

A Generalized Numerical Approach for Modeling Multiphase Flow and Transport in Fractured Porous Media

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Abstract. A physically based numerical approach is presented for modeling multiphase flow and transport processes in fractured rock. In particular, a general framework model is discussed for dealing with fracture-matrix interactions, which is applicable to both continuum and discrete fracture conceptualization. The numerical modeling approach is based on a general multiple-continuum concept, suitable for modeling any types of fractured reservoirs, including double-, triple-, and other multiple-continuum conceptual models. In addition, a new, physically correct numerical scheme is discussed to calculate multiphase flow between fractures and the matrix, using continuity of capillary pressure at the fracture-matrix interface. The proposed general modeling methodology is verified in special cases using analytical solutions and laboratory experimental data, and demonstrated for its application in modeling flow through fractured vuggy reservoirs.

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1 Introduction

Since the 1960s, significant progress has been made in mathematical modeling of flow and transport processes in fractured rock. Research efforts, driven by the increasing need to develop petroleum and geothermal energy in reservoirs, other natural underground resources, and to resolve concerns of subsurface contamination, have developed many numerical modeling approaches and techniques (Barenblatt et al., 1960; Warren

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and Root, 1963; Kazemi, 1969; Pruess and Narasimhan, 1985). Mathematical modeling approaches developed in the past few decades in general rely on continuum approaches and involve developing conceptual models, incorporating the geometrical information of a given fracture-matrix system, setting up mass and energy conservation equations for fracture-matrix domains, and then solving discrete nonlinear algebraic equations. Most computational effort is consumed in solving the governing equations that couple multiphase fluid flow with other physical processes either analytically or numerically. The key issue for simulating flow in fractured rock, however, is how to handle fracture-matrix interaction under different conditions (involving multiple phase flow). This is because the fracture-matrix interaction distinguishes the flow through fractured porous media from the flow through homogeneous or heterogeneous single-porosity porous media.

To model fracture-matrix interaction during flow in fractured porous media, investigators have developed and applied many different conceptual models and modeling approaches (e.g., Berkowitz, 2002; Neuman; 2005). In modeling multiphase flow and transport, and heat transfer in fractured porous media, the most critical issue is how to handle inter-“flow” or interaction of mass and thermal energy at fracture-matrix interfaces under multiphase and non-isothermal condition. Commonly used mathematical methods for dealing with fracture-matrix interaction include:

- an explicit discrete-fracture and matrix model (e.g., Snow, 1969; Stothoff, 2000),
- the dual-continuum method, including double- and multi-porosity, dual-permeability, or the more general “multiple interacting continua” (MINC) method (e.g., Barenblatt et al., 1960; Warren and Root, 1963; Kazemi, 1969; Pruess and Narasimhan, 1985; Wu and Pruess, 1988),
- the effective-continuum method (ECM) (e.g., Wu, 2000a).

The explicit discrete-fracture approach is, in principle, a more rigorous model. However, the application of this method to field studies is currently limited because of the computational intensity involved as well as the lack of detailed knowledge of fracture and matrix geometric properties and their spatial distributions at a given subsurface site. On the other hand, the dual-continuum method is conceptually simpler and computationally much less demanding than the discrete-fracture approach, and is able to handle fracture-matrix interaction more easily than the discrete-fracture model. For these reasons, the dual-continuum approach has been used as the main approach for modeling fluid flow, heat transfer, and chemical transport through fractured reservoirs (e.g., Wu et al., 1999 and 2007).

Dual-continuum approaches, as discussed in this paper, include the classical double-porosity model (Barenblatt et al., 1960; Warren and Root, 1963), the dual-permeability concept, and the more rigorous dual-continuum generalization of the MINC (Pruess and Narasimhan, 1985) for modeling flow in fractured porous media. In the double-porosity model, a flow domain is composed of matrix blocks with low permeability, embedded in a network of interconnected fractures. Global flow and transport in the formation occur only through the fracture system, conceptualized as an effective continuum. This

model treats matrix blocks as spatially distributed sinks or sources to the fracture system without accounting for global matrix-matrix flow. In comparison, the MINC concept (Pruess and Narasimhan, 1985) is able to describe gradients of pressures, temperatures, or concentrations near matrix surface and inside the matrix-by further subdividing individual matrix blocks with one- or multidimensional strings of nested meshes. Therefore, the MINC model in general provides a better numerical approximation for transient fracture-matrix interactions than the double-porosity model.

Because of its computational efficiency and its ability to match many types of laboratory- or field-observed data simultaneously (e.g., Kazemi, 1979; Wu et al., 1999; 2007), the dual-continuum model, such as double-porosity and dual-permeability concept, has perhaps been the most widely used method in petroleum and geothermal engineering, and groundwater hydrogeology. For example, it has also been implemented in many commercially available reservoir simulators. In comparison, the effective continuum approach, as a simplified method, the ECM represents fractures and rock matrix by a single effective continuum. The ECM has long been used for modeling fracture-matrix flow because of its simple data requirements and computational efficiency. This approach may be applicable to modeling multiphase, nonisothermal flow and solute transport in fractured porous media under near-thermodynamic-equilibrium conditions (Wu et al., 1999). When rapid flow and transport processes occur in subsurface fractured reservoirs, however, thermodynamic equilibrium conditions cannot in general hold. Therefore, the instantaneous equilibrium assumption for fracture-matrix systems limits the application of the ECM approach for modeling general multiphase flow, transport, and heat transfer processes.

In this paper, a physically based, unified numerical approach is presented for modeling multiphase flow and transport processes in fractured rock. In particular, we discuss a general mathematical framework model for dealing with fracture-matrix interactions, which is applicable to both continuum and discrete fracture conceptualization. In this approach, a subsurface domain is discretized using an unstructured grid with regular or irregular meshes, followed by time discretization carried out using a backward, first-order, finite-difference method. The final discrete linear or nonlinear equations are handled fully implicitly using Newton iteration. In addition, the fracture medium is handled using a general dual-continuum concept with continuum or discrete modeling approaches.

The main contribution of this work is to show that it is possible to formulate a uniform, generalized mathematical model as well as numerical scheme that can be used to simulate any types of flow and transport in fractured reservoirs, using different fracture-matrix conceptual model. We demonstrate that with this unified approach, modeling a particular process of porous-medium or fractured-media flow and transport becomes simply a matter of defining a set of state variables, along with their interrelations or mutual effects, once a fractured-medium system is discretized using the multi-continuum approach.

2 Generalized governing equations

The physical processes associated with flow and transport in fractured porous media are governed by the same fundamental conservation laws as those used in other branches of the sciences and engineering: conservation of mass, momentum, and energy governs the behavior of fluid flow, chemical transport, and heat transfer in rock. These physical laws are often represented mathematically on the macroscopic level by a set of partial differential or integral equations, called governing equations. These governing equations are generally nonlinear as long as compressible or multiphase fluids or heat transfer is involved and needed to quantitatively model the flow and transport processes occurring in porous or fractured media. Based on the general conservation laws, we present a set of generalized governing equations for multiphase fluid flow, multicomponent transport, and heat transfer in porous and fractured media, providing a framework for numerical formulations to cover all possible scenarios for flow and transport in porous media.

Let us consider a multiphase, nonisothermal system consisting of several fluid phases, such as gas, water, and oil (NAPL), with each fluid phase in turn consisting of a number of mass components. To derive a set of generalized governing equations for multiphase fluid flow, multicomponent transport, and heat transfer, we assume that these processes can be described using a continuum approach within a representative elementary volume (REV) in a porous or fractured medium (Bear, 1972). In addition, a condition of local thermodynamic equilibrium is assumed so that at any time temperatures, phase pressures, densities, viscosities, enthalpies, internal energies, and component concentrations (or mass fractions) are the same locally at each REV of the porous medium.

According to mass and energy conservation principles, a generalized conservation equation of mass components and energy in the porous continuum can be written as follows:

$$\frac{\partial M^k}{\partial t} = G^k + q^k + F^k, \quad (2.1)$$

where superscript k is the index for the components, $k = 1, \dots, N_c$, with N_c being the total number of mass components and with $k = N_c + 1$ for energy "component" (note that heat energy is here regarded as a component for convenience); M is the accumulation term of component k ; G^k is the decay or internal generation (reaction) term of mass or energy components; q^k is an external source/sink term or fracture-matrix exchange term for mass or energy component k and energy; and F^k is the "flow" term of mass or energy movement or net exchange from single-phase and multiphase flow, or diffusive and dispersive mass transport, or heat transfer, as discussed below.

In addition to the conservation or continuity equations of mass and thermal energy, shown in Eq. (2.1), we also need specific relationships or mechanisms that describe why and how fluid flow, solute transport, and heat transfer occur in porous and fractured media. This is to define the "flow" term in Eq. (2.1), and the following specific laws act as such mechanisms by governing local fluid flow, component transport, and heat transfer processes in porous media.

2.1 Single-phase and multiphase flow

For single-phase liquid or gas flow, Richards' equation, two active or three phase flow, if these fluids are treated as immiscible or mass exchange between phases can be ignored, the accumulation terms in Eq. (2.1) for gas (air), water and/or oil (NAPL) components in are evaluated as

$$M^\beta = \sum_{\beta} (\phi \rho_{\beta} S_{\beta}), \quad (2.2)$$

where superscript and subscript β is an index for fluid phase ($\beta = g$ for gas, $= w$ for aqueous phase, $= o$ for oil); ϕ is the porosity of porous media; ρ_{β} is the density of phase β ; and S_{β} is the saturation of phase β . Note that in this special case, component k (by superscript) and phase (by subscript) are interchangeable.

In this case, the decay or generation term is negligible with

$$G^\beta = 0. \quad (2.3)$$

The mass flow term is determined by

$$F^\beta = \nabla \bullet (\rho_{\beta} \mathbf{v}_{\beta}), \quad (2.4)$$

where \mathbf{v}_{β} is a vector of the Darcy's velocity or volumetric flow, defined by Darcy's law to describe the flow of single or multiple immiscible fluids as

$$\mathbf{v}_{\beta} = -\frac{k k_{r\beta}}{\mu_{\beta}} (\nabla P_{\beta} - \rho_{\beta} g \nabla z), \quad (2.5)$$

where P_{β} , μ_{β} , and g are pressure, viscosity of fluid phase β , and gravitational constant, respectively; z is the vertical coordinate; k is absolute or intrinsic permeability (a tensor in general); and $k_{r\beta}$ is the relative permeability to phase β (equal to one for single-phase flow, i.e., single-phase is considered as a special case of multiphase flow in this paper).

2.2 Mass or chemical transport

The movement of dissolved mass components or chemical species in a multiphase porous medium system can also be handled as a special case of Eq. (2.1). The accumulation terms for component k is

$$M^k = \phi \sum_{\beta} (\rho_{\beta} S_{\beta} X_{\beta}^k) + (1 - \phi) \rho_s \rho_w X_w^k K_d^k \quad (k = 1, \dots, N_c), \quad (2.6)$$

where X_{β}^k is the mass fraction of component k in fluid β ; ρ_s is the density of rock solids; and K_d^k is the distribution coefficient of component k between the aqueous phase and rock solids to account for adsorption effects.

In the case in which components are subject to a first-order radioactive decay, the decay/generation term is

$$G^k = \phi \lambda_k \left(\sum_{\beta} (\rho_{\beta} S_{\beta} X_{\beta}^k) + (1 - \phi) \rho_s \rho_w X_w^k K_d^k \right) \quad (k=1, \dots, N_c), \quad (2.7)$$

where λ_k is the radioactive decay constant of component k .

The mass component transport is governed in general by processes of advection, diffusion, and dispersion, and is also subject to other processes such as radioactive decay, adsorption, dissolution and precipitation, mass exchange and partition between phases, or chemical reactions. Advective transport of a component or solute is carried by flow of a fluid, and diffusive and dispersive flux is contributed by molecular diffusion and mechanical dispersion, or hydrodynamic dispersion. These processes are described using a modified Fick's law for transport through a single-phase porous medium (Scheidegger, 1961). Then, the total mass flow term for a component k , by advection and dispersion, is written as

$$F^k = - \sum_{\beta} \nabla \cdot (\rho_{\beta} X_{\beta}^k \mathbf{v}_{\beta}) + \sum_{\beta} \nabla \cdot (\underline{D}_{\beta}^k \cdot \nabla (\rho_{\beta} X_{\beta}^k)) \quad (k=1, \dots, N_c). \quad (2.8)$$

Eq. (2.8) indicates that the mass flow consists of two parts, the first part, i.e., the first term on the left-hand side of (2.8), is contributed by advection in all phases and the second part (the second term on the left-hand side of (2.8)) is diffusive flux by hydrodynamic dispersion. In Eq. (2.8), \underline{D}_{β}^k is the hydrodynamic dispersion tensor accounting for both molecular diffusion and mechanical dispersion for component k in phase β , defined by an extended dispersion model (Scheidegger, 1961) to include multiphase effects (Wu and Pruess, 2000b) as

$$\underline{D}_{\beta}^k = \alpha_T^{\beta} |\mathbf{v}_{\beta}| \delta_{ij} + (\alpha_L^{\beta} - \alpha_T^{\beta}) \frac{\mathbf{v}_{\beta} \mathbf{v}_{\beta}}{|\mathbf{v}_{\beta}|} + \phi S_{\beta} \tau d_{\beta}^k \delta_{ij} \quad (k=1, \dots, N_c), \quad (2.9)$$

where α_T^{β} and α_L^{β} are transverse and longitudinal dispersivities, respectively, in fluid β of porous media; τ is tortuosity of the porous medium; d_{β}^k is the molecular diffusion coefficient of component k within fluid β ; and δ_{ij} is the Kronecker delta function ($\delta_{ij} = 1$ for $i = j$, and $\delta_{ij} = 0$ for $i \neq j$), with i and j being coordinate indices.

2.3 Heat transfer

The accumulation term for the heat equation is usually is defined as

$$M^{N_c+1} = \sum_{\beta} (\phi \rho_{\beta} S_{\beta} U_{\beta}) + (1 - \phi) \rho_s U_s, \quad (2.10)$$

where ρ_s is the density of rock solids; and U_{β} and U_s are the internal energies of fluid β and rock solids, respectively.

Heat transfer in porous media is in general a result of both convective and conductive processes, although in certain cases, radiation may also be involved. These heat-transfer processes are complicated by interactions between multiphase fluids, multicomponents, and associated changes in phases, internal energy, and enthalpy. Heat convection is contributed by thermal energy carried mainly by bulk flow of all fluids as well as by dispersive mass fluxes. On the other hand, heat conduction or radiation is driven by temperature gradients and may follow Fourier's law or Stefan-Boltzmann's law, respectively. Then the combined, overall heat flux term, owe to convection, conduction and radiation in a multiphase, multicomponent, porous medium system, may be described as

$$F^{N_c+1} = - \sum_{\beta} \nabla \bullet (h_{\beta} \rho_{\beta} \mathbf{v}_{\beta}) + \sum_{\beta} \sum_k \nabla \bullet (h_{\beta}^k D_{\beta}^k \bullet \nabla (\rho_{\beta} X_{\beta}^k)) + \nabla \bullet (K_T \nabla T) - \varepsilon \sigma_0 T^4, \quad (2.11)$$

where h_{β} and h_{β}^k are specific enthalpies of fluid phase β and of component k in fluid β , respectively; K_T is the overall thermal conductivity; T is temperature; ε is a radiation emissivity factor, and σ_0 ($= 5.6687 \times 10^{-8} \text{ J/m}^2 \text{ K}^4$) is the Stefan-Boltzmann constant.

As shown in Eq. (2.11), the total heat flow in a multiphase, multicomponent system is determined by heat convection of flow and mass dispersion (the first two terms on the right-hand side of (2.11)), heat conduction (the third term on the right-hand side), and thermal radiation when occurring (the last term on the right-hand side).

2.4 Constitutive relationships

To complete the mathematical description of multiphase flow, multicomponent transport, and heat transfer in porous media, Eq. (2.1), a generalized mass- and energy-balance equation, needs to be supplemented with a number of constitutive equations. These constitutive correlations express interrelationships and constraints of physical processes, variables, and parameters, and allow the evaluation of secondary variables and parameters as functions of a set of primary unknowns or variables selected to make the governing equations solvable. Table 1 lists a commonly used set of constitutive relationships for describing multiphase flow, multicomponent mass transport, and heat transfer through porous media. Many of these correlations for estimating properties and interrelationships are determined by experimental studies.

3 Numerical formulation

The methodology for using numerical approaches to simulate multiphase subsurface flow and transport, and heat transfer consists in general of the following three steps: (1) spatial discretization of mass and energy conservation equations, (2) time discretization; and (3) iterative approaches to solve the resulting nonlinear, discrete algebraic equations. Among various numerical techniques for simulation studies, a mass- and energy-

Table 1: Constitutive relationships and functional dependence.

Definition	Function	Description
Fluid saturation	$\sum_{\beta} S_{\beta} = 1$	Constraint on summation of total fluid saturation.
Mass fraction	$\sum_k X_{\beta}^k = 1$	Constraint on mass fractions within phase β .
Capillary pressure	$P_{C\beta} = P_{C\beta}(S_{\beta})$	In a multiphase system, the capillary pressure relates pressures between the phases and is defined as functions of fluid saturation.
Relative permeability	$k_{r\beta} = k_{r\beta}(S_{\beta})$	The relative permeability of a fluid phase in a multiphase system are normally assumed to be functions of fluid saturation.
Fluid density	$\rho_{\beta} = \rho_{\beta}(P, T, X_{\beta}^k)$	Density of a fluid phase is treated as a function of pressure and temperature, as well as mass compositions ($k = 1, 2, 3, \dots, N_c$).
Fluid viscosity	$\mu_{\beta} = \mu_{\beta}(P, T, X_{\beta}^k)$	The functional dependence or empirical expressions of viscosity of a fluid is treated as a function of pressure, temperature, and composition.
Henry's law	$P_g^k = K_H^k \omega_w^k$	P_g^k is partial pressure of component k in gas phase; K_H^k is Henry's constant for component k ; and ω_w^k is the mole fraction of component k in water phase.
Equilibrium partitioning	$\omega_{\alpha}^k = K_{\alpha:\beta}^k \omega_{\beta}^k$	ω_{α}^k and ω_{β}^k are the mole fraction of component k in phase α and β , respectively; and $K_{\alpha:\beta}^k$ is the equilibrium partitioning coefficient of component k between phases α and β .
Partitioning coefficient	$K_{\alpha:\beta}^k = K_{\alpha:\beta}^k(P_{\beta}, T, X_{\beta}^k)$	Depends on chemical properties of the component and is a function of temperature, pressure and composition.
Specific enthalpy of liquid	$h_{\beta} = U_{\beta} + \frac{P_{\beta}}{\rho_{\beta}}$	Internal energy, U_{β} , of liquid phase β is a function of pressure and temperature.
Specific enthalpies of gas	$h_g^k = U_g^k + \frac{P_g^k}{C_g^k}$	U_g^k the specific internal energy of component k in the gas phase; C_g^k concentration of component k in gas phase (kg/m^3).
Thermal conductivity	$K_T = K_T(S_{\beta})$	The thermal conductivity of the porous medium is treated as a function of fluid saturation.
Porosity	$\phi = \phi^0(1 + C_r(P - P^0) - C_T(T - T^0))$	ϕ^0 is the effective porosity at a reference pressure, P^0 , and a reference temperature, T^0 ; and C_r and C_T are the compressibility and thermal expansion coefficient of the medium, respectively.
Equilibrium adsorption	$X_s^k = K_d^k \rho_{\beta} X_{\beta}^k$	X_s^k is the mass of component k sorbed per mass of solids; and the distribution coefficient, K_d^k , is treated as a constant or as a function of the concentration or mass fraction in a fluid phase under the local chemical equilibrium condition.
Radioactive decay	$C_{\beta}^k = C_{\beta 0}^k e^{-\lambda_k t}$	C_{β}^k is the concentration of component k in phase β and is equal to $C_{\beta 0}^k$ at $t = 0$; λ_k is the radioactive decay constant.
First-order decay constant	$\lambda_k = \frac{\ln(2)}{T_{1/2}}$	$T_{1/2}$ is the half-life of the radioactive component.

conserving discretization scheme, based on finite or integral finite-difference or finite-element methods, is the most commonly used approach, and is discussed here.

3.1 Discrete equations

The component mass- and energy-balance Eq. (2.1) are discretized in space using a control-volume concept. The control-volume approach provides a general spatial discretization scheme that can represent a one-, two- or three-dimensional domain using a set of discrete meshes. Each mesh has a certain control volume for a proper averaging or interpolation of flow and transport properties or thermodynamic variables. The control volume concept includes the conventional finite-difference scheme (Narasimhan and Witherspoon, 1975; Pruess et al. 1999), an integral finite-difference method (Fig. 1) (Pruess, 1991), a control-volume finite element (Forsyth, 1994), and Galerkin finite-element methods (Huyakorn et al. 1994). These are the most widely used discretization schemes for multiphase flow simulation.

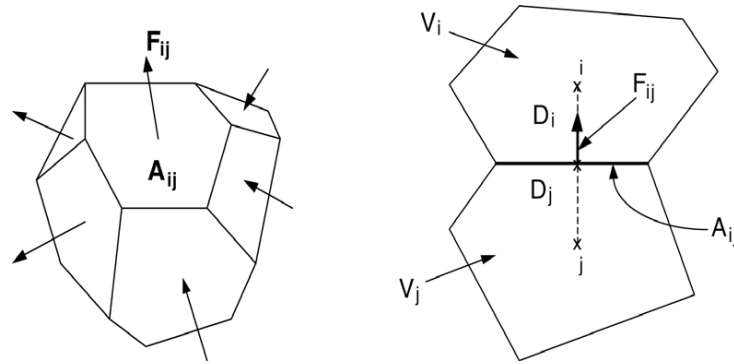


Figure 1: Space discretization and flow-term evaluation in the integral finite difference method (Pruess, 1991).

Time discretization is carried out using a backward, first-order, fully implicit finite-difference scheme. The discrete nonlinear equations for components of water, gas and oil, and heat at gridblock or node i can be written in a general form:

$$\left\{ A_i^{k,n+1} + G_i^{k,n+1} \Delta t - A_i^{k,n} \right\} \frac{V_i}{\Delta t} = \sum_{j \in \eta_i} flow_{ij}^{k,n+1} + Q_i^{k,n+1},$$

$$(k=1, \dots, N_c, N_c+1) \text{ and } (i=1, \dots, N), \tag{3.1}$$

where superscript k serves also as an equation index for all mass components with $k = 1, \dots, N_c$ and $k = N_c + 1$ denoting the heat equation; superscript n denotes the previous time level, with $n + 1$ the current time level to be solved; subscript i refers to the index of gridblock or node I , with N being the total number of nodes in the grid; Δt is time step size; V_i is the volume of node i ; η_i contains the set of direct neighboring nodes (j) of node i ; A_i^k , G_i^k , $flow_{ij}^k$, and Q_i^k are the accumulation and decay/generation terms, respectively, at node i ; the "flow" term between nodes i and j , and sink/source term at node i for component k or thermal energy, respectively, are defined below. Eq. (3.1) has the same

form regardless of the dimensionality of the system, i.e., it applies to one-, two-, or three-dimensional flow, transport, and heat-transfer analyses.

The accumulation and decay/generation terms for mass components or thermal energy are evaluated using Eqs. (2.6), (2.7), and (2.11), respectively, at each node i . The "flow" terms in Eq. (3.1) are generic and include mass fluxes by advective and dispersive processes, as described by Eq. (2.4) or (2.8), as well as heat transfer, described by Eq. (2.11).

The mass flow term of Eq. (3.1) for single-phase, Richards' or multiphase flow is described by a discrete version of Darcy's law, i.e., the mass flux of fluid phase β along the connection is given by

$$flow_{ij}^{\beta} = \lambda_{\beta,ij+1/2} \gamma_{ij} [\psi_{\beta j} - \psi_{\beta i}], \quad (3.2)$$

where $\lambda_{\beta,ij+1/2}$ is the mobility term to phase β , defined as

$$\lambda_{\beta,ij+1/2} = \left(\frac{\rho_{\beta} k_{r\beta}}{\mu_{\beta}} \right)_{ij+1/2}. \quad (3.3)$$

In Eq. (3.2), γ_{ij} is transmissivity and is defined differently for finite-difference or finite-element discretization. If the integral finite-difference scheme (Pruess et al. 1999) is used, the transmissivity is evaluated as

$$\gamma_{ij} = \frac{A_{ij} k_{ij+1/2}}{D_i + D_j}, \quad (3.4)$$

where A_{ij} is the common interface area between connected blocks or nodes i and j (Fig. 1); and D_i is the distance from the center of block i to the interface between blocks i and j (Fig. 1). The flow potential term in Eq. (3.2) is defined as

$$\psi_{\beta i} = P_{\beta i} - \rho_{\beta,ij+1/2} g Z_i, \quad (3.5)$$

where Z_i is the depth to the center of block i from a reference datum.

For mass component transport, the flow term, or the net mass flux by advection and hydrodynamic dispersion of a component along the connection of nodes i and j , is determined by

$$flow_{ij}^k = F_{A,ij}^k + F_{D,ij}^k \quad (k=1, \dots, N_c), \quad (3.6)$$

where $F_{A,ij}^k$ and $F_{D,ij}^k$ are the net mass fluxes by advection and hydrodynamic dispersion along the connection, respectively, with

$$F_{A,ij}^k = A_{ij} \sum_{\beta} \left(X_{\beta}^k \right)_{ij+1/2} F_{\beta,ij}, \quad (3.7)$$

$$F_{D,ij}^k = -\mathbf{n}_{ij} \bullet A_{ij} \sum_{\beta} \underline{D}_{\beta}^k \bullet \nabla \left(\rho_{\beta} X_{\beta}^k \right), \quad (3.8)$$

where \mathbf{n}_{ij} is the unit vector along the connection of the two blocks i and j .

The total heat flux along the connection of nodes i and j , including advective, diffusive, conductive and radiation terms, may be evaluated, when using a finite-difference scheme, by

$$\begin{aligned} flow_{ij}^{N_c+1} = & \sum_{\beta} \left[(h_{\beta})_{ij+1/2} F_{\beta,ij} \right] + \sum_{\beta} \sum_k \left\{ (h_{\beta}^k)_{ij+1/2} F_{D,ij}^k \right\} \\ & + A_{ij} (K_T)_{ij+1/2} \left[\frac{T_j - T_i}{D_i + D_j} \right] + A_{ij} \sigma_0 \varepsilon_{ij+1/2} (T_j^4 - T_i^4). \end{aligned} \quad (3.9)$$

In evaluating the "flow" terms in the above Eqs. (3.2)-(3.5), (3.7) and (3.9), subscript $ij+1/2$ is used to denote a proper averaging or weighting of fluid flow, component transport, or heat transfer properties at the interface or along the connection between two blocks or nodes i and j . The convention for the signs of flow terms is that flow from node j into node i is defined as "+" (positive) in calculating the flow terms. Wu and Pruess (2000b) present a general approach to calculating these flow terms associated with advective and dispersive mass transport and heat transfer in a multiphase system, using an irregular and unstructured, multidimensional grid.

The mass or energy sink/source in Eq. (3.1) at node i , Q_i^k , is defined as the mass or energy exchange rate per unit volume of rocks or soils. It is normally used to treat boundary conditions, such as surface infiltration, pumping, and injection through wells. Note that we present explicit, discrete expressions for estimating all the flow terms above, except for dispersive fluxes in Eq. (3.7). This is because of the numerical difficulties introduced in handling the hydrodynamic tensor of dispersion, which is treated very differently with different numerical approaches, such as finite difference or finite element. In most formulations for solute transport, the off-diagonal terms and contributions of the dispersion tensor are ignored, and dispersive transport is considered only along the principal directions. However, a general procedure for using the integral finite difference to incorporate a full dispersion tensor is presented by Wu and Pruess (2000b).

Note that Eq. (3.1) presents a precise form of the balance equation for each mass component and heat in a discrete form. It states that the rate of change in mass or energy accumulation (plus decay/generation, if existing) at a node over a time step is exactly balanced by inflow/outflow of mass and energy and also by sink/source terms, when existing for the node. As long as all flow terms have flow from node i to node j equal to and opposite to that of node j to node i for fluids, components, and heat, no mass or energy will be lost or created in the formulation during the solution. Therefore, the discretization in (3.1) is conservative.

3.2 Numerical solution scheme

There are a number of numerical solution techniques that have been developed in the literature over the past few decades to solve the nonlinear, discrete equations of reservoir simulations. When handling multiphase flow, multicomponent transport, and heat

transfer in a multiphase flow system, the predominant approach is to use a fully implicit scheme. This is due to the extremely high nonlinearity inherent in those discrete equations and the many numerical schemes with different level of explicitness that fail to converge in practice. In this section, we discuss a general procedure to solve the discrete nonlinear Eq. (3.1) fully implicitly, using a Newton iteration method.

Let us write the discrete non-linear equation (3.1) in a residual form as

$$R_i^{k,n+1} = \left\{ A_i^{k,n+1} + G_i^{k,n+1} - A_i^{k,n} \right\} \frac{V_i}{\Delta t} - \sum_{j \in \eta_i} flow_{ij}^{k,n+1} - Q_i^{k,n+1} = 0$$

$$(k=1, \dots, N_c+1; \quad i=1, \dots, N). \quad (3.10)$$

Eq. (3.9) defines a set of $(N_c+1) \times N$ coupled nonlinear equations that need to be solved for every balance equation of mass components and heat, respectively. In general, (N_c+1) primary variables per node are needed to use the Newton iteration for the associated (N_c+1) equations per node. The primary variables are usually selected among fluid pressures, fluid saturations, mass (mole) fractions of components in fluids, and temperatures. In many applications, however, primary variables cannot be fixed and must be allowed to vary dynamically in order to deal with phase appearance and disappearance (Forsyth, 1994). The rest of the dependent variables, such as relative permeability, capillary pressures, viscosity and densities, partitioning coefficients, specific enthalpies, thermal conductivities, dispersion tensor, etc., as well as nonselected pressures, saturations, and mass (mole) fractions, are treated as secondary variables.

In terms of the primary variables, the residual equation (3.10) at a node i is regarded as a function of the primary variables at not only node i , but also at all its direct neighboring nodes j . The Newton iteration scheme gives rise to

$$\sum_m \frac{\partial R_i^{k,n+1}(x_{m,p})}{\partial x_m} (\delta x_{m,p+1}) = -R_i^{k,n+1}(x_{m,p}), \quad (3.11)$$

where x_m is the primary variable m with $m=1, \dots, N_c+1$, respectively, at node i and all its direct neighbors; p is the iteration level; and $i=1, \dots, N$. The primary variables in Eq. (3.11) need to be updated after each iteration:

$$x_{m,p+1} = x_{m,p} + \delta x_{m,p+1}. \quad (3.12)$$

The Newton iteration process continues until the residuals $R_n^{k,n+1}$ or changes in the primary variables $\delta x_{m,p+1}$ over an iteration are reduced below preset convergence tolerances.

Numerical methods are generally used to construct the Jacobian matrix for Eq. (3.11), as outlined in Forsyth et al. (1995). At each Newton iteration, Eq. (3.11) represents a system of $(N_c+1) \times N$ linearized algebraic equations with sparse matrices, which are solved by a linear equation solver.

3.3 Treatment of initial and boundary conditions

A set of initial conditions is required to start a transient simulation, i.e., a complete set of primary variables need to be specified for every gridblock or node. A commonly used procedure for specifying initial conditions is the restart option, in which a complete set of initial conditions or primary unknowns is generated in a previous simulation with proper boundary conditions described.

Because of more physical and chemical constraints, boundary conditions for a multiphase flow and transport problem are generally much more difficult to handle than for a single-phase situation. When using a block-centered grid, first-type or Dirichlet boundary conditions, can be effectively treated with the "inactive cell" or "big-volume" method, as normally used in the TOUGH2 code (Pruess et al. 1999). In this method, a constant pressure/saturation/concentration/temperature node is specified as an inactive cell or with a huge volume, while keeping all the other geometric properties of the mesh unchanged.

With finite-element or edge-centered finite-difference grids, first-type boundary conditions and Neuman boundary conditions can be treated using a generalized, sink/source term approach (Wu et al. 1996a). Certain flux-type boundary conditions are easy to handle for a situation where flux distribution along the boundary is known, such as in dealing with surface infiltration. However, a description of more general types of flux- or mixed-boundaries, such as seepage faces and multilayered wells, is part of the solution, and general procedures of handling such boundary conditions are discussed in (Wu et al. 1996a; Wu 2000).

4 Treatment of fracture-matrix interaction

The mathematical and numerical formulations discussed above are applicable to both single-continuum and multi-continuum media using the generalized multicontinuum concept, as long as the physical processes concerned can be described in a continuum sense within either continuum. Fig. 2 shows several commonly used conceptual models for modeling fracture-matrix flow in fractured reservoirs. Fig. 3 presents an example of extended multi-continuum concept to include small fractures and vugs in petroleum reservoirs (Kang et al. 2006). All these cases and scenarios could all be considered to be special cases of the model formulation we discussed above.

The technique used in this paper for handling multiphase flow through fractured rock follows the dual-continuum methodology (Warren and Root, 1963; Pruess and Narasimhan, 1985; Wu and Pruess, 1988). This method treats fracture and matrix flow and interactions using a multi-continuum numerical approach, including the double- or multiporosity method, the dual-permeability method, and the more general MINC method (Fig. 2). Note that in the following discussion, we focus only on multiphase flow simulation. The multiphase flow formulation, Eq. (3.2) is applicable to both single-continuum and multi-continuum media. Using the dual-continuum concept, Eqs. (2.1)

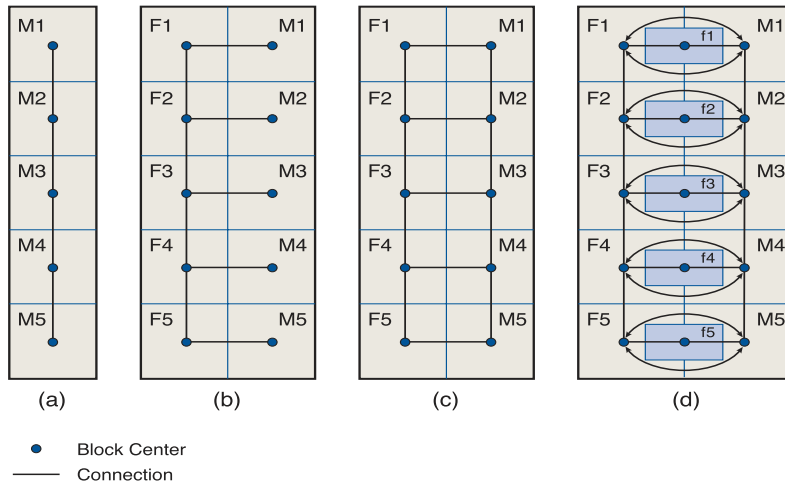


Figure 2: Schematic of different conceptualizations for handling fracture-matrix interactions: (a) effective-continuum model (ECM); (b) double-porosity model; (c) dual-permeability model; and (d) triple-continuum model. (M=matrix; F=large-fractures; f=small-fractures).

and (3.2) can be used to describe multiphase flow both in fractures and inside matrix blocks, as well as fracture-matrix interaction. However, special attention needs to be paid to treating fracture-matrix flow. The flow between fractures and the matrix is still evaluated using Eq. (3.2); however, the transmissivity for the fracture-matrix flow is given by

$$\gamma_{ij} = \frac{A_{FM}k_M}{l_{FM}}, \tag{4.1}$$

where A_{FM} is the total interfacial area between fractures and the matrix of elements i

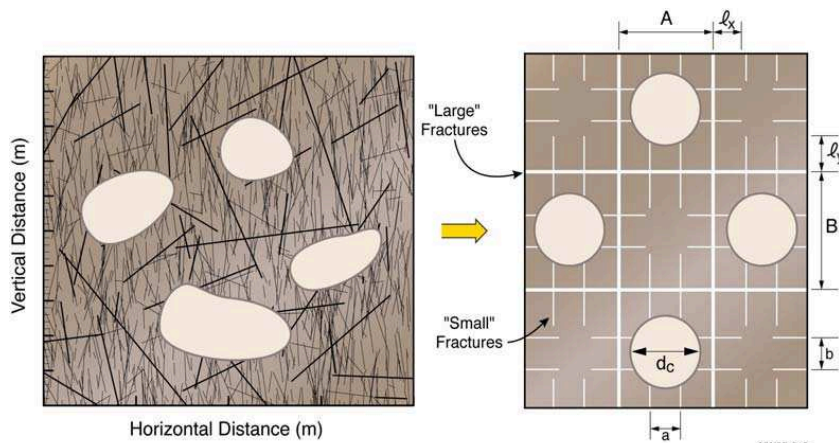


Figure 3: Conceptualization of vuggy fractured rock as a triple-continuum system with vugs indirectly connected to fractures through small fractures (Kang et al.2006).

Table 2: Characteristic distances* for evaluating flow terms between fractures (F), vugs (V), and matrix (M) systems.

Fracture Sets	Dimensions of Matrix Blocks (m)	Characteristic F-M Distances (m)	Characteristic F-V Distances (m)	Characteristic V-M Distances ¹ (m)	Characteristic V-M Distances ² (m)
1-D	A	$l_{FM} = A/6$	$l_{FV} = l_x$	$l_{VM} = a/6$	$l_{VM} = (A - d_c)/2$
2-D	A, B	$l_{FM} = AB / 4(A + B)$	$l_{FV} = \frac{l_x + l_y}{2}$	$l_{VM} = ab / 4(a + b)$	$l_{VM} = \frac{A + B - 2d_c}{4}$
3-D	A, B, C	$l_{FM} = 3ABC/10 / (AB + BC + CA)$	$l_{FV} = \frac{l_x + l_y + l_z}{3}$	$l_{VM} = 3abc/10 / (ab + bc + ca)$	$l_{FV} = \frac{A + B + C - 3d_c}{6}$

* Note in Table 2, A, B, and C are dimensions of matrix blocks along x, y, and z directions, respectively.

¹ Characteristic V-M distances are estimated for the case (Fig. 3), i.e., vuggy-matrix connections are dominated by small fractures, where dimensions a, b, and c are fracture-spacings of small fractures along x, y, and z directions, respectively.

² Characteristic V-M distances are used for the case that vugs are isolated from fractures.

and j (one of them is a fracture and the other a matrix block); k_M is the matrix absolute permeability along the fracture-matrix connection; and l_{FM} is a characteristic distance for flow crossing fracture-matrix interfaces, which can be determined for idealized 1-D, 2-D and 3-D dimensional rectangular matrix blocks when using the double-porosity model (Warren and Root, 1963). Table 2 lists several correlations for determining the characteristic distance in a fracture-vug-matrix system (Kang et al. 2006).

The appropriate spatial weighting scheme for averaging flow properties, such as the mobility of Eq. (3.2), in a heterogeneous formation has been an important issue in reservoir simulation and groundwater-modeling literature (Peaceman, 1977; Huyakorn and Pinder, 1983). Single-point or fully upstream weighting has been the exclusive approach for averaging mobility or relative permeability in calculating flow term, using a discrete Darcy's law for multiphase flow in heterogeneous petroleum reservoirs (Aziz and Settari, 1979). Recently, several theoretical studies (Forsyth et al., 1995; Forsyth and Kropinski, 1997) have shown that the upstream weighting scheme, if used with the control-volume discretization of the Richards' equation, will satisfy monotonicity conditions regardless of time step or mesh size. It will guarantee that converged numerical solutions are physically correct, while other weighting schemes, such as central weighting, may converge to an incorrect, unphysical solution (Forsyth and Kropinski, 1997). However, determining flow along fracture-matrix connections (i.e., flow across fracture-matrix interfaces in the direction perpendicular to fracture planes) is different from fracture-fracture flow and the conventional upstream weighting scheme may no longer be applicable. This is because fracture relative permeability functions are fracture flow properties describing flow along fractures, determined independently from matrix flow, while fracture-matrix flow or in-

teraction normally occurs along the directions perpendicular to fractures and is largely controlled by matrix properties or by flow resistance within the matrix block. The physical inconsistency in selecting fracture relative permeability for calculating fracture-matrix flow may lead to unphysical solutions or significant numerical errors.

To overcome these limitations, Wu et al. (2004a) presents a modified upstream weighting scheme to select appropriate mobility for fracture-matrix interaction. This new scheme is based on the principle that the capillary pressure is continuous at the fracture-matrix interface, and the assumption that there is instantaneous local equilibrium in pressure for each phase on the matrix surface between fracture and matrix systems. This should hold true for most subsurface fractured reservoirs, because fracture aperture is normally very small and fracture lateral boundaries are defined by matrix surfaces. Any dynamic changes in fractures, such as capillary pressures, could be instantaneously equilibrated locally with that at contacted matrix surfaces. As a result, the matrix relative permeability at the matrix surface can be readily determined as a function of fracture capillary pressure, or the matrix saturation corresponding to that fracture capillary pressure. Therefore, the new scheme, when the upstream direction for fracture-matrix flow is at the fractures, uses the matrix relative permeability function (instead of the fracture relative permeability function, as in the conventional upstream weighting scheme) to calculate the mobility. Physically, this is equivalent to evaluating flow through the fracture-matrix interface into the matrix with the effective matrix permeability at that interface.

The proposed weighting scheme is still dependent on the upstream fracture condition, and therefore does not lose the advantages of upstream schemes. In addition, in case fracture-matrix flow is from matrix to fractures, such as in a situation of drainage or flow between globally connected fractures or along global or local matrix-matrix connections, the conventional upstream weighting scheme should still be used. We call this hybrid mobility-averaging scheme physically based upstream weighting to determine mobility terms for fracture-matrix flow. Mathematically, the proposed mobility-weighting scheme requires the appropriate selection of relative permeability for fracture-matrix flow, used for calculating the mobility term in Eq. (3.3), as

$$k_{r\beta,FM} = k_{r\beta,M}(S_{\beta,M}^*) \quad \text{for } \Psi_{\beta F} \geq \Psi_{\beta M} \quad (4.2)$$

and

$$k_{r\beta,FM} = k_{r\beta,M}(S_{\beta,M}) \quad \text{for } \Psi_{\beta M} > \Psi_{\beta F}, \quad (4.3)$$

where $k_{r\beta,FM}$ is the physically upstream relative permeability for estimating fracture-matrix flow of phase β ; $k_{r\beta,M}$ is relative permeability of phase β in matrix, a function of matrix saturation ($S_{\beta,M}$); and $S_{\beta,M}^*$ is matrix saturation of phase β on matrix surface, determined from inverting the matrix capillary pressure function by setting matrix capillary pressure equal to fracture capillary pressure.

Within the context of the dual-continuum concept, the proposed approach can be applied to different matrix discretizations, such as double-porosity, dual-permeability,

or MINC grids. The proposed physical upstream weighting scheme has been tested in two multidimensional reservoir simulators with a series of numerical experiments conducted for commonly used dual-continuum models. In all test cases, this new weighting scheme is found to work efficiently, similarly to using the traditional single-point upstream weighting, without serious numerical difficulties. This new scheme should be applicable for discrete fracture-network models as well.

When handling flow and transport through a fractured rock using the generalized numerical formation of this paper, fractured media (including explicit fracture, dual, or multiple continuum models) can be considered as special cases of unstructured grids (e.g., Pruess, 1991). Then, a large portion of the work of modeling flow in fractured rock consists of generating a mesh that represents both the fracture system and the matrix system under consideration. Several fracture and matrix subgridding schemes exist for designing different meshes for different fracture-matrix conceptual models (Pruess and Narasimhan, 1985; Pruess 1983).

Once a proper grid of a fracture-matrix system is generated, fracture and matrix blocks are identified to represent fracture and matrix domains, separately. Formally they are treated identically for the solution in the model simulation. However, physically consistent fracture and matrix properties, parameter weighting schemes, and modeling conditions must be appropriately specified for both fracture and matrix systems.

5 Application

In an effort to demonstrate usefulness of the proposed generalized modeling approach in fractured reservoir simulation, we present two application examples. In the case of multiphase flow in isothermal condition, the proposed model formulation has been implemented and tested in the general-purpose reservoir simulator of MSFLOW (Wu, 2000), which is used in the following application examples. The first example is to match published laboratory experiment results of water imbibition and oil displacement conducted on fractured cores (Kazemi, 1979). The second problem is simulating single-phase flow through fractured vuggy rock with comparison with the existing analytical solution.

In the literature, there are several more examples for demonstrations, in which the work can be or were done using the model formulation discussed in this paper. They include (1) unsaturated multiphase fluid and heat flow in unsaturated porous or fractured media (Forsyth et al., 1995; Wu et al., 1999); (2) multi-phase flow in triple-continuum fractured system with small-fracture effect (Wu et al., 2004b); (3) multiphase flow in fractured-vuggy reservoirs (Kang et al., 2006); and (4) multiphase and heat flow and trace transport in fractured rock (Wu and Pruess, 2000).

5.1 Comparison with laboratory experimental results

Kazemi (1979) presented a series of laboratory experimental results of water imbibition into fractured matrix cores to displace oil. The laboratory tests were conducted on three

sets of artificial fractured cores using cylindrical and rectangular blocks, with one fracture along the long axis for each set. The cylindrical and rectangular matrix blocks were actually cut from Berea sandstone. The laboratory model we consider here consists of a fractured core with two brick-type matrix blocks. Each matrix block has a brick shape with dimension of width, height, and length ($50.8 \times 50.8 \times 101.6$ mm's) as shown in Fig. 4. The fracture formed between the two matrix cores has an aperture of 0.30 mm. The experimental data used in this study was from Test 38423 (Kazemi, 1979) as an example. In the experiment, flow channels were left open only at the inlet and outlet ends of the fracture (i.e., for water injection and for oil and water flow out), and side fracture and matrix surfaces were sealed. Initially, the fracture and matrix system was fully saturated uniformly with oil (diesel), and then water was injected with a constant rate at the inlet (Fig. 4) to displace the oil.

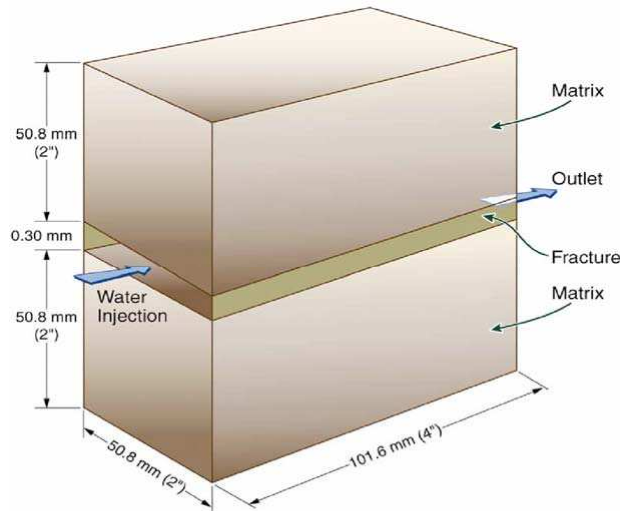


Figure 4: Schematic of fractured cores used the experimental studies (Kazemi, 1979; Wu et al. 2004).

Basic model experimental and modeling parameters are listed in Table 3. The relative permeability and capillary pressure curves used in this case are presented in Wu et al. (2004), using the equations given in Kazemi (1979), and the matrix capillary pressure curve was taken from the capillary-pressure curve on the Berea core of Figure 12 in Kazemi (1979). However, several important parameters were not provided in Kazemi (1979), including residual water saturation, residual oil saturation, and fracture capillary pressure curves. Actual values used for these missing parameters were determined in this work by model calibration, with the final estimates given in Table 3.

Here, this test is analyzed using a double-porosity approach (equivalent to the explicit-fracture model in this case) to examine the numerical scheme for handling fracture-matrix interaction under multiphase flow conditions. The fracture-matrix set of Fig. 4 is treated as a 2-D system along the longitudinal (x) direction (from inlet to outlet). Because of the symmetry, only half of the 2-D model domain (one matrix block and

Table 3: Parameters used in the comparison with laboratory testing results.

Parameter	Value	Unit
Fracture aperture	$b = 0.0003$	m
Fracture porosity	$\phi_F = 1.0$	
Matrix porosity	$\phi_M = 0.21$	
Absolute fracture permeability	$k_F = 1 \times 10^{-11}$	m^2
Absolute matrix permeability	$k_M = 4,23 \times 10^{-13}$	m^2
Water density	$\rho_w = 1,000$	kg/m^3
Water viscosity	$\mu_w = 1 \times 10^{-3}$	$Pa \cdot s$
Oil (diesel) density	$\rho_w = 828$	kg/m^3
Oil (diesel) viscosity	$\mu_w = 4.6 \times 10^{-3}$	$Pa \cdot s$
Residual fracture water saturation	$S_{wr,F} = 0.10$	
Residual matrix water saturation	$S_{wr,M} = 0.20$	
Residual fracture oil saturation	$S_{or,F} = 0.0001$	
Initial fracture water saturation	$S_{wi,F} = 0.00$	
Initial matrix water saturation	$S_{wi,M} = 0.00$	
Water injection rate	$q = 2.568 \times 10^{-5}$	m^3/d

half the fracture) is discretized into a double-porosity grid, using a 1-D parallel fracture concept, with one (actually half) fracture element corresponding to one matrix element in the transverse direction (perpendicular to the fracture plane). Along the x direction, a uniform linear grid of 10 elements is generated for both the fracture and the matrix block, with a uniform grid spacing of $\Delta x = 10.16$ mm. The final simulation results using the proposed physical upstream weighting scheme are compared with the laboratory experimental data in Fig. 5. Fig. 5 shows excellent agreement between measured and simulated volumetric fractional oil recovery versus pore volume of water injected. This result indicates that the numerical model formulation is able to capture the main factors that control fracture-matrix interaction during the oil-water displacement for this test problem.

5.2 Comparison with analytical solution

In this example, the numerical model results are examined using an analytical solution (Lui et al, 2003; Wu et al. 2004b). The problem concerns typical transient flow towards

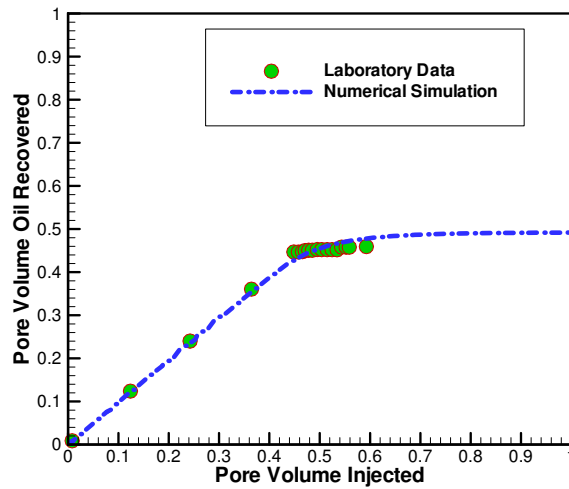


Figure 5: Comparison of simulation results with experimental data (Kazemi, 1979).

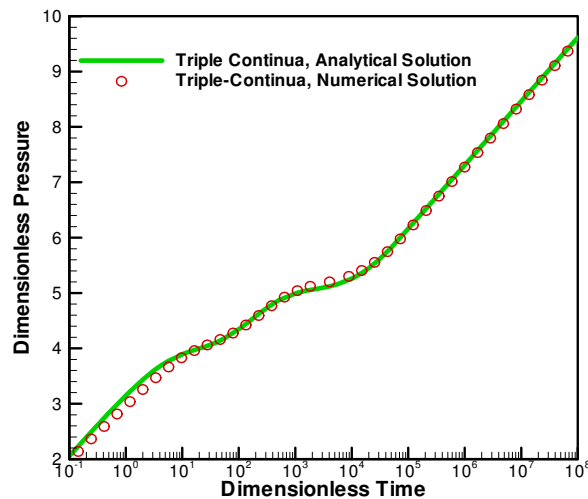


Figure 6: Comparison between analytical and numerical solutions for single-phase transient flow through vuggy fractured formation.

a well that fully penetrates a radially infinite, horizontal, and uniformly vuggy fractured reservoir. Numerically, a radial reservoir ($r_e = 10,000$ m) of 20 m thick is represented by a 1-D (primary) grid of 2,100 intervals. A triple-continuum mesh is then generated using a 1-D vuggy-fracture-matrix conceptual model, consisting of a horizontal large-fracture plate network with a uniform disk-shaped matrix block. Uniform spherical vugs are contained inside the matrix and connected to fractures through small fractures. Fracture, vugs and matrix parameters are given in Table 4.

Fig. 6 compares numerical-modeling results with the analytical solution for a single-

Table 4: Parameters used in the second problem of flow in the triple-continuum, vuggy fractured reservoir.

Parameter	Value	Unit
Matrix porosity	$\phi_M = 0.263$	
Fracture porosity	$\phi_F = 0.001$	
Vuggy porosity	$\phi_V = 0.01$	
Fracture spacing	$A = 5$	m
Small-fracture spacing	$a = 1.6$	m
F characteristic length	$l_x = 3.472$	m
F-M/F-V areas per unit volume rock	$A_{FM} = A_{FV} = 0.61$	m^2/m^3
Reference water density	$\rho_i = 1,000$	kg/m^3
Water phase viscosity	$\mu = 1 \times 10^{-3}$	Pa•s
Matrix permeability	$k_M = 1.572 \times 10^{-16}$	m^2
Fracture permeability	$k_F = 1.383 \times 10^{-13}$	m^2
Small-fracture or vug permeability	$k_V = 1.383 \times 10^{-14}$	m^2
Water Production Rate	$q = 100$	m^3/d
Total compressibility of three media	$C_F = C_M = C_V = 1.0 \times 10^{-9}$	1/Pa
Well radius	$r_w = 0.1$	m
Formation thickness	$h = 20$	m

phase transient flow case (in terms of dimensionless variables). Excellent agreement exists between the two solutions, which provides some verification of the numerical formation and its implementation.

6 Summary

A unified, generalized numerical formulation has been discussed for modeling fluid flow, mass transport, and heat-transfer processes through fractured porous media. This work takes advantage of the fact that governing equations used for describing various flow and transport phenomena in porous media are all generally based on the same form of mass and/or energy conservation laws. This indicates that there may exist a unified formulation and numerical scheme applicable to all of these physical processes. This paper explores such a possibility by proposing a generalized framework as well as mathematical formulation for modeling all known transport phenomena in fractured porous media.

As demonstrated in this paper, the proposed unified numerical modeling approach, based on a general multiple-continuum concept, is suitable for modeling any types of fractured reservoirs, including double-, triple-, and other multiple-continuum concep-

tual models. In addition, a new, physically correct mathematical scheme is discussed to calculate multiphase flow between fractures and the matrix, using continuity of capillary pressure at the fracture-matrix interface. The numerical implementation of the unified formulation is based on a control-volume spatial discretization with an unstructured grid and time discretization with a fully implicit finite-difference method. The final discrete linear or nonlinear equations are handled fully implicitly, using Newton iteration. The proposed general modeling methodology is demonstrated for its application in special cases where analytical solutions and laboratory experimental data.

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