{II}^*}{\Delta t} \rho_w \delta_{IJ} \quad (16d)$$

$$\frac{\partial R_I^n}{\partial S_{nJ}} = \Phi_{nL} \frac{\partial A_{IL}^n}{\partial S_{nJ}} - A_{IL}^n \frac{\partial \bar{p}_{cgnL}}{\partial S_{nJ}} + \frac{B_{II}^*}{\Delta t} \rho_n \delta_{IJ} \quad (16e)$$

$$\frac{\partial R_I^g}{\partial S_{nJ}} = 0 \quad (16f)$$

$$\frac{\partial R_I^w}{\partial S_{gJ}} = \Phi_{wL} \frac{\partial A_{IL}^w}{\partial S_{gJ}} - A_{IL}^w \frac{\partial \bar{p}_{cgwL}}{\partial S_{gJ}} - \frac{B_{II}^*}{\Delta t} \rho_w \delta_{IJ} \quad (16g)$$

$$\frac{\partial R_I^n}{\partial S_{gJ}} = \Phi_{nL} \frac{\partial A_{IL}^n}{\partial S_{gJ}} - A_{IL}^n \frac{\partial \bar{p}_{cgnL}}{\partial S_{gJ}} \quad (16h)$$

$$\frac{\partial R_I^g}{\partial S_{gJ}} = \Phi_{gL} \frac{\partial A_{IL}^g}{\partial S_{gJ}} + \frac{B_{II}^*}{\Delta t} \rho_g \delta_{IJ} \quad (16i)$$

where  $B_{II}^* = \phi^0 B_{II}$ ,  $\beta_{Tl} = \beta_l + \beta_s$ ,  $\bar{p}_{cgwL} = p_{gL} - p_{wL}$ ,  $\bar{p}_{cgnL} = p_{gL} - p_{nL}$  ( $L =$  a dummy nodal subscript), and  $\delta_{IJ}$  is the Kronecker delta.

In constructing the Jacobian matrix for the numerical flow model, two additional options may be provided, which consider the three-phase fluid system with a passive gas phase, and the two-phase liquid system of water and NAPL, respectively. Both options only deal with the flow equations for water and NAPL. The first option is referred to as a “pseudo three-phase formulation” and the second option is just a regular two-phase formulation for flow in the saturated zone. The primary variables selected for each option are  $p_n$  and  $S_n$ . The Jacobian matrix elements can be derived in a similar manner to the most general fully three-phase formulation. Further degeneration of the two optional formulations can readily be obtained for other simpler cases involving water–air flow or water or vapor flow only. For certain practical situations (e.g., air sparging or vapor extraction), the passive-liquid-phase formulation may be used to provide an efficient analysis of the variably saturated flow problem.

#### 2.4. Incorporation of initial and boundary conditions

The initial conditions required to start a transient simulation are introduced by specifying the values of the primary variables at all nodes. These initial values may be derived from the information about the initial state of the system. In some instances, the initial conditions for a current simulation correspond to the final results of a previous simulation.

Boundary conditions for the multiphase flow equations may be specified in terms of nodal values of fluid pressures and mass fluxes. Prescribed flux conditions are treated simply by adding the specified nodal flux values to the right-hand side of the



corresponding nodal equations. Prescribed pressure conditions of  $p_{\ell I} = \bar{p}$  are incorporated into the matrix system by first considering a no-flow condition at node  $I$  then using a source/sink term,  $\Lambda_I^\ell$ , to inject or produce the correct amount of fluid so that  $p_{\ell I}$  approaches the prescribed value  $\bar{p}$  (Forsyth, 1988). Physically,  $\Lambda_I^\ell$  may be regarded as the mass flux of phase  $\ell$  through a skin layer of porous material adjacent to the boundary portion covered by node  $I$ .

The above scheme for treating pressure boundary conditions is chosen in preference of the more straightforward matrix manipulation scheme used in the mixed formulation ( $p_w, S_n$ ) of the pseudo three-phase models of Faust (1985) and Faust et al. (1989). In the latter scheme, the first-type condition at node  $I$  is satisfied simply by setting the diagonal term of the corresponding model equation to 1 and the off-diagonal terms to 0, and setting the right-hand side to the prescribed value. The major shortcoming of such a scheme is that certain practical boundary conditions involving nodal unknowns that are non-primary variables cannot be handled. For instance, if  $p_w$  and  $S_n$  are the primary variables, then the boundary conditions  $\bar{p}$  cannot be directly imposed.

After the boundary conditions have been incorporated into the matrix system, the water-phase nodal equations are replaced by the phase-summed nodal equations obtained by summing the contributions of all phases. This is done to ensure non-zero diagonal coefficients of the pressure unknowns. Because of the fact that we associate the pressure variable,  $p_g$ , with the water flow governing equation, zero diagonal terms may occur in a zone of residual water saturation for cases where the compressibility factor  $\beta_{Tw}$  is assumed to be zero (see Eq. 16a).

### 2.5. Treatment of well conditions

Withdrawal and injection wells may be used in the remediation of soil and groundwater contamination problems, and need to be incorporated in the numerical solution of the governing equations. It should be noted that two simplifying assumptions are commonly employed in the treatment of well boundary conditions. The first assumption concerns the allocation of the total well flow rate to the individual well nodes. Via this assumption, the allocation is performed in proportion to the transmissivity values at the nodes. Such an approximation may be inaccurate for cases involving partially penetrating wells or multi-screen wells in layered formations. The second assumption concerns the evaluation of nodal fluid flux of a particular phase. Via this assumption, the nodal flux evaluation is made on the basis of fractional mobility of the phase. For the assumption to be valid, the nodal pressures of all fluid phases must be identical (i.e.  $p_{wI} = p_{nI} = p_{gI}$ ). This will not be the case if capillary effects are appreciable near the well.

We consider two cases involving withdrawal wells operating under prescribed total rate of production and prescribed bottom pressure conditions, respectively. Treatment procedures developed for the withdrawal wells can be readily adapted to the corresponding cases of injection wells. The schemes presented below are rigorous schemes that do not require the two simplifying assumptions just mentioned.

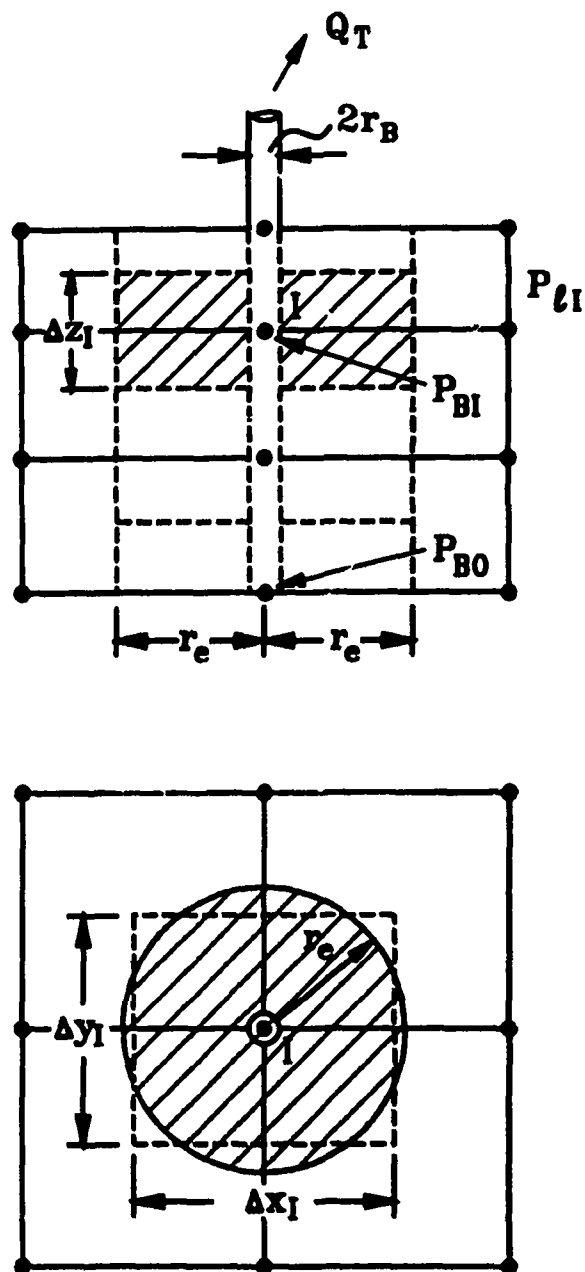


Fig. 1. Wellbore configuration and boundary condition [ $\ell = (w, n, a)$ ];  $P_{B0}$  = bottom hole pressure;  $r_B$  = wellbase radius]. Note:  $n_e = (\Delta k_1, \Delta y_1, / \pi)^{1/2}$ .

### 2.6. Prescribed total production rate

Consider the general situation depicted in Fig. 1 where a well is withdrawing fluids from several grid blocks and the total volumetric production rate is specified as  $\bar{Q}_T$ . The total volumetric production rate as contributed by the nodes along the well screen is given by:

$$\bar{Q}_T = \sum_{I=1}^{n_s} q_{TI} \tag{17}$$

where  $q_{TI}$  is the total volumetric fluid flux at node  $I$ ; and  $n_s$  is the number of nodes on the well screen.

The total fluid flux at node  $I$  is the sum of contributions from all fluid phases. Thus:

$$q_{TI} = \sum_{\ell} q_{\ell I} \tag{18}$$

where  $q_{\ell I}$  is the  $\ell$ -phase fluid flux at node  $I$ . Note that  $q_{\ell I} = M_{\alpha} / \rho_{\ell}^0$ , where  $\rho_{\ell}^0$  is the

reference density of phase  $\ell$ . The control volume associated with node  $I$  is depicted in Fig. 1. Within this volume, the flow of each phase is assumed to be in a quasi-steady state and the average phase pressure is  $p_{\ell I}$ . To facilitate an analytical solution of the local grid-block well flow problem, we introduce a concentric circle of radius  $r_e$ . The analytical solution domain is thus bounded by  $r_B \leq r \leq r_e$ . Formulas for determining  $r_e$  can be found in several references (Pritchett and Garg, 1980; Peaceman, 1983; Abou-Kassem and Aziz, 1985). At the well boundary,  $r = r_B$  and  $p_\ell = p_{BI}$  (the wellbore pressure at node  $I$ ). Using the radial flow analytical solution given by Dake (1978, p.146)  $q_{\ell I}$  may be expressed as:

$$q_{\ell I} = G_{BI} \lambda_{\ell I} (p_{\ell I} - p_{BI}) \tag{19}$$

where  $\lambda_{\ell I}$  is a mobility factor for phase  $\ell$  at node  $I$ ; and  $G_{BI}$  is the wellbore index for node  $I$ . These coefficients are defined as follows:

$$\lambda_{\ell I} = \frac{k_{r\ell I}}{\mu_\ell B_{\ell I}} \tag{20a}$$

$$G_{BI} = \frac{2\pi k \Delta Z_I}{\ln(r_e/r_B) + S_F - f} \tag{20b}$$

where  $B_\ell$  is the formation volume factor for phase  $\ell$ ;  $r_B$  is the wellbore radius;  $f$  is a constant set equal to 0.75 for transient flow solution;  $\Delta Z_I$  is the thickness of the control volume surrounding node  $I$ ; and  $S_F$  is a skin factor of the well ( $S_F$  is usually set = 0). The formation factor for phase  $\ell$  is a dimensionless quantity reflecting the volume that a unit volume of fluid phase  $\ell$  occupies under reservoir conditions (see G.W. Thomas, 1982, pp. 38 and 39). Note that  $p_{BI}$  can be evaluated in terms of the bottom hole pressure  $p_{BO}$  by using the hydrostatic assumption as follows:

$$p_{BI} = p_{BO} - \bar{\rho}g(Z_I - Z_0) \tag{21a}$$

and

$$p_{BO} = \frac{-\bar{Q}_T + \sum_{I=1}^{n_s} \sum_{\ell} G_{BI} \lambda_{\ell I} [p_{\ell I} + \bar{\rho}g_T(Z_T - Z)]}{\sum_{I=1}^{n_s} \sum_{\ell} G_{BI} \lambda_{\ell I}} \tag{21b}$$

where  $\bar{\rho}$  is an average density of the column of fluid mixture in the wellbore.

A fully implicit treatment of the production term of nodal equation for fluid phase  $\ell$  is obtained by evaluating  $\Delta q_{\ell I}$  as follows:

$$\Delta q_{\ell I} = \frac{\partial q_{\ell I}}{\partial p_{gI}} \Delta p_{gI} + \frac{\partial q_{\ell I}}{\partial S_{nI}} \Delta S_{nI} + \frac{\partial q_{\ell I}}{\partial S_{gI}} \Delta S_{gI} + \frac{\partial q_{\ell I}}{\partial p_{BI}} \Delta p_{BI} \tag{22}$$

Next, we need to eliminate  $\Delta p_{BI}$  from Eq. 22. This is achieved by making use of Eqs. 17 and 18 to obtain:

$$\Delta \bar{Q}_T = 0 = \sum_{I=1}^{n_s} \sum_{\ell} \Delta q_{\ell I} \tag{23}$$

which upon combining with Eq. 22 gives:

$$\sum_{I=1}^{n_s} \sum_{\ell} \frac{\partial q_{\ell I}}{\partial p_{BI}} \Delta p_{BI} = - \sum_{I=1}^{n_s} \sum_{\ell} \left[ \frac{\partial q_{\ell I}}{\partial p_{gI}} \Delta p_{gI} + \frac{\partial q_{\ell I}}{\partial S_{nI}} \Delta S_{nI} + \frac{\partial q_{\ell I}}{\partial S_{gI}} \Delta S_{gI} \right] \quad (24)$$

Noting from Eqs. 21 that  $\Delta p_{BI}$  is independent of  $I$  (i.e.  $\Delta p_{BI} = \Delta p_{BO}$ ), we obtain:

$$\Delta p_{BI} = \frac{- \sum_{I=1}^{n_s} \sum_{\ell} \left[ \frac{\partial q_{\ell I}}{\partial p_{gI}} \Delta p_{gI} + \frac{\partial q_{\ell I}}{\partial S_{nI}} \Delta S_{nI} + \frac{\partial q_{\ell I}}{\partial S_{gI}} \Delta S_{gI} \right]}{\sum_{I=1}^{n_s} \sum_{\ell} \frac{\partial q_{\ell I}}{\partial p_{BI}}} \quad (25)$$

The gradients of  $q_{\ell I}$  may be directly evaluated from Eq. 19 as follows:

$$\frac{\partial q_{\ell I}}{\partial p_{BI}} = -G_{BI} \lambda_{\ell I} \quad (26a)$$

$$\frac{\partial q_{\ell I}}{\partial p_{gI}} = G_{BI} \lambda_{\ell I} \frac{\partial p_{\ell I}}{\partial p_{gI}} \quad (26b)$$

$$\frac{\partial q_{\ell I}}{\partial S_{nI}} = G_{BI} (p_{\ell I} - p_{BI}) \frac{\partial \lambda_{\ell I}}{\partial S_{nI}} + G_{BI} \lambda_{\ell I} \frac{\partial p_{\ell I}}{\partial S_{nI}} \quad (26c)$$

$$\frac{\partial q_{\ell I}}{\partial S_{gI}} = G_{BI} (p_{\ell I} - p_{BI}) \frac{\partial \lambda_{\ell I}}{\partial S_{gI}} + G_{BI} \lambda_{\ell I} \frac{\partial p_{\ell I}}{\partial S_{gI}} \quad (26d)$$

In summary, the treatment of the well boundary conditions at node  $I$  involves the following calculation for each iteration:

(1) Evaluation of  $q_{\ell I}^k$  using Eqs. 19–21a and the nodal values from the previous iteration, and addition of  $q_{\ell I}^k$  to the residual.

(2) Evaluation of  $\Delta q_{\ell I}$  using Eqs. 22, 25 and 26a–26d.

(3) Incorporation of the terms resulting from the  $\Delta q_{\ell I}$  evaluation into the Jacobian matrix, and solution of the resulting matrix equation.

(4) Evaluation of  $\Delta p_{BI}$  using Eq. 25, and addition of  $\Delta p_{BI}$  to  $p_{BI}^k$  to obtain  $p_{BI}^{k+1}$ .

(5) Updating the well bottom hole pressure  $p_{BO}^{k+1}$  using Eq. 21b.

A constraint may be imposed on the calculated value of the well bottom hole pressure to ensure that it does not fall below the minimum practically allowable value for the well to maintain the prescribed production rate. If this constraint is violated the well may be switched from prescribed flow rate to prescribed bottom hole pressure condition.

## 2.7. Prescribed bottom hole pressure

In the case where  $p_{BO}$  is specified ( $p_{BO} = \bar{p}_{BO}$ ), it follows from Eqs. 21 that:

$$p_{BI} = \bar{p}_{BO} - \bar{\rho}g(Z_I - Z_0) \quad (27a)$$

and

$$\Delta p_{BI} = 0 \quad (27b)$$

Thus  $q_{\ell I}^k$  and  $\Delta q_{\ell I}$  are given by:

$$q_{\ell I}^k = G_{BI} \lambda_{\ell I}^k (p_{\ell I}^k - \tilde{p}_{BI}) \quad (28)$$

and

$$\Delta q_{\ell I} = \frac{\partial q_{\ell I}}{\partial p_{gI}} \Delta p_{gI} + \frac{\partial q_{\ell I}}{\partial S_{nI}} \Delta S_{nI} + \frac{\partial q_{\ell I}}{\partial S_g} \Delta S_g \quad (29)$$

where the three partial derivatives are evaluated using Eqs. 26b, 26c and 26d, respectively.

The treatment of the well boundary conditions at node  $I$  involves the following calculation for each iteration:

(1) Evaluation of  $q_{\ell I}^k$  using Eq. 28 and the nodal values from the previous iteration, and addition of  $q_{\ell I}^k$  to the residual.

(2) Evaluation of  $\Delta q_{\ell I}$  using Eqs. 29 and 26b–26d.

(3) Incorporation of the terms resulting from the  $\Delta q_{\ell I}$  evaluation into the Jacobian matrix, and solution of the resulting matrix equation.

## 2.8. Iterative solution and time-stepping schemes

In a multiphase flow simulation, nonlinear iterations must be performed within each time step to obtain a stable numerical solution. At the beginning of the current time step, the converged nodal values from the previous time step are used as the initial estimate to compute the Jacobian matrix elements. The resulting linearized system of algebraic equations is solved for current nodal values of the primary variable  $\chi_I$ . Iteration is then performed following the updating of the Jacobian matrix. The iteration is continued until the residuals,  $\Delta \chi_I$ , are reduced to within prescribed tolerances.

To enhance convergence of the numerical solution, we use an under-relaxation procedure whereby the current unknown vector  $\chi_I^{r+1}$  is computed from:

$$\chi_I^{r+1} = \chi_I^r + \Omega^{r+1} \Delta \chi_I^{r+1} \quad (30)$$

where  $\Omega^{r+1}$  is an automatically computed under-relaxation factor. The value of  $\Omega^{r+1}$  is determined as follows:

$$\Omega^{r+1} = \min \left[ \frac{0.2}{|e_s^{r+1}|}, 1 \right] \quad (31)$$

subject to

$$0.1 \leq \Omega^{r+1} \leq 1 \quad (32)$$

$$|e_s^{r+1}| = \max \left[ \max_I |\Delta S_{\ell I}^r|, \quad \ell = w, n, g \right] \quad (33)$$

Computational time steps for the transient flow simulation are determined using the following procedure:

(1) Start the numerical solution for the first time step with a specified value of  $\Delta t_1$ . Perform the nonlinear Newton–Raphson iterations. If satisfactory convergence is obtained, then determine the subsequent computational time steps using the following algorithm:

$$\Delta t_{k+1} = \text{TMUL} * \Delta t_k \leq \Delta t_{\max}, \quad k \geq 1$$

where  $\Delta t_{\max}$  is the maximum allowable time step size prescribed a priori; and TMUL is the time step multiplier. The value of TMUL is given by:

$$\text{TMUL} = \min \left[ \frac{\text{DSWISH}}{\sum |\Delta' S_{\ell}|_{\max}}, 5 \right]; \quad \ell = \text{active phases}$$

$$|\delta' S_{\ell}|_{\max} = \max_l |S_{\ell l}^{k+1} - S_{\ell l}^k|$$

and the desired incremental change in saturation value over the time step (DSWISH) may be specified as 0.2.

(2) If convergence of the solution is not achieved within the allowable maximum number of nonlinear iterations, NITMAX, then reduce the computational time step size according to the following scheme:

$$\Delta t_k = \Delta t_k / \text{TDIV}$$

where TDIV is the time step divider set equal to 2, 5 and 10 for  $k = 1, 2$  and  $\geq 3$ , respectively.

(3) If necessary, adjust the computational time step,  $\Delta t_k$ , to obtain  $t_{k+1}$ -value that coincides with a target time value at which simulation output is required.

## 2.9. Variable scaling and matrix solution

In computing the Jacobian matrix and right-hand-side vector, certain variables and physical parameters are scaled to minimize floating-point round-off errors in the matrix solution. The following scaling factor is introduced:

$$\xi = \rho_{fw} g \quad (34)$$

where  $\xi$  is the specific weight of fresh water.

The scaled quantities are defined in terms of their original counterparts as follows:

$$p_{\ell}^* = p_{\ell} / \xi \quad (35a)$$

$$\Phi_{\ell}^* = \Phi_{\ell} / \xi \quad (35b)$$

$$k_{ij}^* = \xi k_{ij} \quad (35c)$$

$$\beta_{\ell}^* = \xi \beta_{\ell} \quad (35d)$$

$$\beta_s^* = \xi \beta_s \quad (35e)$$

$$g^* = g / \xi \quad (35f)$$

By operating in terms of the scaled quantities, the contrast in orders of magnitude of the real numbers are greatly reduced.

In obtaining the numerical solution of a given flow problem, we adopt the following procedure:

(1) Scale material parameters,  $k_{ij}$ ,  $\beta_\ell$ ,  $\beta_s$  and the gravitational constant,  $g$ , using Eqs. 35c, 35d, 35e and 35f, respectively. This step may be performed after the material properties have been read and printed.

(2) Introduce local arrays in the element matrix computation subroutine to store scaled values of fluid potentials, pressures and their derivatives. Use these local arrays (instead of their corresponding global arrays) in the evaluation of Jacobian matrix and right-hand-side vector.

(3) Solve the matrix equation and use Eqs. 35a and 35b to compute the unscaled pressure and potential values,  $p_\ell$  and  $\Phi_\ell$ .

Note that step (1) is performed only once but steps (2) and (3) are performed for each iteration. For the solution of the linearized system of algebraic equations we use an iterative matrix solver based on an incomplete factorization with Orthomin<sup>©</sup> acceleration (Behie and Forsyth, 1984). The computational time and memory requirements of the iterative matrix solver used is directly dependent on the choice of model lattice option. In three dimensions, the 27-point finite-element lattice option requires substantially more memory and computational effort in the matrix solution than the 7-point finite-difference lattice option. However, the latter may be prone to grid orientation problem. The 11-point option provides a viable alternative by combining the salient features of finite-element and finite-difference approximations.

### 3. Extension to fractured media

Fractured formations can be conceptually represented using two approaches referred to as the discrete-fracture and the dual-porosity modeling approaches, respectively (Huyakorn et al., 1983; Pinder et al., 1993). Both approaches and their formulations are described below for the general situation of three-phase flow.

#### 3.1. Discrete-fracture modeling approach

In the discrete-fracture modeling approach, each individual fracture is idealized as a pair of parallel plates. The fracture may contain only fluids or both fluids and granular solid materials (i.e. its internal porosity,  $\phi^f$ , may be  $\leq 1$ ). The fluid potentials are assumed to be uniform across the fracture aperture. The governing equations for three-phase, planar flow of water, NAPL and air in a non-deformable fracture of aperture  $b^f$  can be written in the form:

$$\frac{\partial}{\partial x_i^*} \left[ k_{ij}^f b^f \tau_\ell^f \frac{\partial \Phi_\ell^f}{\partial x_j^*} \right] = b^f \frac{\partial}{\partial t} (\phi^f \rho_\ell S_\ell), \quad i, j = 1, 2; \quad \ell = w, n, g \quad (36)$$

where superscript f is used to denote the planar fracture domain;  $x_i^*$  ( $i = 1, 2$ ) are

local coordinates parallel to the fracture planes, and the remaining symbols are as defined previously. The fracture intrinsic permeability,  $k_{ij}^f$ , is defined as:

$$k_{ij}^f = \frac{(b^f)^2}{12} \delta_{ij} \quad (37)$$

Multiphase constitutive relations for the fractures are needed to describe their fluid retention characteristics. Such relations have not yet been determined experimentally for NAPL contamination problems. However, several theoretical studies have been performed to characterize the nature of the relationships (Wang and Narasimhan, 1985; Pruess and Tsang, 1990; Mendoza and Sudicky, 1993).

Eq. 36 is discretized using the Galerkin finite-element procedure with a fully implicit time integration scheme. The fractures are represented using plane rectangular elements if the overall flow problem is 3-D. For 2-D analyses, the fractures are represented by 1-D line elements. For a typical fracture element, the discretized set of algebraic equations take the form:

$$R_I^{wf} \equiv A_{IJ}^{wf} \Phi_{wJ} + \frac{B_{II}^f}{\Delta t} [\Delta'(\phi^f \rho_w S_w)_I] = 0 \quad (38)$$

$$R_I^{nf} \equiv A_{IJ}^{nf} \Phi_{nJ} + \frac{B_{II}^f}{\Delta t} [\Delta'(\phi^f \rho_n S_n)_I] = 0 \quad (39)$$

$$R_I^{gf} \equiv A_{IJ}^{gf} \Phi_{gJ} + \frac{B_{II}^f}{\Delta t} [\Delta'(\phi^f \rho_g S_g)_I] = 0 \quad (40)$$

where the assumption of  $\Phi_{\ell J}^f = \Phi_{\ell J}$  has been incorporated.

The Jacobian matrix for each of the variably saturated flow formulations can be derived in the same manner as that described previously for the porous medium case. The three-phase pressures are the primary variables at nodes that represent both fracture and matrix, since there is continuity of pressure (but not of phase saturations), across the fracture–matrix boundary. The contributions of the fracture elements can be directly added to the global matrix system using the standard procedure for matrix assembly.

### 3.2. Dual-porosity approach

In the dual-porosity modeling approach, the reservoir formation is assumed to be comprised of a continuous network of fractures in direct contact with porous matrix blocks. The fractured porous medium is represented by two completely overlapping continua, one representing the fracture domain and the other representing the porous matrix. Primary flow in the reservoir formation is assumed to occur within the fractures with local exchanges of fluids between the fractures and the porous matrix blocks.

The governing equations for three-phase flow in the fracture continuum may be



written as:

$$\frac{\partial}{\partial x_i} \left[ k_{ij} \tau_\ell \frac{\partial \Phi_\ell}{\partial x_j} \right] = \frac{\partial}{\partial t} (\phi \rho_\ell S_\ell) - \dot{M}_\ell - \Gamma_\ell, \quad \ell = w, n, g; \quad i, j = 1, 2, 3 \quad (41)$$

where  $\Gamma_\ell$  is the rate of fluid mass transfer from the fracture to porous matrix domain, and the remaining symbols are as defined previously for the conventional porous-medium flow except that all quantities in Eq. 41 now refer to the fracture continuum. Note that  $\phi$  in Eq. 41 now denotes the fracture (or secondary) porosity defined as the ratio of the volume of fractures to the bulk volume of the medium. The matrix/fracture fluid exchange term,  $\Gamma_\ell$ , is evaluated using a quasi-steady approximation for inter-porosity flow (Barenblatt et al., 1960). The expression for  $\Gamma_\ell$  is given by:

$$\Gamma_\ell = \Lambda^m k^m \tau_\ell^m (\Phi_\ell - \Phi_\ell^m) \quad (42)$$

where superscript m refers to the matrix block domain; and  $\Lambda^m$  is a geometrical shape factor which depends on the matrix-block specific surface and a characteristic length associated with matrix/fracture flow.

The governing equations for flow in the porous matrix blocks are given by:

$$-\Lambda^m k^m \tau_\ell^m (\Phi_\ell^m - \Phi_\ell) = \frac{\partial}{\partial t} (\phi^m \rho_\ell S_\ell^m) \quad (43)$$

where  $\phi^m$  denotes the matrix (primary) porosity. In addition to the governing equations, two sets of multiphase constitutive relations are needed to describe fluid retention characteristics of the fractures and matrix blocks.

The governing equations represented by Eqs. 41 and 43 are discretized using the Galerkin finite-element procedure with a fully implicit time-stepping scheme. The discretized system of equations for flow in the fracture domain takes the form:

$$R_I^{w*} \equiv R_I^w + \Gamma_{wI} = 0 \quad (44)$$

$$R_I^{n*} \equiv R_I^n + \Gamma_{nI} = 0 \quad (45)$$

$$R_I^{g*} \equiv R_I^g + \Gamma_{gI} = 0 \quad (46)$$

where the expressions for  $R_I^w$ ,  $R_I^n$  and  $R_I^g$  are as given previously for the porous-medium case,

$$\Gamma_{\ell I} = \Lambda^m k^m \tau_{\ell u}^m B'_{II} (\Phi_{\ell I} - \Phi_{\ell I}^m), \quad \ell = w, n, a \quad (47)$$

where  $B'_I$  is the grid bulk volume for node  $I$ ; and  $\tau_{\ell u}^m$  is the upstream mobility evaluated using the porous matrix fluid retention characteristic curves. The discretized system of equations for flow in the matrix block takes the form:

$$R_I^{wm} \equiv -\Gamma_{wI} + \frac{B'_{II}}{\Delta t} [\Delta t (\phi^m \rho_w S_w^m)_I] = 0 \quad (48)$$

$$R_I^{nm} \equiv -\Gamma_{nI} + \frac{B'_{II}}{\Delta t} [\Delta t (\phi^m \rho_n S_n^m)_I] = 0 \quad (49)$$

$$R_I^{gm} \equiv -\Gamma_{gI} + \frac{B'_{II}}{\Delta t} [\Delta t (\phi^m \rho_g S_g^m)_I] = 0 \quad (50)$$

For a situation of three-phase flow, the selected primary variables are  $p_g$ ,  $S_n$ ,  $S_g$ ,  $p_g^m$ ,  $S_n^m$  and  $S_g^m$ . It is best to begin the Jacobian matrix evaluation by applying the Newton–Raphson procedure to Eqs. 48–50. The resulting matrix system may be written in the form:

$$[G]_{II}\{\Delta\chi^m\}_I = -[H]_{II}\{\Delta\chi\}_I - \{R^{wm}\}_I^k \quad (51)$$

where  $[G]_{II}$ ,  $[H]_{II}$  are  $3 \times 3$  submatrices given by:

$$[G]_{II} = \begin{bmatrix} \frac{\partial R_I^{wm}}{\partial p_{gl}^m} & \frac{\partial R_I^{wm}}{\partial S_{nl}^m} & \frac{\partial R_I^{wm}}{\partial S_{gl}^m} \\ \frac{\partial R_I^{nm}}{\partial p_{gl}^m} & \frac{\partial R_I^{nm}}{\partial S_{nl}^m} & \frac{\partial R_I^{nm}}{\partial S_{gl}^m} \\ \frac{\partial R_I^{gm}}{\partial p_{gl}^m} & \frac{\partial R_I^{gm}}{\partial S_{nl}^m} & \frac{\partial R_I^{gm}}{\partial S_{gl}^m} \end{bmatrix} \quad (52a)$$

$$[H]_{II} = \begin{bmatrix} \frac{\partial R_I^{wm}}{\partial p_{gl}} & \frac{\partial R_I^{wm}}{\partial S_{nl}} & \frac{\partial R_I^{wm}}{\partial S_{gl}} \\ \frac{\partial R_I^{nm}}{\partial p_{gl}} & \frac{\partial R_I^{nm}}{\partial S_{nl}} & \frac{\partial R_I^{nm}}{\partial S_{gl}} \\ \frac{\partial R_I^{gm}}{\partial p_{gl}} & \frac{\partial R_I^{gm}}{\partial S_{nl}} & \frac{\partial R_I^{gm}}{\partial S_{gl}} \end{bmatrix} \quad (52b)$$

$$\{\Delta\chi^m\}_I = \begin{Bmatrix} \Delta p_{gl}^m \\ \Delta S_{nl}^m \\ \Delta S_{gl}^m \end{Bmatrix}; \quad \{\Delta\chi\}_I = \begin{Bmatrix} \Delta p_{gl} \\ \Delta S_{nl} \\ \Delta S_{gl} \end{Bmatrix} \quad (53)$$

Using Eq. 51 the unknown vector  $\Delta\chi^m_I$  may be expressed in terms of  $\Delta\chi_I$  as follows:

$$\{\Delta\chi^m\}_I = -[\underline{H}]_{II}\{\Delta\chi\}_I - \{\underline{R}^{wm}\}_I^k \quad (54)$$

where

$$[\underline{H}]_{II} = [G]_{II}^{-1}[H]_{II} \quad (55)$$

and

$$\{\underline{R}^{wm}\}_I^k = [G]_{II}^{-1}\{R^{wm}\}_I^k \quad (56)$$

In a similar manner, the Newton–Raphson procedure is applied to the residual equations of fracture flow (44)–(46). This yields the following global matrix equation:

$$\left[ \frac{\partial R^{\ell*}}{\partial \chi} \right]_{IJ} \{\Delta\chi\}_J = -\{R^{\ell*}\}_I^k \quad (57)$$

where

$$\left[ \frac{\partial R^{\ell*}}{\partial \chi} \right]_{IJ} = \begin{bmatrix} \frac{\partial R_I^{w*}}{\partial p_{gJ}} & \frac{\partial R_I^{w*}}{\partial S_{nJ}} & \frac{\partial R_I^{w*}}{\partial S_{gJ}} \\ \frac{\partial R_I^{n*}}{\partial p_{gJ}} & \frac{\partial R_I^{n*}}{\partial S_{nJ}} & \frac{\partial R_I^{n*}}{\partial S_{gJ}} \\ \frac{\partial R_I^{g*}}{\partial p_{gJ}} & \frac{\partial R_I^{g*}}{\partial S_{nJ}} & \frac{\partial R_I^{g*}}{\partial S_{gJ}} \end{bmatrix} \quad (58)$$

$$\{\Delta \chi\}_J = \begin{Bmatrix} \Delta p_{gJ} \\ \Delta S_{nJ} \\ \Delta S_{gJ} \end{Bmatrix}, \quad \{\underline{R}^{\ell*}\}_I = \begin{Bmatrix} \underline{R}_I^{w*} \\ \underline{R}_I^{n*} \\ \underline{R}_I^{g*} \end{Bmatrix} \quad (59)$$

and the Jacobian submatrix elements may be evaluated as follows:  
for  $J \neq I$ ,

$$\left[ \frac{\partial R^{\ell*}}{\partial \chi} \right]_{IJ} = \left[ \frac{\partial R^{\ell}}{\partial \chi} \right]_{IJ} \quad (60)$$

and for  $J = I$ ,

$$\left[ \frac{\partial R^{\ell*}}{\partial \chi} \right]_{II} = \left[ \frac{\partial R^{\ell}}{\partial \chi} \right]_{II} + \left[ \frac{\partial \Gamma^{\ell}}{\partial \chi} \right]_{II} + \left[ \frac{\partial \Gamma^{\ell}}{\partial \chi^m} \right]_{II} [\underline{H}]_{II} \quad (61)$$

The elements of the right-hand-side vector are given by:

$$\{\underline{R}^{\ell*}\}_I^k = \{R^{\ell*}\}_I^k + \{\underline{R}^{\ell m}\}_I^k \quad (62)$$

For each computational time step, the system of algebraic equations represented by Eq. 57 is solved for the nodal unknowns of the fracture domain,  $\Delta \chi_J$ . The determined values of  $\Delta \chi_J$  are then substituted into Eq. 56 to evaluate the nodal unknowns of the porous matrix domain.

#### 4. Summary and conclusion

The formulation and numerical solution techniques of a comprehensive 3-D model for analyzing the subsurface flow of NAPL contaminants have been developed. The three-phase governing and supplementary equations for a general contamination or remediation scenario involving water, NAPL, and vapor have been discussed. The various boundary conditions implemented in the code include prescribed phase pressures and/or fluxes, total well production rate, and bottom hole pressure conditions. Fracture flows are significant for many kinds of subsurface materials, and these have been treated via the discrete-fracture and dual-porosity conceptual

approaches. Coupling of the porous matrix and fracture domains has been taken into account, and an efficient scheme has been presented for Jacobian evaluation and nonlinear solution. The numerical techniques have been derived with an emphasis on practical applicability of the model to various field contamination/remediation assessment scenarios. Orthogonal curvilinear grids consisting of distorted brick elements may be used to accommodate irregular soil layering or other complex features of the flow boundaries. The Galerkin procedure has been used to approximate the governing equations, with upstream weighting of fluid mobilities, storage matrix mass lumping, and fully implicit time stepping. The Newton–Raphson linearization with fully implicit representation of nonlinear coefficients and the under-relaxation updating scheme provide stable solutions for large time steps and severely nonlinear conditions. The mixed selection of primary variables (one pressure and two saturations for the three-phase problem) ensures mass-conservative numerical results. In view of its superior mass-balance behavior and robustness, such a mixed formulation is preferable to a formulation with only pressures or equivalent freshwater heads as the primary variables. Term-by-term evaluation of the Jacobian matrix prevents unwarranted computations. The general three-phase formulation of the present model collapses to the passive air-phase and two-phase formulations for efficient simulations of simpler scenarios. Finally, aggressive time-stepping scheme and robust block-Orthomin<sup>©</sup> solver provides efficient and accurate solutions to the complex equation set. A comprehensive, flexible and robust simulator is essential for practical investigations; from pilot studies, calibration, and sensitivity analyses to predictive simulations and examination of alternative remediation scenarios.

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