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Mathematical and Numerical Formulation of Nonisothermal Multicomponent Three-Phase Flow in Porous Media

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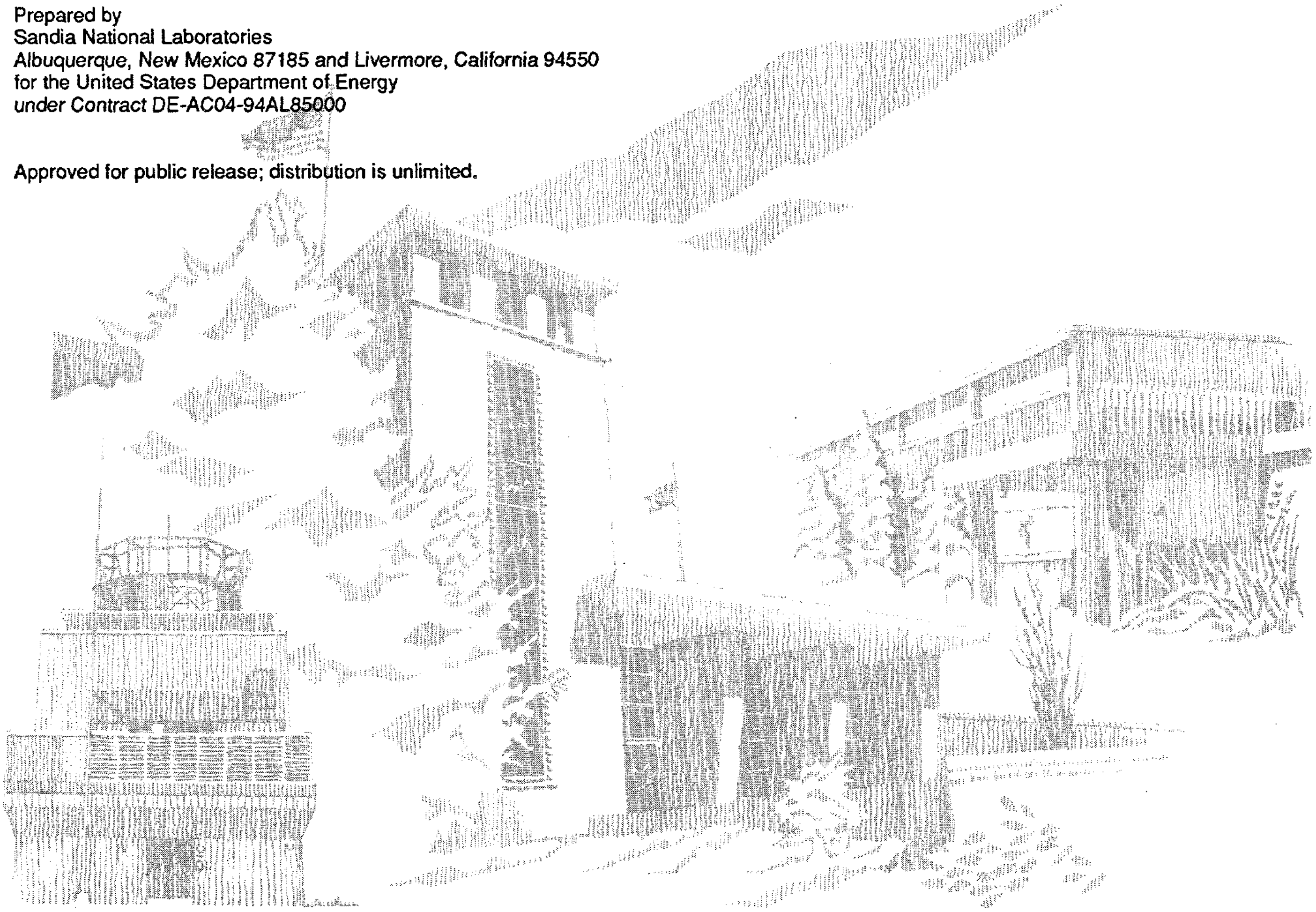

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Mathematical and Numerical Formulation of Nonisothermal Multicomponent Three-Phase Flow in Porous Media

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Abstract

A mathematical formulation is presented for describing the transport of air, water, NAPL, and energy through porous media. The development follows a continuum mechanics approach. The theory assumes the existence of various average macroscopic variables which describe the state of the system. Balance equations for mass and energy are formulated in terms of these macroscopic variables. The system is supplemented with constitutive equations relating fluxes to the state variables, and with transport property specifications. Specification of phase equilibrium criteria, various mixing rules and thermodynamic relations completes the system of equations. A numerical simulation scheme based on finite-differences is described.

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1. Introduction

Many new and established remediation techniques for subsurface contaminant spills or leaks involve multiphase, multicomponent transport of fluids in geologic materials. Emerging thermal techniques introduce even more complexity owing to heat-driven transport processes and phase transitions. Evaluation and analysis of such technologies is greatly enhanced by numerical simulation. This report forms the basis for the development of numerical simulation capability for this class of transport problem. Problems of this type have been considered in the oil industry, especially in enhanced oil recovery processes such as steam injection and chemical flooding techniques (see Lake, 1989). The emphasis in the oil industry is different from remediation. In the former the emphasis is on recovering as much free product as is economically feasible, whereas the latter is to recover residual (often measured in parts-per-million) quantities of contaminants (usually organics). Chemical flooding techniques are concerned with recovering residuals. However, these treatments typically involve isothermal transport of trace additives (surfactants for example), for which interphase transport is not significant. Therefore, numerical simulators developed in the oil industry may not include physics relevant to groundwater quality problems, such as multicomponent diffusion or interphase transport.

There are several approaches leading to the development of a mathematical description of multiphase flow in porous media. This fact in itself is indicative of a state of flux in the development and understanding of multiphase flow in porous media. The basic problem lies in the fact that a pore scale description is impractical due to the complex geometries of the interstitial passages through which the fluids must flow. A more practical approach is to develop a description applicable to the macroscale, and herein lies the source of the problem. The equations governing multiphase flow on the microscale (Williams, 1985) are fairly well-established, although by no means fully settled. However, the problem of taking the microscale continuum equations to the macroscale is a formidable task. The approaches taken to date involve averaging methods, use of mixture theory, and a macroscale continuum approach (see Hassanizadeh and Gray, 1990). By the latter we refer to an approach where certain macroscale quantities are assumed to exist at the outset. These quantities are conceptualized as values averaged over a representative elementary volume (REV). In the present work, we will follow a continuum mechanics approach based on postulates regarding relations between microscale and macroscale quantities, although we make use of findings from all the aforementioned approaches. Balance equations for mass and energy are supplemented with constitutive equations, transport property specifications, and thermodynamic relations to complete the system of equations.

Because the resulting system of partial differential equations require numerical treatment, a numerical scheme, based on finite difference techniques is described. The temporal integration is accomplished using implicit backward-difference formulae. The resulting nonlinear system of equations can be solved via Newton's method, and this procedure is also described in some detail.

2. Balance Equations

2.1 Kinematics

The system under consideration is composed of a porous matrix or skeleton whose interstitial volume is occupied by fluid in motion under various forces. The porosity (interstitial volume fraction) is denoted ϕ and is occupied by two liquid phases, water and a nonaqueous-phase-liquid (NAPL), and a gas phase. The NAPL will be interchangeably referred to as an oil as well. For definiteness, we take the fluid components to be water, air, and an oil. Each component can partition into each phase. A distinguishing feature of this system is that the liquid phases are partially miscible. That is, the water phase is mostly water, but can have small amounts of oil and air in solution. On the other hand, the gas phase is a mixture of air, water and oil vapor, where each constituent may exist in any fraction between zero and one. In the remainder of this work, subscript g refers to gas, w to water, and o to oil. In order to avoid introducing interphase mass transfer terms, component balances will be developed.

Component balance equations for water, air, and oil (NAPL), respectively, take the form:

$$\frac{\partial d_w}{\partial t} + \nabla \bullet \boldsymbol{F}_w = Q_w, \tag{1}$$

$$\frac{\partial d_a}{\partial t} + \nabla \bullet \boldsymbol{F}_a = Q_a, \tag{2}$$

$$\frac{\partial d_o}{\partial t} + \nabla \bullet \boldsymbol{F}_o = Q_o. \tag{3}$$

where d_α is the bulk density of component α, and $\boldsymbol{F}_\alpha$ is the net mass flux vector of component α, relative to stationary coordinates. The bulk densities are given by:

$$d_w = \phi\,(x_{ww}\rho_w S_w + x_{wo}\rho_o S_o + x_{wg}\rho_g S_g)\,, \tag{4}$$

$$d_a = \phi\,(x_{aw}\rho_w S_w + x_{ao}\rho_o S_o + x_{ag}\rho_g S_g)\,, \tag{5}$$

$$d_o = \phi\,(x_{ow}\rho_w S_w + x_{oo}\rho_o S_o + x_{og}\rho_g S_g)\,, \tag{6}$$

where $x_{\alpha\beta}$ denotes the mass fraction of component α in phase β, ρ_β are phase densities, which in general are each a mixture of the components, and S_β are the phase saturations, the fraction of the interstitial volume occupied by phase β. The pore space is assumed to be fully occupied by fluid,

$$S_w + S_o + S_g = 1\,. \tag{7}$$

The multiphase system is assumed to be in thermal equilibrium. In particular, the thermal energy state of the fluids and solid in a REV is described by a single average temperature, T. An energy balance takes the form

$$\frac{\partial e}{\partial t} + \nabla \bullet \boldsymbol{q} = Q_e \ , \tag{8}$$

where the bulk internal energy is given by

$$e = (1-\phi)\,\rho_s e_s + \phi\,(S_w \rho_w e_w + S_o \rho_o e_o + S_g \rho_g e_g)\ , \tag{9}$$

where e_β denotes the specific internal energy of phase β, and e_s is the internal energy of the solid phase. Each phase energy is, in general, dependent on pressure, temperature and composition. Also, $\boldsymbol{q}$ denotes the net heat flux vector, including diffusive and advective transport of heat, and Q_e is an extraneous heat source.

3. Constitutive and Thermodynamic Relations

In order to close the system of equations, one must now propose constitutive equations which provide relations between the kinematic variables appearing in the balance equations and the state variables.

3.1 Mass flux relations

In describing flow through porous media, one must necessarily pose average quantities (defined with respect to an REV) rather than pore-scale continuum values. For example, even though the Darcy fluxes, $\boldsymbol{v}_\beta$, have units of velocity, they represent the local volume flux per unit area of porous medium. As such, they cannot satisfy the no-slip condition on boundaries. The flux relations to follow take the place of the momentum balance in continuum equations; they are the average momentum balances under conditions of "creeping flow," i.e., inertia-free, slow viscous flow.

The advective fluxes are assumed to be adequately described by the extended Darcy law, in which relative permeabilities are introduced to account for the multiphase motion of fluids. Thus the mass flux of water, oil, and gas phases are, respectively,

$$\rho_w \boldsymbol{v}_w = \boldsymbol{f}_w = -\frac{\rho_w k k_{rw}}{\mu_w}(\nabla P_w + \rho_w g \nabla z)\ , \tag{10}$$

$$\rho_o \boldsymbol{v}_o = \boldsymbol{f}_o = -\frac{\rho_o k k_{ro}}{\mu_o}(\nabla P_o + \rho_o g \nabla z)\ , \tag{11}$$

$$\rho_g \boldsymbol{v}_g = \boldsymbol{f}_g = -\frac{\rho_g k k_{rg}}{\mu_g}(\nabla P_g + \rho_g g \nabla z)\ , \tag{12}$$

where P is pressure, g is the gravitational acceleration, and μ is dynamic viscosity. Note that we have assumed that each phase has its own phase pressure. The intrinsic permeability of the medium is k and the relative permeabilities are denoted $k_{r\beta}$. The intrinsic permeability is assumed to be a property of the material under consideration, and as such is a spatially heterogeneous quantity.

Each component net mass flux is assumed to be a superposition of component fluxes in each phase,

$$\boldsymbol{F}_{\alpha} = \boldsymbol{F}_{\alpha w} + \boldsymbol{F}_{\alpha o} + \boldsymbol{F}_{\alpha g}\ , \tag{13}$$

and each component phase-flux can be written as a sum of an advective (pressure-driven) flux and a diffusive flux,

$$\boldsymbol{F}_{\alpha\beta} = x_{\alpha\beta}\boldsymbol{f}_{\beta} + \boldsymbol{J}_{\alpha\beta}\ . \tag{14}$$

Because the gas is a mixture, each component will undergo interdiffusion whenever a gradient in concentration exists (see, for example, Bird, Stewart and Lightfoot, 1960). The diffusive fluxes in the gas are approximated by

$$\boldsymbol{J}_{\alpha g} = -\rho_{g} D_{\alpha g} \nabla x_{\alpha g}\ . \tag{15}$$

We note here that this form is only strictly valid for binary mixtures. In a multicomponent system with more than two components, the diffusion fluxes appear in the so-called Stefan-Maxwell form (see Appendix E of Williams, 1985) which is an implicit system of equations for the diffusive fluxes in terms of the gradients of mass fraction. On average, the gas mixture as a whole moves with the average mass flux given by,

$$\boldsymbol{f}_{g} = (\boldsymbol{F}_{wg} + \boldsymbol{F}_{og} + \boldsymbol{F}_{ag})\ . \tag{16}$$

In view of the expression (14), the diffusive fluxes in the gas phase must satisfy,

$$\sum_{\alpha} \boldsymbol{J}_{\alpha g} = 0\ . \tag{17}$$

In a similar manner, the diffusive fluxes of components dissolved in the liquid phases can be described in the form

$$\boldsymbol{J}_{\alpha\beta} = -D_{\alpha\beta} \nabla \rho_{\alpha\beta}, \qquad \beta \neq g, \tag{18}$$

where $\rho_{\alpha\beta}$ is the concentration of component α in phase β. Because the dissolved components in the liquid phases are presumed only slightly soluble, $D_{\alpha\beta} = 0$ when $\alpha = \beta$. That is, air or oil dissolved in the water phase can diffuse relative to the bulk motion of the water phase, but the diffusion of water in the water phase is supposed negligible.

3.2 Heat flux relations

The total heat flux vector includes conductive and convective contributions,

$$\boldsymbol{q} = -\lambda \nabla T + \sum_{\beta} \left(\sum_{\alpha} h_{\alpha\beta} \boldsymbol{F}_{\alpha\beta} \right) \tag{19}$$

where λ is an effective thermal conductivity. The second term on the right-hand-side is the convective flux, and is the sum over all components and phases of the product of the component enthalpy and net flux of component in a particular phase. The phase enthalpies (h_β) are also defined via superpositions of component enthalpies in each phase,

$$\sum_{\alpha} h_{\alpha\beta} F_{\alpha\beta} = \sum_{\alpha} h_{\alpha\beta} (x_{\alpha\beta} f_\beta + J_{\alpha\beta}) = h_\beta f_\beta + \sum_{\alpha} h_{\alpha\beta} J_{\alpha\beta} , \tag{20}$$

where $h_{\alpha\beta}$ is the enthalpy of component α as it would exist pure at the same temperature and pressure of the phase β, and the phase enthalpy is $h_\beta = \sum_{\alpha} h_{\alpha\beta} x_{\alpha\beta}$. For example, h_{og} is the enthalpy of oil vapor (TCE, say) at the prevailing temperature and gas pressure. Thus, the convective part of the heat flux vector can be written in the (familiar) form

$$q_{conv} = \sum_{\beta} \left(\rho_\beta v_\beta h_\beta + \sum_{\alpha} h_{\alpha\beta} J_{\alpha\beta} \right) . \tag{21}$$

3.3 Thermodynamics

3.3.1 Mixture rules

Ideal gas mixing rules are used to approximate the thermodynamics of the gaseous phase,

$$P_g = \sum_{\alpha} P_{\alpha g} \qquad \rho_g = \sum_{\alpha} \rho_{\alpha g} , \tag{22}$$

where $P_{\alpha g}$ and $\rho_{\alpha g}$ are the partial pressure and density of each component in the gas phase. The mass fractions in each phase must sum to unity,

$$x_{w\beta} + x_{a\beta} + x_{o\beta} = 1 \qquad \beta = w, o, g . \tag{23}$$

3.3.2 Capillary pressure

Because the transport problem under consideration involves multiple, partially miscible phases, capillary forces must be considered. The Darcy flux laws given earlier were expressed with respect to phase pressure gradients. The various phase pressures are related via the capillary pressure relations,

$$P_g - P_w = P_{c,gw} (S_w, S_g) , \tag{24}$$

$$P_o - P_w = P_{c,ow} (S_w, S_o) , \tag{25}$$

which, as indicated, are assumed to be empirically specified as functions of the phase saturations of each phase pair. We note that the capillary pressures as defined are well motivated on the microscale. Their interpretation on the macroscale is not so easily motivated, and involves postulating the existence of the relations relative to REV-averaged pressures.

However, the capillary pressure-saturation relation is commonly assumed to hold for flow in porous media. See Scheidegger (1974), Bear (1972), and Aziz & Settari (1979) for the "traditional" viewpoint on the role of capillary pressure in porous media. Some more recent discussions can be found in Hassanizadeh and Gray (1990), and references therein.

3.3.3 Equations of state

Equations of state must be specified to complete the P-V-T (pressure-volume-temperature) description of the system. For the gas phase, the equations of state take the general form,

$$\begin{aligned} \rho_{\alpha g} &= \rho_{\alpha g}(P_{\alpha g}, T) \\ h_{\alpha g} &= h_{\alpha g}(T) \end{aligned} , \tag{26}$$

for the concentration (partial density) and enthalpy of component α. Notice that the gas phase is approximated as a mixture of ideal gases and the enthalpy is independent of pressure under this approximation. The energies are found from the definition of the enthalpy, $h_{\alpha g} = e_{\alpha g} + P_{\alpha g}/\rho_{\alpha g}$. Because of the low solubility of oil in water and vice-versa, the liquid phase density and enthalpy can be computed as though they were pure phases of oil or water. This assumes that the liquid solubilities oil in water and vice versa are low enough to safely neglect their contribution to the calculation of these properties; the dissolved quantities are conserved in the balance equations for each component.

3.4 Transport parameters

3.4.1 Relative permeability functions

The three-phase relative permeabilities are specified in the form,

$$k_{r\beta} = k_{r\beta}(S_\beta) . \tag{27}$$

In view of the relation (7) among the phase saturations, the β-phase relative permeability is presumed to depend on the two independent phase saturations.

The measurement of three-phase flow relative permeabilities is a demanding task. Consequently, a variety of methods have been proposed for developing three-phase relative permeabilities from two-phase relative permeabilities, see Stone (1973), and Aziz and Settari (1979). Each of these models requires a variety of experimentally determined data, such as residual saturations. The particular model used will depend on the available data for the materials being modeled.

3.4.2 Gas diffusion

It was stated in section 3.1 that the multicomponent diffusion model, equation (15), is an approximation, even though an oft-used approximation. The reason for its appeal is that the exact model, the so-called Stefan-Maxwell equation (see Williams, 1985, Appendix

E), is complicated and time-consuming computationally. Similarly, the diffusion coefficients appropriate for the model in equation (15) are often approximated according to,

$$D^0_{\alpha g} = (1-\chi_\alpha) / \sum_{\substack{\gamma \\ \gamma \neq \alpha}} (\chi_\gamma / D_{\alpha\gamma}) \ , \tag{28}$$

where $D_{\alpha\gamma}$ are binary diffusion coefficients. Unfortunately, this approximation can only be applied to $N_{cmp} - 1$ components, where N_{cmp} is the number of components (which is 3 for the present case), because the diffusion coefficients are not independent (see p. 637 of Williams, 1985)[1]. The foregoing model applies to diffusion in free-space. To account for the fact that diffusion is taking place in a porous medium, and to account for the temperature and pressure dependence, the diffusion coefficients applied in (15) can be modeled according to,

$$D_{\alpha g} = \frac{\phi S_g}{\tau} D^0_{\alpha g} \frac{P_{ref}}{P_g} \left(\frac{T}{T_{ref}} \right)^{\upsilon} , \tag{29}$$

where τ is tortuosity and $D^0_{\alpha g}$ is the diffusivity in free space at temperature T_{ref} and pressure P_{ref}, which is given in (28). The term $\phi S_g / \tau$ modifies the expression for free diffusion to account for the porous skeleton.

3.4.3 Effective thermal conductivity

The saturation-dependent effective thermal conductivity can be specified as an *ad hoc* generalization of the two-phase conductivity defined by Somerton, *et al.*, (1974), taking the form

$$\lambda = \lambda_{dry} + S_w (\lambda_{w,wet} - \lambda_{dry}) + S_o (\lambda_{o,wet} - \lambda_{dry}) \ , \tag{30}$$

where λ_{dry} is the conductivity under all-gas conditions, $\lambda_{w,wet}$ is the conductivity under water-saturated conditions, and $\lambda_{o,wet}$ is the conductivity under oil-saturated conditions.

3.4.4 Viscosity

The gas phase viscosity can be computed as

$$\mu_g = \sum_\alpha x_{\alpha g} \mu_{\alpha g} \tag{31}$$

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[1] For the 3-component model presented here, the full Stefan-Maxwell equation could be applied without incurring an unmanageable computational expense. Bird, *et al.*, (1960), give the required diffusion coefficients in terms of binary coefficients on p. 570.

where $\mu_{\alpha g}$ is the viscosity of component α in the gas phase, generally a strong function of temperature. Because of the low mutual solubilities of water and oil, the liquid phase viscosities can be computed as though they consisted of pure water and oil.

4. Phase Equilibria

Since each component can partition into all phases, relationships for determining composition must be developed from phase equilibrium considerations. The general principal invoked is the assumption that the system is in thermochemical equilibrium at all times. In this case, equilibrium dictates that the chemical potential of each component must be the same in all the phases in which it exists (Callen, 1985). In applications, the equilibrium criteria are more conveniently restated as requiring the fugacity of each component be the same in all phases (see van Ness, 1964, for a detailed derivation). Equilibrium relationships to follow are derived in this way. The derivation is not elaborated upon here, but can be found in Adenekan *et al.* (1994), or Ho (1995).

In the current model, the three phase system includes two partially miscible liquid phases and a gas phase. The constituents making up this system include water, air, and an oil (NAPL). The air is presumed a noncondensible component under conditions relevant to the current model. The oil component is slightly miscible in the water and vice-versa. Because of the possibility of appearance and disappearance of phases, the equilibrium conditions for all the possible states must be considered. In the following, we first discuss the three two-phase states and finally the three-phase state.

4.1 Water-gas equilibrium

The following relations can be applied to compute equilibrium phase compositions when water and gas phases are present, but the oil phase does not exist. There can be oil in the system, distributed in solution between the gas and water phases, but its concentration is not sufficient to produce an oil phase. Under the assumption that vapor-liquid equilibria can be described via Henry's law (Reid, et al., 1987), the composition in the water phase can be related to the partial pressure of the component in the gas phase (Falta, *et al.*, 1990),

$$P_{\alpha g} = H_{\alpha, gw}\chi_{\alpha w}, \qquad \alpha \neq w \tag{32}$$

where $H_{\alpha, gw}$ is the temperature- and composition-dependent Henry's "constant" for the distribution of component α in the gas-water phases, and $\chi_{\alpha w}$ is the mole fraction of component α in the water phase. This equation gives the required relationship between the mole fraction of component in solution in the liquid phase and its partial pressure in the gas phase. For noncondensables, like air, the Henry's constant is described as a temperature-dependent function (or a constant). For condensable components (NAPL), the parameter $H_{\alpha, gw}$ is estimated by evaluating the formula in the limit of pure NAPL,

$$P_{vap, \alpha} = H_{\alpha, gw}\chi_{\alpha w}^{sol} \tag{33}$$

where $P_{vap,\alpha}$ is the saturated vapor pressure at the prevailing temperature, and $\chi_{\alpha w}^{sol}$ is the solubility of component α in the water phase, expressed as a mole fraction. Implicit in this approximation is that the Henry's constant is assumed independent of composition. Thus, the compositions of air and oil in the water phase are given by

$$P_{ag} = H_{a,gw}\chi_{aw} \tag{34}$$

$$P_{og} = P_{vap,o}\frac{\chi_{ow}}{\chi_{ow}^{sol}}. \tag{35}$$

Raoult's law (van Ness, 1964) can be applied to determine the water vapor pressure in the gas phase,

$$P_{wg} = (1-\chi_{aw}-\chi_{ow})P_{vap,w}. \tag{36}$$

Equations of state for the components in the gas phase can be used to compute the partial densities and then the mass fractions in the gas phase, completing the calculation of equilibrium compositions in the two phase system.

4.2 Oil-gas equilibrium

In situations where the oil and gas phases are in equilibrium, the use of Henry's laws for the air and water compositions dissolved in the oil phase result in,

$$P_{ag} = H_{a,go}\chi_{ao} \tag{37}$$

$$P_{wg} = P_{vap,w}\frac{\chi_{wo}}{\chi_{wo}^{sol}}. \tag{38}$$

These relations would be used when only the oil and gas phases exist, but there is water and air dissolved in each, although at concentrations less than the solubility of water in the oil phase. If the concentration of water in the oil rises to or above its solubility, a (liquid) water phase would form. The mole fraction of oil in the oil phase is given by the fact that the mole fractions must sum to unity. Application of Raoult's law, gives the partial pressure of oil vapor,

$$P_{og} = (1-\chi_{ao}-\chi_{wo})P_{vap,o}, \tag{39}$$

which through the use of (22) completes the calculation of gas pressure. Equations of state for the vapors results in completion of the calculation of gas composition in terms of mole fractions. Mass fractions can be determined from the mole fractions of a particular phase via

$$x_{\alpha\beta} = \chi_{\alpha\beta}w_{\alpha}/\Sigma_{\gamma}\chi_{\gamma\beta}w_{\gamma} \tag{40}$$

where w_α is the molecular weight of component α. Finally, capillary pressure functions for oil and gas can be used to find the oil pressure, completing the calculations of the secondary thermodynamic variables.

4.3 Water-oil equilibrium

For the calculation of water-oil equilibrium, the primary variables will include the mole fraction of air in the water phase, χ_{aw}. Henry's law gives the composition of air in the oil phase,

$$\chi_{ao} = \frac{H_{a,gw}}{H_{a,go}} \chi_{aw}. \tag{41}$$

Expressions relating the equilibrium mole fraction of oil in solution in the water phase and the mole fraction of oil in the oil phase can be derived by combining (35) and (39). A similar relation for water in solution in the oil phase is found by combining (36) and (38), which together result in the equations,

$$\chi_{oo} = \frac{\chi_{ow}}{\chi_{ow}^{sol}}, \qquad \chi_{ww} = \frac{\chi_{wo}}{\chi_{wo}^{sol}}. \tag{42}$$

Using relation (23) and the foregoing equations, results in the 2x2 system,

$$\begin{bmatrix} 1 & \chi_{ow}^{sol} \\ \chi_{wo}^{sol} & 1 \end{bmatrix} \begin{bmatrix} \chi_{ww} \\ \chi_{oo} \end{bmatrix} = \begin{bmatrix} 1 - \chi_{aw} \\ 1 - \chi_{ao} \end{bmatrix}. \tag{43}$$

Solving for χ_{ww} and χ_{oo}, the relations (42) can then be used to complete the composition of the water and oil phases. If the primary variables include the oil pressure and water saturation, the oil-water capillary pressure relations can be used to compute the water pressure.

4.4 Three-phase equilibrium

In this case, all three phases are present, two are partially miscible liquid phases and a gas phase. The Henry's laws in equations (34) and (37) specify the molar concentration of air in solution in the two liquid phases. The water and oil composition in the liquid phases can be determined in the same way as discussed in the previous subsection, once again leading to the system (43). The partial pressures of water and oil in the gas phase are also computed from Raoult's law, using equations (36) and (39). The only additional calculation is to determine the liquid phase pressures. The capillary equations (24) and (25) can be used, if the primary variables include two of the phase saturations.

4.5 Equilibrium coefficients

The foregoing relationships can be summarized by defining the so-called K-factors, or distribution ratios (Peaceman, 1977),

$$K_{\alpha\beta\gamma} = \frac{\chi_{\alpha\beta}}{\chi_{\alpha\gamma}}, \tag{44}$$

which relates the equilibrium composition of component α between phases β and γ. The K-factors are recorded here for reference and can be summarized as follows:

Water-gas:

$$K_{agw} = \frac{H_{a,gw}}{P_g} \qquad K_{ogw} = \frac{P_{vap,o}}{P_g}\frac{1}{\chi_{ow}^{sol}} \qquad K_{wgw} = \frac{P_{vap,w}}{P_g} \tag{45}$$

Oil-gas:

$$K_{ago} = \frac{H_{a,go}}{P_g} \qquad K_{ogo} = \frac{P_{vap,o}}{P_g} \qquad K_{wgo} = \frac{P_{vap,w}}{P_g}\frac{1}{\chi_{wo}^{sol}} \tag{46}$$

Water-oil:

$$K_{\alpha wo} = \frac{K_{\alpha go}}{K_{\alpha gw}}, \qquad \alpha = a, o, w. \tag{47}$$

5. Numerical Treatment

In this section we discuss a numerical method, based on finite difference techniques, for obtaining approximate solutions to the mathematical model. The flow equations describing the transport of water, air oil, and energy are comprised of the component and energy balances given in the foregoing, which together with equations of constitution and transport parameters, form a closed system of equations. These governing equations constitute a coupled set of highly nonlinear partial differential equations (PDEs). Numerical techniques must be employed in order to obtain approximate solutions to this system of initial-boundary value problems. This state of affairs motivates the present discussion, which is not meant as a definitive exposition on the numerical solution of the system. However, it seems appropriate to at least discuss how the system may be solved numerically.

The numerical method presented for solving the initial-boundary value problem formed by the coupled system of PDEs is a finite difference technique. The effective treatment of the highly nonlinear system considered here is made possible by the use of Newton iteration. In the present work, the spatial derivatives are approximated by a centered difference approximation. The resulting system of ODEs can be integrated forward in time by a variable-step backward-difference predictor-corrector scheme. The backward-difference formulae result in systems of nonlinear algebraic equations to be solved for nodal quantities. These equations are solved via an inexact Newton algorithm, which is especially effective for the structured grid scheme discussed here.

5.1 Numerical discretization

Approximating the spatial divergences by centered differences, the system of discrete ODEs describing the temporal variation of primary variables at node points takes the form

$$\begin{bmatrix} \dot{d}_w \\ \dot{d}_a \\ \dot{d}_o \\ \dot{u} \end{bmatrix}_{ijk} = -\frac{\delta_x}{\delta x_i}\begin{bmatrix} F_{wx,\,ijk} \\ F_{ax,\,ijk} \\ F_{ox,\,ijk} \\ q_{x,\,ijk} \end{bmatrix} - \frac{\delta_y}{\delta y_j}\begin{bmatrix} F_{wy,\,ijk} \\ F_{ay,\,ijk} \\ F_{oy,\,ijk} \\ q_{y,\,ijk} \end{bmatrix} - \frac{\delta_z}{\delta z_k}\begin{bmatrix} F_{wz,\,ijk} \\ F_{az,\,ijk} \\ F_{oz,\,ijk} \\ q_{z,\,ijk} \end{bmatrix} + \begin{bmatrix} Q_w \\ Q_a \\ Q_o \\ Q_e \end{bmatrix}_{ijk} \tag{48}$$

on a structured grid of mesh points with coordinates (x_i, y_j, z_k), on which a grid function is denoted $f_{ijk} = f(x_i, y_j, z_k, t)$. Vector components in the three coordinate directions are denoted by the x, y, and z subscripts; for example $\boldsymbol{F}_w(\boldsymbol{x}) = (F_{wx}, F_{wy}, F_{wz})^T$. The central difference operator notation is defined such that $\delta_x f_{ijk} = f_{i+1/2,j,k} - f_{i-1/2,j,k}$, etc., and $\delta x_i = x_{i+1/2} - x_{i-1/2}$. For example,

$$\frac{\delta_y F_{wy,\,ijk}}{\delta y_j} = \frac{F_{wy,\,i,j+1/2,k} - F_{wy,\,i,j-1/2,k}}{y_{j+1/2} - y_{j-1/2}}. \tag{49}$$

The net fluxes of a component appearing in Eqn. (48) are defined by Eqn. (13). Because of the relation given in Eqn. (14), each component flux will be expressed in terms of the phase fluxes defined in Eqns. (10)-(12). For the numerical approximation, each phase flux is also expressed as a centered difference (on a staggered mesh), for example the water phase mass flux is approximated by

$$f_{wx,\,i+1/2,j,k} = -\left(\frac{\rho_w k k_{rw}}{\mu_w}\right)_{i+1/2,j,k}\left(\frac{\Delta_x P_{wx,\,ijk}}{\Delta x_i} + \rho_{w,\,i+1/2,j,k}\, g\frac{dh}{dx}\right), \tag{50}$$

where Δ denotes the forward difference operator, defined similarly to the central difference operator used above ($\Delta_x P_{wx,\,ijk} = P_{wx,\,i+1,j,k} - P_{wx,\,i,j,k}$), and dh/dx is the direction cosine for the gravitational component acting along the x-coordinate direction. The diffusive and conductive fluxes can be approximated by centered differences in a similar fashion.

Time integration can be performed with a backward difference formula. Denoting the forgoing system in vector notation, the time-discretized equations are given by

$$D_l^{n+1} = D_l^n + \Delta t_n F_l\left(D^{n+1}\right), \tag{51}$$

where $D_l = (d_w, d_a, d_o, u)_l^T$ is the mass and energy density vector at grid point l, the n subscript or superscript denotes the time level, and F_l denotes the right-hand-side of (48) for grid point l. For a structured grid, the l-th grid point can be related to the ijk notation as $l = i + (j-1)N_x + (k-1)N_xN_y$, where N_x and N_y are the number of grid points in the x and y directions, respectively. This time discretization results in a nonlinear system of equations, which can be solved by Newton iteration. The objective is to find the solution vector that satisfies,

$$\|R(D)\| \le \tau_R, \qquad \text{where} \qquad R_l(D) = D_l - D_l^n - \Delta t_n F_l(D), \tag{52}$$

$\| \ \|$ denotes a vector norm, and τ_R is the numerical tolerance to which the system is computed.

5.2 Primary variables and Newton iteration

The system of nonlinear equations is to be solved for a set of primary variables, which by definition are a set of variables which allow the remaining secondary variables to be calculated. The three-component system under consideration may exist in seven possible configurations or states. Table 1 shows the seven configurations and a set of primary variables for each state consistent with the equilibrium relations given in the previous section. These sets of primary variables are not unique; other variables could also be used. These sets were chosen for convenience in the numerical calculation of secondary variables from these primary variables. These primary variable sets form the solution vector for each state. For example, in the case of three-phase flow the solution vector is

Table 1: Primary Variables

Existing Phases	Solution Vector
water	$(P_w, T, \chi_{ow}, \chi_{aw})$
oil	$(P_o, T, \chi_{wo}, \chi_{ao})$
gas	$(P_g, T, \chi_{wg}, \chi_{ag})$
water-gas	$(P_{ag}, T, S_w, \chi_{ow})$
oil-gas	$(P_{ag}, T, S_o, \chi_{wo})$
water-oil	(P_o, T, S_w, χ_{aw})
water-oil-gas	(P_{ag}, T, S_o, S_w)

$U = (S_w, P_{ag}, S_o, T)^T$. The discretized system of nonlinear equations can be solved for these variables by Newton's method. By Taylor series expansion of the system of nonlinear equations about the desired solution (i.e. the value of U that minimizes the vector of residual equations), the system to be solved is found to be

$$J\left(U^q\right)\delta U^{q+1} = -R\left(U^q\right), \tag{53}$$

where J is the Jacobian matrix,

$$J_{ij} = \frac{\partial R_i}{\partial U_j}, \tag{54}$$

and R is the residual vector defined in (52), except here we acknowledge that the residual equations depend on the solution vector U, since $D=D(U)$. The solution vector is updated at each iteration according to

$$U^{q+1} = U^q + \delta U^{q+1}. \tag{55}$$

In the finite-difference form used for approximation of spatial and temporal derivatives, the Jacobian can be computed efficiently via forward difference approximations. (This is particularly efficient for the block-tridiagonal systems generated for a one-dimensional system of equations. In this case, the Jacobian can be computed in *IBAND* evaluations of the residual, and $IBAND = 3*NPDE$, where $NPDE$ is the number of degrees of freedom per node.) This inexact Newton scheme is a convenient method of determining the Jacobian because any new transport parameter function or equation of state can be implemented without the need for the user to also program the gradient of the functions with respect to the solution vector variables. This is particularly helpful in this problem where the primary variables, and hence the solution vector variables, change depending on the phases present at a particular node point. However, special care must be taken in computing the forward differences to minimize finite-precision errors (see for example, Gill et al. 1981, or Press et al., 1992).

For the structured grid system, the Jacobian matrix will be block septa-diagonal. Furthermore, the bandwidth is $N_x x N_y$ (in practice the numbering of nodes would be chosen to minimize the bandwidth), making direct solution methods for the linear systems impractical for general use in three dimensions. Two methods can be employed to overcome this problem; use of splitting methods or use of iterative solution methods coupled with sparse matrix storage. By splitting methods we refer to ADI-like methods (Aziz and Settari, 1979) which result in block tri-diagonal linear equations, but require treating each of the coordinate directions implicitly in succession. The use of iterative methods requires schemes applicable to unsymmetric systems. The success of iterative methods often depends heavily on an appropriate preconditioner, and remains a topic of current research. However, success with these schemes is being reported (van der Vorst, 1990) and it appears to be an effective approach.

The switching of variables must be considered during the Newton iteration. If the update in Eqn. (55) indicates a phase appearance or disappearance, the definition of the solution vector is changed according to Table 1. This necessitates re-initializing the solution vector at the affected grid point (or points). Depending on which phase appears or disappears, the initialization may require a so-called flash calculation (Walas, 1985) in order to find accurate values for the new solution vector at the considered node point. More accurate values will reduce the number of Newton iterations required at a time step in which variable switching is indicated. Changing the solution vector definition at a grid point also means the corresponding block column of the Jacobian is the gradient of all the residual equations with respect to the new grid point solution vector.

5.3 Boundary conditions

Both Dirichlet and specified flux boundary conditions can be imposed on the discrete equations. Several combinations of Dirichlet and flux conditions are also allowable. The several types are discussed in the following.

5.3.1 Dirichlet conditions

Fixed values for all degrees-of-freedom at a particular boundary node (cell) can be specified directly into the residual equation for that cell. For the Newton iteration, the block diagonal entry in the Jacobian matrix corresponding to the boundary node is replaced by the identity matrix. This procedure sets the correct Dirichlet values and forces the updates to zero for the matrix solution. This technique can obviously be applied to the discretized system for both constant and time-varying Dirichlet values. Several techniques can be employed in several variants of the implementation of this technique. A general implementation method is to simply specify the residual equation for the boundary node as $R_l = u_l - g(t)$, where u_l is the current value of the unknown, which for the first iteration in a time step may be the value from the previous time step, and $g(t)$ is the Dirichlet value to be set. Clearly, the corresponding Jacobian entry is unity on the diagonal and zero elsewhere. Each matrix solution and update will force the desired Dirichlet value.

5.3.2 Flux conditions

Specified values of flux, normal to the computational boundary, for all degrees-of-freedom at a particular boundary node can also be imposed. In general the fluxes are time dependent, and can depend on the solution vector at the considered node. For example, wells are often approximated by setting fluxes which are proportional to the difference between the boundary pressure in the computation and a wellbore pressure. The coefficient for the flux may also depend on the boundary pressures, temperature, and fluid saturations, see Aziz and Settari (1979). By setting the coefficient to a sufficiently large value, the flux condition essentially becomes a Dirichlet condition for the wellbore pressure.

By performing a material or energy balance on the half-cell adjacent to the boundary on the plane at $x = 0$, fluxes of the conserved quantities can be imposed,

$$\begin{bmatrix}\dot{d}_w\\ \dot{d}_a\\ \dot{d}_o\\ \dot{u}\end{bmatrix}_{1jk} = \frac{2}{x_2-x_1}\begin{bmatrix}F_{wx,1,j,k}-F_{wx,3/2,j,k}\\ F_{ax,1,j,k}-F_{ax,3/2,j,k}\\ F_{ox,1,j,k}-F_{ox,3/2,j,k}\\ q_{x,1,j,k}-q_{x,3/2,j,k}\end{bmatrix} - 2\frac{\delta_y}{\delta y_j}\begin{bmatrix}F_{wy,ijk}\\ F_{ay,ijk}\\ F_{oy,ijk}\\ q_{y,ijk}\end{bmatrix} - 2\frac{\delta_z}{\delta z_k}\begin{bmatrix}F_{wz,ijk}\\ F_{az,ijk}\\ F_{oz,ijk}\\ q_{z,ijk}\end{bmatrix} + 2\begin{bmatrix}Q_w\\ Q_a\\ Q_o\\ Q_e\end{bmatrix}_{1jk} \tag{56}$$

where the 1-subscripted fluxes are specified (or set to zero for no-flux conditions). Note that these fluxes can be general functions of time. Similar equations apply at other boundaries on which fluxes are specified.

Note that in specifying any of these fluxes, there are several physical fluxes which are superposed in these definitions. For example, one may want to specify the injection of cold water at a mass flux rate F_{in}, at temperature T_{cold} together with an additional heat flux imposed at the same boundary. The mass flow rate of water is specified as $F_{wx,1,j,k} = F_{in}$. The net heat flux is specified by superposing the convected enthalpy of the injected fluid with the conducted heat flux, q_{cond}, by specifying $q_{x,1,j,k} = q_{cond} + C_{pl}(T_{cold} - T_0)F_{in}$.

5.3.3 Mixed conditions

In many applications one may want to specify mixed boundary conditions, i.e., certain combinations of fluxes and primary variables. This can be accomplished by a combination of the procedures discussed in the preceding subsections on Dirichlet and flux boundaries.

As a particular example, one may want to specify a temperature and impervious flow conditions on the fluids. Assuming the conditions are specified at x=0, the specified time-varying temperature is imposed directly in the matrix as discussed in the section on Dirichlet conditions. This condition is imposed on the heat equation, i.e., the balance equation which is associated with the temperature variable. This identity replaces the last equation in the block matrix for that degree of freedom, for example the last equation in the matrix shown in Eqn. (56). Setting values of $F_{wx,1,j,k}$, $F_{ax,1,j,k}$, and $F_{ox,1,j,k}$ (equal zero for impervious conditions) in the remaining equations for that block completes the specification of boundary conditions. This procedure generalizes for any combination of flux and Dirichlet DOFs to be applied.

6. Concluding Remarks

We have presented a formulation describing nonisothermal three-phase transport of air, water, oil, and energy through porous media. The formulation employs component mass balances, and a heat balance encompassing all phases, assuming thermal equilibrium. This formulation conveniently includes phase transitions, as well as phase appearances and disappearances without the need to explicitly define mass transfer sources between phases. The three components are allowed to partition into all three phases, and the discussion includes the required phase equilibrium relations necessary to determine composition for each of seven possible phase configurations. The calculation of the required transport properties is also discussed.

A numerical method is required for solving the resulting system of highly nonlinear equations. For completeness such a numerical procedure is presented, including the treatment of boundary conditions. The numerical procedure ultimately relies on Newton iteration for solving the set of discretized nonlinear system of equations. Even though the numerical method presented involved the use of finite differences for approximating spatial gradients, the general algorithmic approach can be applied to control volume or finite element methods.

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