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Publication Date

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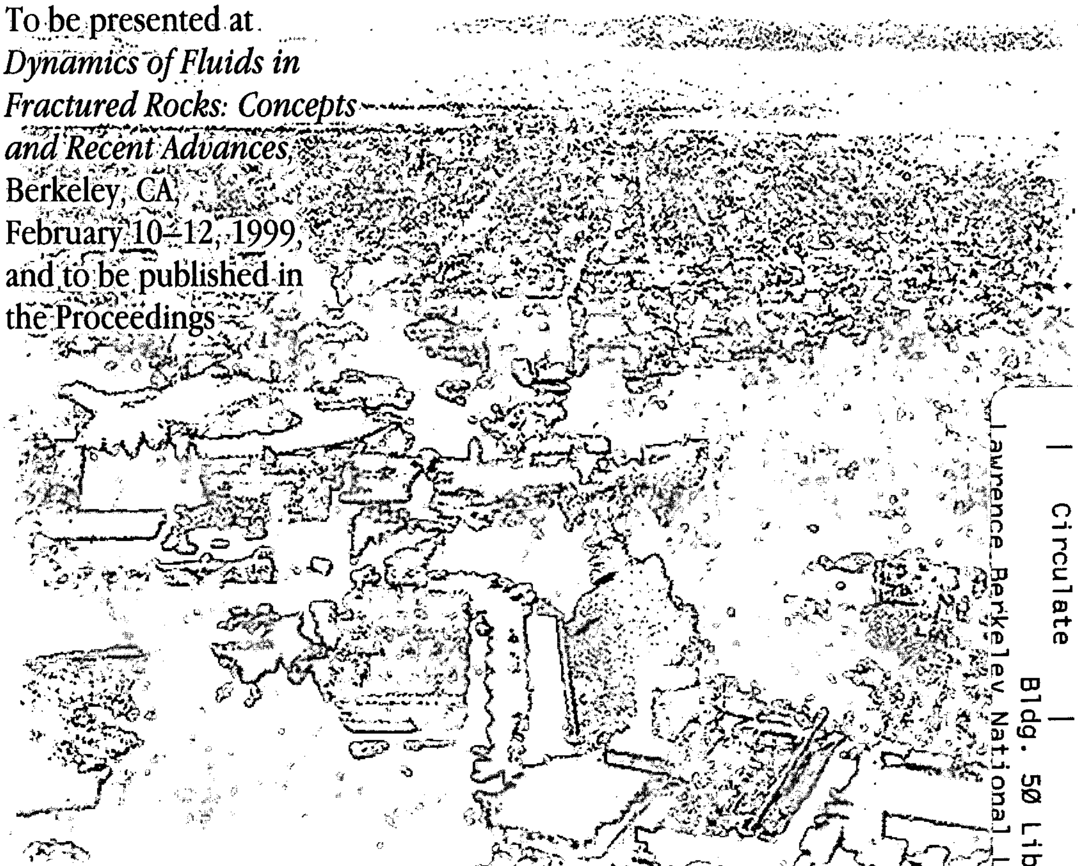
January 1999

To be presented at
Dynamics of Fluids in Fractured Rocks: Concepts and Recent Advances,
Berkeley, CA,
February 10–12, 1999,
and to be published in
the Proceedings



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LBNL - 42720

On the Effective Continuum Method for Modeling Multiphase Flow, Multicomponent Transport and Heat Transfer in Fractured Rock

International Symposium

Dynamics of Fluids in Fractured Rocks: Concepts and Recent Advances

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This work was supported by the Assistant Secretary for Energy Efficiency and Renewable Energy, Geothermal Division, of the US Department of Energy under contract No. DE-AC03-76SF00098.

Abstract

Flow and transport through fractured porous media occurs in many subsurface systems and has received considerable attention in recent years due to the importance in the areas of underground natural resource recovery, waste storage, and environmental remediation scheme. Among the methods of handling fracture/matrix flow and transport through geological media, the effective continuum method (ECM) has been widely used, and misused in some cases, because of its simplicity in terms of data requirements and computational efficiency.

This paper presents a rigorous, generalized effective continuum formulation, which has been implemented into the TOUGH2 code (Pruess, 1991) for modeling multiphase, multicomponent, non-isothermal flow and transport in fractured rocks. Also included in the paper are discussions of the conditions under which the ECM approach applies and the procedures for evaluating the effective parameters for both flow and transport simulations. Three application examples, one multiphase flow, one heat flow and one chemical transport problem, are given to demonstrate the usefulness of the ECM method.

1. Introduction

Flow and transport through fractured porous media occurs in many subsurface systems and has received considerable attention in recent years due to the importance in the areas of underground natural resource recovery, waste storage, and environmental remediation schemes. Since the 1960's, significant progress has been made in understanding and modeling fracture flow phenomena in porous media (Barenblatt et al., 1960; Warren and Root, 1963; Kazimi, 1969; Pruess and Narasimhan, 1985). Despite these advances, modeling the coupled processes of multiphase fluid flow, heat transfer, and chemical migration in a fractured porous medium remains a challenge conceptually and mathematically. This is primarily due to the nature of inherent heterogeneity and uncertainties associated with fracture/matrix systems for any given field problem, as well as the computational intensity required. Numerical modeling approaches currently used for simulating multiphase fluid flow, heat transfer, and chemical transport processes are generally based on methodologies developed for geothermal and petroleum reservoir simulations. They involve solving coupled multiphase fluid and heat flow, mutli-chemical component migration formulations based on finite difference or finite element schemes with a volume averaging approach.

A key issue for simulating fluid and heat flow and chemical transport in the fractured porous rocks is how to handle fracture and matrix interactions under multiphase, non-isothermal conditions. The available methods for treatment of fracture and porous matrix interactions using a numerical model include: (1) an explicit, discrete fracture and matrix model (Sudicky and McLaren, 1992); (2) the dual-continua method including double- and multi-porosity, dual-permeability, or the more general "multiple interacting continua" (MINC) method (Pruess and Narasimhan, 1985); and (3) the effective continuum method (ECM) (Wu et al. 1996a).

The discrete fracture modeling approach is, in general, computationally intensive and requires a detailed knowledge of fracture and matrix geometric properties and their spatial distributions, which are rarely known at a given site. For these reasons, it has found limited field applications in modeling multiphase, non-isothermal flow and transport in fractured rock for large-scale problems. On the other hand, the dual-continua method is conceptually appealing and computationally much less demanding than the discrete fracture modeling approach, and therefore has become the main approach used in handling fluid flow, heat transfer and chemical transport through fracture/matrix systems. However, this approach also requires detailed fracture and matrix geometric properties and their spatial distributions, such as fracture networks, connection and fracture/matrix interface areas, and is much less efficient computationally than the ECM method.

The ECM approximation has long been used for modeling fracture/matrix flow problems. However, there is a lack, in the literature and in applications, on the clear definition of the effective continuum or equivalent porous medium approach. Many different types of ECM models have been prsented and used, based on different assumptions and approximations, such as for isothermal, unsaturated flow (Peter and Klavetter, 1988), for coupled fluid and heat flow (Pruess et al. 1988; 1990; Nitao, 1989), for single phase flow and transport (Kool and Wu, 1991; Berkowitz et al., 1988), and for coupled multi-phase fluid and heat flow and solute transport (Wu et al., 1996a and 1996b).

This paper presents a generalized, rigorous ECM formulation for modeling multiphase, non-isothermal flow and solute transport. The focus of this work is to discuss the theoretical basis for the ECM methodology and the procedures to estimate effective parameters and constitutive relations in order to apply the method. Also included is a discussion on the conditions under which the ECM model can be used. In addition, three application examples, one multiphase flow, one heat flow and one chemical transport problem, are given to demonstrate the usefulness of the ECM method.

2. Formulation

In concept, the effective continuum approach uses an "effective" porous medium to approximate a fractured/matrix system, and calculations for flow and transport are then simplified and performed by a single-porosity continuum approach with a set of "effective" parameters. The ECM relies on a critical assumption that there is approximate thermodynamic equilibrium (locally) between fracture and matrix at all times in the formation. This implies that the local fracture/matrix interactions (fluid, heat and concentration exchanges) are simultaneously completed in a time scale relative to the time needed for the global flow and transport occurring through surrounding fracture-fracture/matrix-matrix connections. Based on the local equilibrium condition, the ECM approach does not require detailed knowledge of distributions and interface areas of fracture and matrix geometric properties and provides a simple, alternative conceptual model. The favorable conditions for the porous medium-like behavior are when rock matrix blocks are relatively small and permeable, the fracture network is intensive and relatively uniformly distributed, and fracture/matrix interactions are rapid. The continuum method will be particularly suitable for a situation when a long-term, averaged, or steady-state solution is sought. However, the effective continuum approximation may break down under certain unfavorable conditions, such as for a very tight, large and low-permeability matrix blocks subject to rapid transient flow, because it may take a long time to reach a local equilibrium under such an environment, which violates the fundamental assumption of local equilibrium for the ECM.

Let us derive fluid and heat flow, and solute transport governing equations starting from a dual-permeability conceptual model. At first, it is assumed that multiphase fluid flow, multicomponent transport and heat transfer processes can be described using a continuum approach in both fractures and matrix, respectively, within a representative elementary volume (REV) of a formation. Each REV contains enough fractures and matrix for such a continuum representation. The condition of local thermodynamic equilibrium requires that temperatures, phase pressures, densities and viscosities, enthalpies, and component concentrations in fracture and matrix systems are the same locally at any REV of the formation. Therefore, governing equations for component mass and energy conservation can be much simplified by adding the fluxes of mass and heat through fracture and matrix, respectively. Darcy's law is still used to describe flow terms of a fluid phase, a mass component is transported by advection and diffusion/dispersion, and heat is transferred by convection and conduction mechanisms in fracture and matrix, respectively. This results in a set of partial differential equations in the ECM formulation for flow and transport in fractured media, which may be written in the same forms as those for a single continuum porous medium (Wu et al. 1996a; Panday et al., 1995; and Forsyth, 1994):

For compositional transport equation of each species κ within a REV:

$$\frac{\partial}{\partial t}\left\{\phi \sum_{\beta}\left(\rho_{\beta} S_{\beta} X_{\beta}^{\kappa}\right)+(1-\phi)\, \rho_{s}\, \rho_{w}\, X_{w}^{\kappa}\, K_{d}^{\kappa}\right\}+\lambda_{\kappa}\left\{\phi \sum_{\beta}\left(\rho_{\beta} S_{\beta} X_{\beta}^{\kappa}\right)+(1-\phi)\, \rho_{s}\, \rho_{w}\, X_{w}^{\kappa}\, K_{d}^{\kappa}\right\}$$
$$=-\sum_{\beta} \nabla \bullet\left(\rho_{\beta} X_{\beta}^{\kappa} \vec{v}_{\beta}\right)+\sum_{\beta} \nabla \bullet\left(\rho_{\beta} \underline{D}^{\kappa} \bullet \nabla X_{\beta}^{\kappa}\right)+q^{\kappa} \tag{1}$$

where β is an index for fluid phase [β = 1, …, NP (total number of phases)]); κ is an index for components [κ = 1, 2, …, NK (total number of components)]; and the rest of symbols are defined below. The left hand of side of Equation (1) consists of (a) an accumulation term of component mass summed over all dissolved phases and adsorption on rock solids and (b) a first order decay term. The right hand of side of (1) is (a) an advection term contributed by all flowing phases; (b) diffusive and dispersive terms within all phases; and (c) a source/sink term.

The energy conservation equation is

$$\frac{\partial}{\partial t}\left\{\sum_{\beta}\left(\phi\, \rho_{\beta} S_{\beta} U_{\beta}\right)+(1-\phi)\, \rho_{s}\, U_{s}\right\}=-\sum_{\beta} \nabla \bullet\left(h_{\beta}\, \rho_{\beta}\, \vec{v}_{\beta}\right)$$
$$+\sum_{\beta} \sum_{\kappa} \nabla \bullet\left(\rho_{\beta}\, h_{\beta}^{\kappa} \underline{D}^{\kappa} \bullet \nabla X_{\beta}^{\kappa}\right)+\nabla \bullet\left(K_{th} \nabla T\right)+q^{E} \tag{2}$$

Similarly, the left hand of side of Equation (2) is an energy accumulation term of summation over all phases and solids, and the right hand of side contains (a) a heat advection term contributed by all flowing phases; (b) diffusive and dispersive heat transfer term within all phases; (c) a heat conduction term; and (d) a source/sink term.

Equations (1) and (2) contain many "effective" or "equivalent" parameters and constitutive correlations that need to be determined before the ECM approach can be used, as discussed in this and the following sections.

Terms and symbols in Equations (1) and (2) are defined as follows:

ϕ is effective porosity, defined as

$$\phi = \phi_f + \phi_m \tag{3}$$

where ϕ_f and ϕ_m are porosities of fracture and matrix continua, respectively.

ρ_β, ρ_s and ρ_w are densities of fluid β, rock solids, and water phase, respectively.

S_β is effective saturation of fluid β, defined as,

$$S_\beta = \frac{S_{\beta,f}\phi_f + S_{\beta,m}\phi_m}{\phi_f + \phi_m} \tag{4}$$

where $S_{\beta,f}$ and $S_{\beta,m}$ are saturation of fluid β, in fracture and matrix continua, respectively.

X_β^κ is mass fraction of component κ in fluid β.

K_d^κ is effective distribution coefficient of component κ between the water phase and rock solids of fracture and matrix, defined as,

$$K_d^\kappa = \frac{A_s K_d^f + (1 - \phi_m - \phi_f) K_d^m}{1 - \phi} \tag{5}$$

where A_s is the ratio of fracture surface areas to a bulk rock (fracture + matrix) volume, representing total fracture surface areas per unit volume of rock; K_d^f and K_d^m are distribution coefficients of component κ between the water phase and rock solids of fracture and matrix continua, respectively. It should be mentioned that here we use different definitions of solid-water partitioning coefficients, K_d, for fracture and matrix. K_d^f has a dimension of ($M/L^2 \bullet L^3/M$) or (L), while K_d^m is a volume concept with a dimension of (L^3/M) (Freeze and Cherry, 1979).

$\vec{v}_\beta$ is the effective Darcy velocity of fluid β, defined as,

$$\vec{v}_\beta = -\frac{k\,k_\beta}{\mu_\beta}\left(\nabla P_\beta - \rho_\beta \vec{g}\right) \tag{6}$$

where P_β, μ_β and $\vec{g}$ are pressure and viscosity of fluid β, and gravity vector, respectively; k is effective continuum permeability, defined as,

$$k = k_f + k_m \tag{7}$$

with k_f and k_m are absolute permeabilities of fracture and matrix continua, respectively; and the effective relative permeability to fluid phase β, k_β, is defined as,

$$k_\beta = \frac{k_f\, k_{\beta,f} + k_m\, k_{\beta,m}}{k_f + k_m} \tag{8}$$

$\underline{D}^\kappa$ is the combined fracture/matrix, diffusion-dispersion tensor accounting for both molecular diffusion and hydrodynamic dispersion for component κ, weighted by total porosity,

$$\underline{D}^\kappa = \frac{\phi_f\, \underline{D}_f^\kappa + \phi_m\, \underline{D}_m^\kappa}{\phi_f + \phi_m} \tag{9}$$

where the fracture diffusion-dispersion tensor is,

$$\underline{D}_f^\kappa = \left(\alpha_{T,f}\left|\vec{v}_{\beta,f}\right|\right)\delta_{ij} + \left(\alpha_{L,f} - \alpha_{T,f}\right)\vec{v}_{\beta,f}\,\vec{v}_{\beta,f} / \left|\vec{v}_{\beta,f}\right| + \left(\phi_f\, S_{\beta,f}\tau_f\, d_f\right)\delta_{ij} \tag{10}$$

and the matrix diffusion-dispersion tensor is,

$$\underline{D}_m^\kappa = \left(\alpha_{T,m}\left|\vec{v}_{\beta,m}\right|\right)\delta_{ij} + \left(\alpha_{L,m} - \alpha_{T,m}\right)\vec{v}_{\beta,m}\,\vec{v}_{\beta,m} / \left|\vec{v}_{\beta,m}\right| + \left(\phi_m\, S_{\beta,m}\tau_m\, d_m\right)\delta_{ij} \tag{11}$$

where $\alpha_{T,f}$, $\alpha_{L,f}$, $\alpha_{T,m}$ and $\alpha_{L,m}$ are the transverse and longitudinal dispersivities, respectively, for fracture and matrix continua; τ_f and τ_m is tortuosities of fracture and matrix continua, respectively; d_f and d_m is the molecular diffusion coefficients in phase β of fracture and matrix continua, respectively; $\vec{v}_{\beta,f}$ and $\vec{v}_{\beta,m}$ are Darcy's velocities of fluid β of fracture and matrix continua, respectively; and δ_{ij} is the Kroneker delta function. (δ_{ij}=1 for i = j, and δ_{ij}=0 for i $\neq$ j).

q^κ and q^E are source/sink terms for component κ and energy, respectively.

h_β and h_β^κ are enthalpies of fluid phase β and of component κ in fluid phase β, respectively.

U_β and U_s are internal energy of fluid β and rock solids, respectively.

K_{th} is effective thermal conductivity, defined as,

$$K_{th} = \frac{\phi_f\, K_{th,f} + \phi_m\, K_{th,m}}{\phi_f + \phi_m} \tag{12}$$

where $K_{,th,f}$ and $K_{th,m}$ are the thermal conductivities of fracture and matrix continua, respectively, and they may be functions of liquid saturations of each continuum.

T is temperature.

3. Evaluation of Effective Parameters and Constitutive Relations

In solving the governing equations (1) and (2) with the ECM approach, the primary variables selected in a numerical solution are normally fluid pressures, P_β, effective saturations, S_β, temperature, T, and mass fraction, X_β^κ. Once the primary variables are chosen, all the secondary variables must be evaluated using the primary variables, effective parameters and correlations to set up a set of solvable numerical equations. Special attention needs to be paid to evaluating the secondary variables, effective constitutive relations and parameters in this process. Many rock and fluid properties, such as porosities, absolute permeability, dispersitities, thermal conductivities, totuosities, and diffusion coefficients of fracture and matrix continua, fluid viscosities and densities, should be determined from site-characterization studies. The key effective constitutive correlations, such as capillary pressures, relative permeability, dispersion tensor and thermal conductivity relation for the ECM formulation are discussed in this section.

The numerical implementation of the ECM scheme for evaluating the effective constitutive relations, as given in the previous section, is straightforward once we know fluid saturations in matrix and fracture, separately. This can be achieved by introducing a fracture/matrix combined (or composite) capillary pressure (P_c) curve (using tabulated values, based on the individual fracture and matrix P_c curves from the input data for a given rock type). Under local equilibrium conditions, the combined P_c curve is

$$P_c(S_\beta) = P_{c,m}(S_{\beta,m}) = P_{c,f}(S_{\beta,f}) \tag{13}$$

as a function of an effective or average liquid saturation, S_β, defined in (4).

During a Newton iteration in a numerical simulation, the liquid saturation obtained from the solution is exactly the effective saturation (4), as a primary variable. This effective saturation value can be used with the combined P_c curve to calculate the value of the effective capillary function, which is the same as that of fracture or matrix systems, based on the ECM, local equilibrium assumption. The fracture and matrix saturations can then be determined by inverting the input capillary pressure functions of fracture and matrix, respectively.

Once fluid saturations, $S_{\beta,m}$ and $S_{\beta,f}$, in fracture and matrix system are determined, separately, the effective relative permeabilities for the ECM calculations are evaluated using Equation (8), in which the relative permeabilities $k_{\beta,m}$ and $k_{\beta,f}$ have to be also evaluated at saturations $S_{\beta,m}$ and $S_{\beta,f}$, respectively.

Equation (5) can be directly used for estimating the effective K_d for adsorption terms of a component, contributed by both fractures and matrix. Similarly, Equation (12) should be used for calculating an effective thermal conductivity, in which fracture and matrix thermal conductivities, needed in (12), can be handled as functions of fracture and matrix liquid saturations, respectively.

One of the primary difficulties in determining "effective" parameters for the ECM formulation is the evaluation of the effective dispersion tensor. In general, Equations (9), (10) and (11) can be used for this purpose. In addition to phase saturations in fracture and matrix continua, these equations require Darcy's velocities in fractures and matrix, separately. These velocities can be approximated by,

$$\vec{v}_{\beta,f} = -\frac{k_f\, k_{\beta,f}}{\mu_\beta}\left(\nabla P_\beta - \rho_\beta \vec{g}\right) \tag{14}$$

for fractures and

$$\vec{v}_{\beta,m} = -\frac{k_m\, k_{\beta,m}}{\mu_\beta}\left(\nabla P_\beta - \rho_\beta \vec{g}\right) \tag{15}$$

for matrix. The two velocities for a phase can be calculated per time step or per Newton iteration.

For a 2-D transport in a regular, two-orthogonal, parallel fractures system, Kool and Wu (1991) provide an alternative, approximate correlation for effective dispersivities as,

$$\alpha_L = \frac{\phi_m (L_x - b)^2}{3\phi^2\, d_m}\left(\frac{R_m}{R_e}\right)^2 |v_x| \tag{16}$$

for effective longitudinal dispersivity along the x-direction and

$$\alpha_T = \frac{\phi_m (L_y - b)^2}{3\phi^2\, d_m}\left(\frac{R_m}{R_e}\right)^2 |v_y| \tag{17}$$

for effective transverse dispersivity to the x-direction. These two dispersivities were derived using a two-region type model of transport in an aggregated soil (van Genuchten and Dalton, 1986). In (16) and (17), L_x and L_y are the half spacings between parallel fractures in the x-direction and the y-direction, respectively; b is half the aperture of fractures; v_x and v_y are effective Darcy's velocities in the x-direction and the y-direction, respectively; and the retardation factors are then

$$R_m = 1 + \frac{(1-\phi_m)\rho_s K_d^m}{\phi} \tag{18}$$

for matrix and

$$R_e = \frac{\phi_f R_f + \phi_m R_m}{\phi} \tag{19}$$

for the effective continuum with

$$R_f = 1 + \frac{K_d^f}{b} \tag{20}$$

for fractures.

4. Model Implementation and Application

The ECM formulation of Section 2 has been implemented into the TOUGH2 code, a multiphase, multicomponent, nonisothermal reservoir simulator (Pruess, 1991). It includes (a) the EOS3 and EOS4 modules for two-phase (water and gas), two components (water and air) and heat; (b) the EOS9 module for two-phase, isothermal flow by solving Richards' equation; and (c) the EOS1G module for single gas flow in a two-phase condition with aqueous phase as a passive phase (Wu et al., 1996a). In addition, a two-phase, three-component and non-isothermal version is implemented into a solute transport code, T2R3D (Wu et al., 1996b; Wu and Pruess, 1998).

Because of computational efficiency and simplicity in data requirement with the ECM method, the implemented modules of the TOUGH2 code and the T2R3D code have found a wide range of applications in field characterization studies at the Yucca Mountain site, a potential underground repository for high-level radionuclide wastes. The ECM methodology has been used as a main modeling approach in 3-D, large-scale unsaturated zone model calibrations (Wu et al., 1996c), in perched water studies (Wu et al., 1997a), and in ambient geothermal condition investigation (Wu et al., 1998). It is also be used for pneumatic data analyses (Ahlers et al., 1997), in modeling geochemical transport (Sonnenthal and Bodvarsson, 1997) and in thermal loading studies (Haukwa and Wu, 1996).

During these applications, several comparative and validation studies have also been carried out to investigate the accuracy and applicability of the ECM approach to field problems (Doughty and Bodvarsson, 1997; Wu et a., 1996a and 1996c). These studies conclude that the ECM concept is adequate to modeling steady-state moisture and ambient heat flow, and transient gas flow in fractured unsaturated zones of Yucca Mountain, as long as there are strong fracture-matrix interactions in the system. However, the ECM approximation will introduce larger errors for the cases where a strong non-equilibrium condition exists between fracture and matrix systems, such as within fast flow pathways along high-permeability flow channels.

Another important application of the ECM model in field studies is to use its results as initial conditions for the dual-permeability simulations. This has been proven to be extremely helpful in performing large-scale moisture flow simulations at Yucca Mountain (Wu et al., 1998). In this case, many 3-D steady-state dual-permeability simulations were needed to study the wide-range uncertainties for parameters arranging from surface infiltration rates to fracture/matrix properties. Due to the more non-linear nature in the dual-permeability formulation in handling fracture/matrix and the doubling in size of the model grid relative to the ECM, a direct use of the dual-permeability modeling approach was impractical for completing all the simulations with the time constraint. Since the ECM and dual-permeability approaches give very similar results in terms of moisture distributions in fractures and matrix at steady state, as demonstrated in the following section, the initial condition for a dual-permeability run was estimated using the results of a corresponding ECM steady-state simulation. With a good initial guess, it was relatively easy for a dual-permeability to converge to a steady-state solution. This approach provided an order of magnitude improvement in computer CPU times relative to those dual-permeability simulations without using ECM results as initial conditions.

5. Application Examples

Three application examples are given in this section for demonstrating the applicability of the ECM approach, and they are:

(1) Comparison of the ECM and the more rigorous, dual-permeability modeling approaches for liquid flow through unsaturated, fracture rocks.

(2) Two-phase, 3-D non-isothermal fluid and heat flow at ambient geothermal condition.

(3) A single-phase, 2-D flow and transport with comparison with a result from a discrete fracture model.

5.1 Example 1 – Comparison with the Dual-Permeability Model Results

The first example is a one-dimensional vertical flow problem in the unsaturated zone of Yucca Mountain and the vertical column grid is extracted directly from the 3-D site-scale model (Wu et al., 1996c). The grid consists of a set of 1-D vertical grid blocks, representing four hydrogeologic units (named as TCw, PTn, TSw, and CHn), and an overlying and underlying boundary block representing the atmosphere and the water table conditions, respectively. The fracture system in the unsaturated zone of the mountain is also subdivided into the same four units. The properties of fractures are taken from Wilson et al. (1993) for the four units, as listed in Table 1.

Table 1. The fracture continuum porosity and spacing data used for the comparison study (Wilson et al., 1993)

Unit	Porosity	Spacing (m)
TCw	1.38e-3	0.618
PTn	4.12e-3	2.220
TSw	2.75e-3	0.740
CHn	9.98e-4	1.618

Since few fractures exist in the PTn unit, the effects of fractures on moisture flow in the PTn are ignored in this simulation, and the PTn formation is treated as a single porous medium rock. The same set of matrix and fracture properties, as listed in Table 2 (Bandurraga and Bodvarsson, 1996), are used for both ECM and dual-permeability simulations.

Table 2. The rock properties of matrix and fractures used in the ECM comparison study.

Unit/ Layer	$k_m (m^2)$	$k_f (m^2)$	$\alpha_m (Pa^{-1})$	$\alpha_f (Pa^{-1})$	m_m	m_f	ϕ_m	ϕ_f
tcw11	0.160E-18	0.910E-11	0.147E-04	0.518E-03	0.238	0.182	0.062	0.290E-03
tcw12	0.540E-15	0.575E-11	0.174E-05	0.977E-03	0.233	0.223	0.082	0.290E-03
tcw13	0.220E-16	0.575E-11	0.129E-05	0.123E-02	0.463	0.437	0.207	0.290E-03
ptn21	0.400E-12	n/a	0.244E-04	n/a	0.215	n/a	0.435	n/a
ptn22	0.240E-12	n/a	0.159E-04	n/a	0.310	n/a	0.222	n/a
ptn23	0.111E-12	n/a	0.445E-04	n/a	0.243	n/a	0.406	n/a
ptn24	0.880E-13	n/a	0.341E-04	n/a	0.295	n/a	0.499	n/a
ptn25	0.105E-11	n/a	0.138E-03	n/a	0.243	n/a	0.490	n/a
tsw31	0.261E-12	0.400E-11	0.237E-04	0.122E-02	0.206	0.203	0.048	0.243E-03
tsw32	0.194E-12	0.445E-11	0.172E-04	0.969E-03	0.248	0.249	0.156	0.243E-03
tsw33	0.796E-17	0.743E-11	0.573E-05	0.243E-03	0.247	0.250	0.154	0.243E-03
tsw34	0.100E-14	0.159E-11	0.754E-06	0.686E-03	0.321	0.325	0.110	0.243E-03
tsw35	0.423E-15	0.400E-11	0.234E-05	0.108E-02	0.231	0.226	0.130	0.243E-03
tsw36	0.776E-16	0.400E-11	0.522E-06	0.122E-02	0.416	0.416	0.112	0.243E-03
tsw37	0.316E-15	0.400E-11	0.804E-06	0.122E-02	0.368	0.368	0.036	0.243E-03
ch1vc	0.160E-11	0.723E-12	0.760E-04	0.122E-02	0.221	0.227	0.273	0.111E-03
ch2vc	0.550E-13	0.723E-12	0.980E-04	0.122E-02	0.223	0.227	0.344	0.111E-03
ch3zc	0.450E-17	0.100E-12	0.394E-05	0.388E-03	0.225	0.225	0.332	0.525E-04
ch4zc	0.210E-16	0.100E-12	0.150E-06	0.730E-03	0.475	0.470	0.266	0.525E-04
pp3vp	0.542E-14	0.300E-13	0.194E-04	0.122E-02	0.316	0.313	0.322	0.111E-03
pp2zp	0.269E-15	0.100E-12	0.126E-05	0.730E-03	0.311	0.312	0.286	0.525E-04

In this table, k_m and k_f are matrix and fracture continuum permeabilities; α_m and α_f are van Genuchten's parameters (van Genuchten, 1980)) of capillary pressure of matrix and fracture; m_m and m_f are van Genuchten's parameters of soil retention curves; and ϕ_m and ϕ_f are porosities of matrix and fracture systems, respectively.

The same type boundary conditions are specified for both models as Dirichlet-type conditions, i.e., constant pressures, temperatures and saturation. Also the surface boundary is subject to a constant water infiltration of 3.6 mm/year. However, the water infiltration on the ground surface is only added as a source term into the fracture elements on the top boundary for the dual-permeability model. It is distributed between fracture and matrix in the ECM model because, realistically, infiltration is expected almost entirely entering through the fractures on the land surface, but the continuum approach of the ECM uses equilibrium partitioning for the infiltration. Also an isothermal condition was assumed to exist under two-phase flow conditions for this comparison.

Both models are run to steady-state and Figure 1 presents the steady-state liquid saturation profiles for fractures and matrix, obtained using the ECM and the dual-permeability models. Figure 1 shows that almost identical results of matrix saturations are obtained from the two modeling approaches. The only differences between the two solutions may be noticed at near the top (TCw unit), or along the interfaces at an elevation of 1,200 m (between the PTn and the TSw). The reasons for these minor differences are from the conceptual model, rather than from the modeling approaches. First, the water infiltration is imposed into fractures only on the top boundary in the dual-permeability simulation, while the ECM model puts the infiltration into both fracture and matrix systems. Second, the PTn unit is treated as a single porous medium, and this creates certain discontinuities in matrix/fracture vertical connections across the interfaces.

The comparison, as shown in Figure 1, indicates that as long as the local equilibrium condition is satisfied between the fracture and matrix systems, the ECM formulation will give accurate predictions of saturation distributions. We can create a situation under which the local equilibrium condition is not well satisfied, and the ECM approach will introduce considerable errors into the solution. Figure 2 shows such a comparison for simulated liquid saturation profiles also using the ECM and the dual-permeability methods. However, the interface areas between the fracture and matrix systems in this case were reduced by a factor of 10, 100, and 1,000, respectively, to reduce fracture/matrix interactions. The interface areas become 10%, 1%, and 0.1% of the geometric area of the fracture and matrix systems, as shown in Figure 2. As the fracture-matrix interface areas get smaller, the local equilibrium conditions are less satisfied, and the figure shows more differences between the predictions using the ECM and the dual-permeability approaches in the certain units/layers (at elevations between 1,000 and 1,200 m).

However, Figure 2 shows that even with several orders of magnitude reduction in the fracture-matrix interface areas, the comparisons are still reasonably well between the ECM and the dual-permeability results for the lower unit of the layers. The reason is that the matrix are relatively permeable in that unit, compared with the fractures, and the local equilibrium conditions are still reasonable. It should be mentioned that many 3-D comparisons between the ECM and dual-permeability model results have been made and very similar results to this 1-D model are obtained (Wu et al., 1996c).

5.2 Example 2 - Comparisons with Measured Temperature Profiles

Several 3-D unsaturated zone fluid and heat flow models have been developed using the ECM approach to estimate geothermal conditions of the Yucca Mountain site (Wu et al., 1998). Measured temperature data (Sass et al., 1988; Rousseau et al., 1996) were compared with the 3-D simulation results for about 25 boreholes within and near the study area of the Yucca Mountain site. The 3-D model also uses the land surface and the water table as the top and bottom boundaries, with constant or spatially varying pressures, saturations and temperatures described based on the field data. In addition, a spatially varying, steady-state water infiltration map is specified to the top model boundary. The detailed on the model grid, parameters and conditions are provided by Wu et al. (1998). In general, it has been found that that the 3-D ECM models are able to match temperature data from all the boreholes. We present only one of the 25 comparisons conducted in the model calibration as a demonstration example. The selected borehole is H-5 and the comparison between the modeled results and observations is shown in Figure 3.

5.3 Example 3 – Single-Phase, 2-D Flow and Transport

This problem is used to test the ECM formulation in simulating a combined flow and transport case (Kool and Wu, 1991), and the effective dispersivities for transport are described by Equations (16) to (20) of Section 3. The vertical 2-D domain, hypothetical waste site, depicted in Figure 4 is discretized into a rectangular element grid with a total of 1,768 elements. The ECM simulation was performed using a finite element code (Huyakorn et al., 1991) and the ECM results were examined against the results from a discrete fracture code (Sudicky and McLaren, 1992). Th detailed information on effective parameters and their evaluation, and model conditions is given in the report (Kool and Wu, 1991) for this problem. The flow and transport simulation was carried out by a decoupled approach, in which a steady-state flow run was conducted first, then followed by the transient transport calculation. The model flow and transport boundary conditions are shown in Figures 5 and 6, respectively.

Figure 7 presents a comparison of simulated hydraulic head contours from the two models, and the agreement is quite good, indicating the ECM approximation is reasonable in this case for describing the steady-state flow field. The results for transport simulation are shown in Figures 8 and 9, respectively, for a conservative and reactive species. Figure 8 shows that the comparison of the ECM and the discrete fracture model results is very favorable for this case. The extent of the contaminant plume, as indicated by the 0.005 relative concentration contour, is predicted well by the ECM model, as compared with the "true" solution by the discrete fracture model. However, the ECM model tends to somehow overpredict the downward extent of the plume at this time.

The comparison of the ECM and discrete fracture model results for a sorbing species, displayed in Figure 9, also shows a similar pattern of the plume at the same time of 2,500 year. The large time values reflect the much slower contaminant migration rates with adsorption/reactive effects. The jaggedness in the concentration contours of the discrete fracture model results is due to effects of fast advection transport through fractures and a non-equilibrium condition between fractures and matrix. The comparisons in Figures 8 and 9 are quite favorable with regard to the applicability of the ECM approach for modeling single-phase flow and transport in fractured rocks. However, this is a limited validation of the ECM method, because the study system is very simple with known fracture characteristics.

6. Conclusions

This paper presents a rigorous derivation of the generalized ECM formulation and defines a complete set of the effective ECM parameters for modeling multiphase flow, multicomponent transport, and heat transfer in fractured rocks. Also included are the discussions on implementation of the ECM formulation into a multidimensional, multiphase flow and transport reservoir simulators. In addition, three examples are provided for examining the ECM approach.

The ECM modeling approach is an efficient, alternative conceptual model for studies of flow and transport phenomena in fractured porous media. As discussed in this work, the ECM concept, relative to the dual-permeability approach, is built on one critical assumption that there is approximate local thermodynamic equilibrium between fracture and matrix at all times in the formation. As long as this assumption is a reasonable approximation for a given application, the ECM approach will provide a reasonable solution with substantial improvement in both computational intensity and requirement of detailed fracture geometric properties. The effective continuum approach is particularly suitable for the case in which a long-term, steady-state solution is sought on large time and spatial scales of concern. In a situation when no detailed fracture characteristic data (this may never be known), such as fracture network distributions and fracture/matrix interface areas, use of the more rigorous modeling approach, the dual-permeability or other multi-continua method, may not gain more advantages than using a simple ECM model due to the uncertainties in fracture/matrix data. Because of these reasons, the ECM approach has been widely used as a practical tool in many field investigations of fracture flow problems.

However, the limitation of the effective continuum approximation must be recognized and examined before its proper use. The single continuum method may break down under certain unfavorable conditions, such as for a very tight, large and low-permeability matrix blocks subject to rapid transient flow and transport, because it may take too long to reach thermodynamic equilibrium between fracture and matrix systems under such an condition. It is recommended that sensitivity and comparison studies be made using the ECM approach against multi-continua model results on a smaller-scale model before ECM approach to a large-scale application for a given site.

Acknowledgments

The author is grateful to H. H. Liu and M. Cushey for review of this paper. Thanks are due to J. Kool for the opportunity of working together on the 2-D flow and transport problem for NRC. This work was in part supported by the Assistant Secretary for Energy Efficiency and Renewable Energy, Office of Geothermal Technologies of the U. S. Department of Energy, under Contract No. DE-AC03-76SF00098.

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Figures

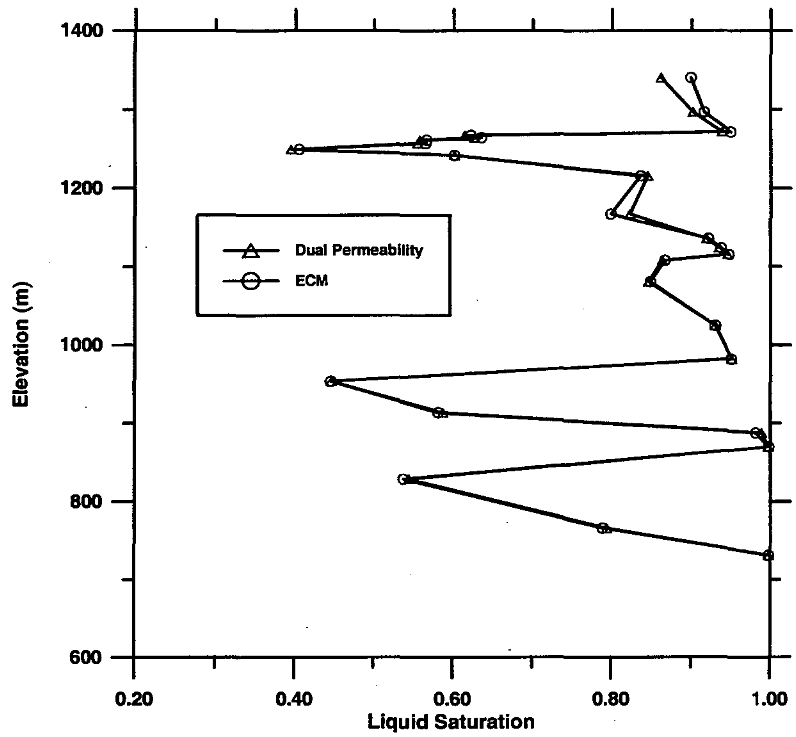


Figure 1. Comparison of the simulated matrix liquid saturation profiles using the ECM and the Dual-permeability models.

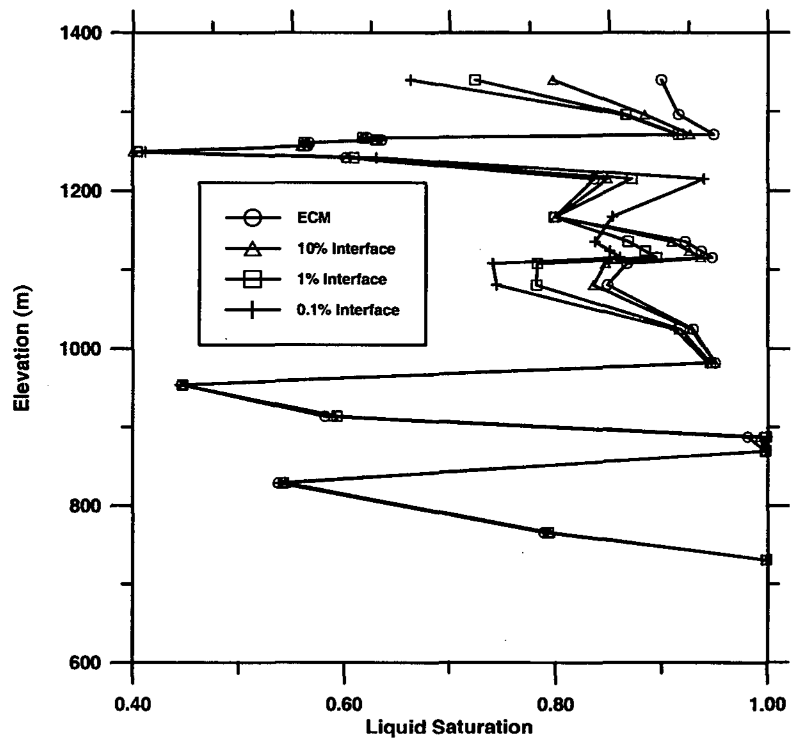


Figure 2. Comparison of the simulated matrix liquid saturation profiles using the ECM and the Dual-permeability models with reduction of fracture/matrix interface areas.

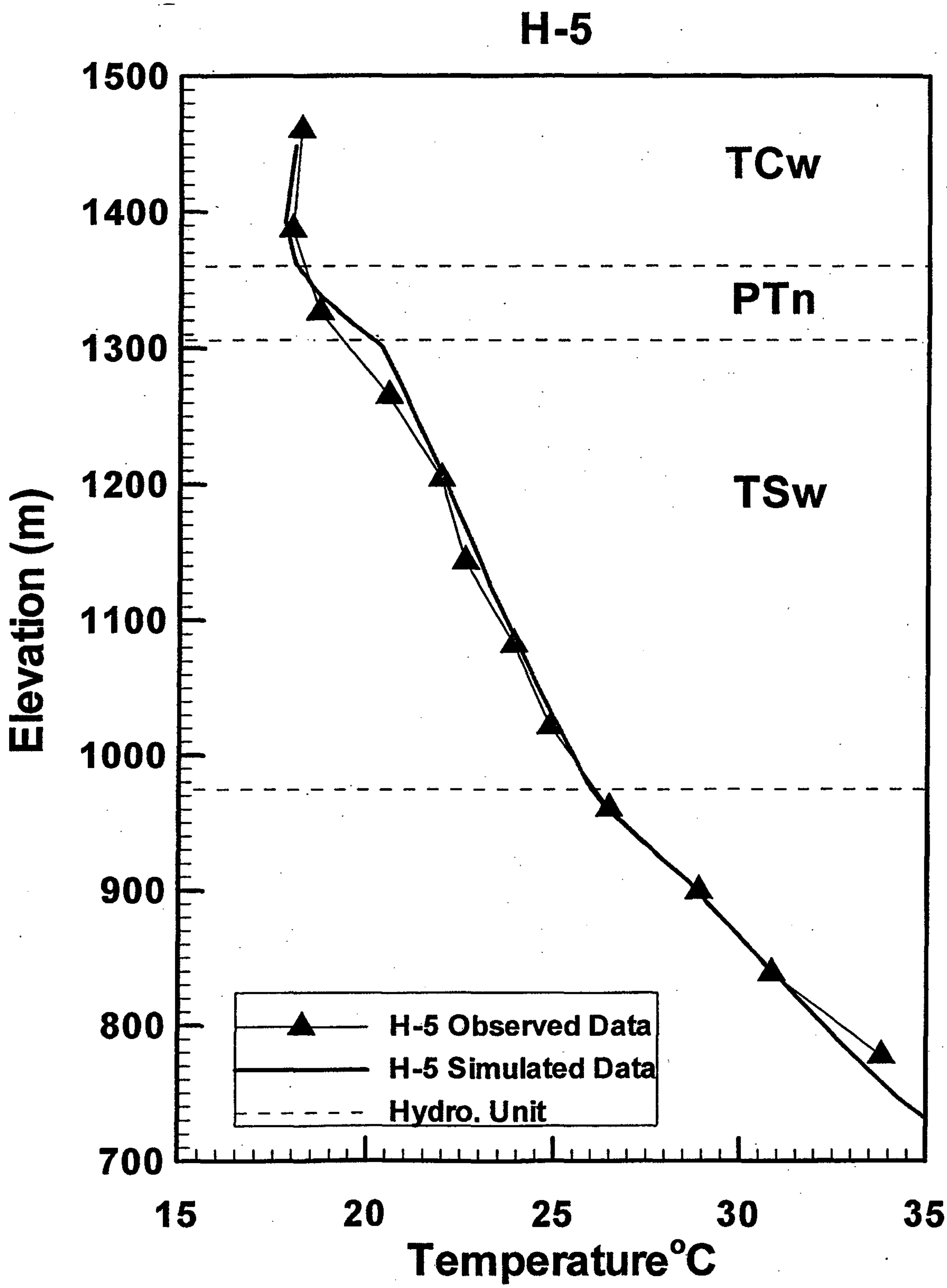


Figure 3. Comparison between measured and simulated temperatures for borehole H-5 in the unsaturated zone of Yucca Mountain.

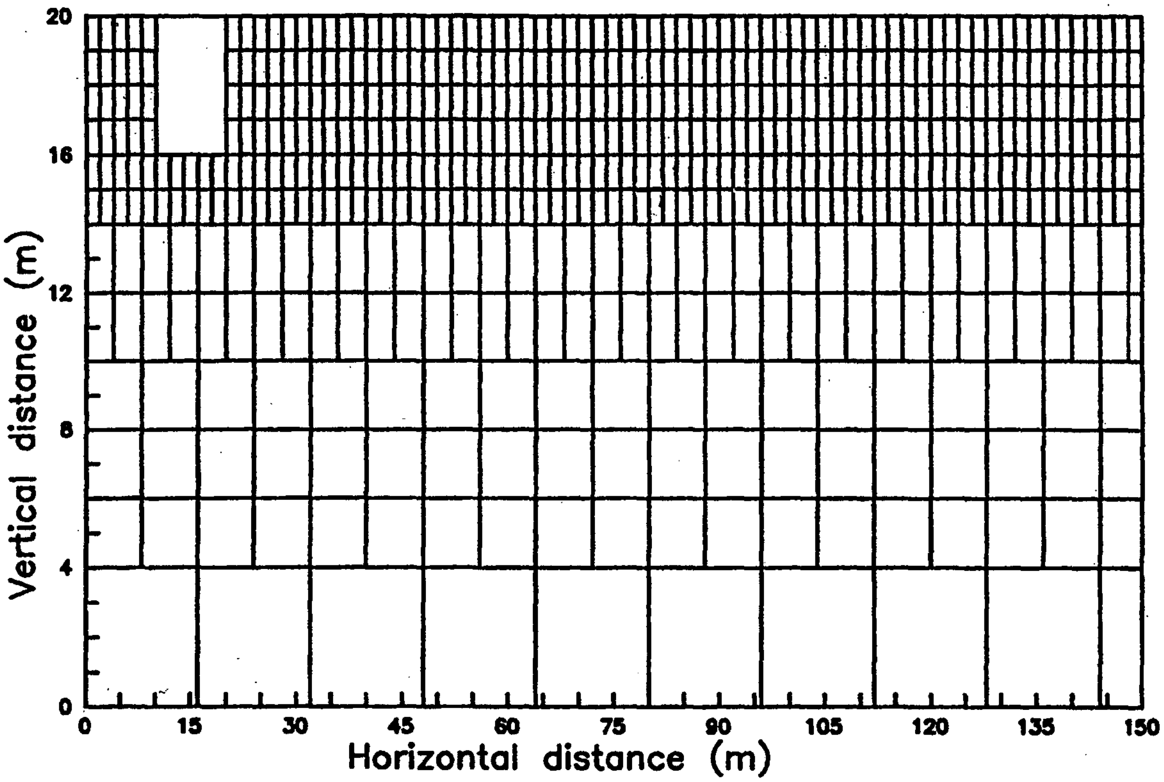


Figure 4. Fracture network and 2-D domain at hypothetical waste disposal site (Note 5x vertical exaggeration).

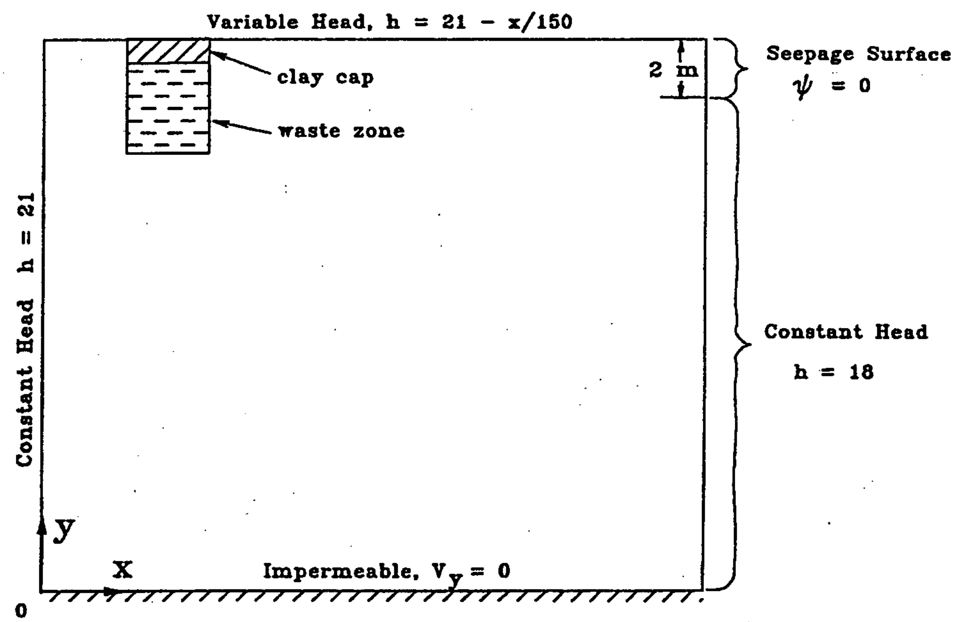


Figure 5. Boundary conditions and coordinates used in the ECM flow simulation.

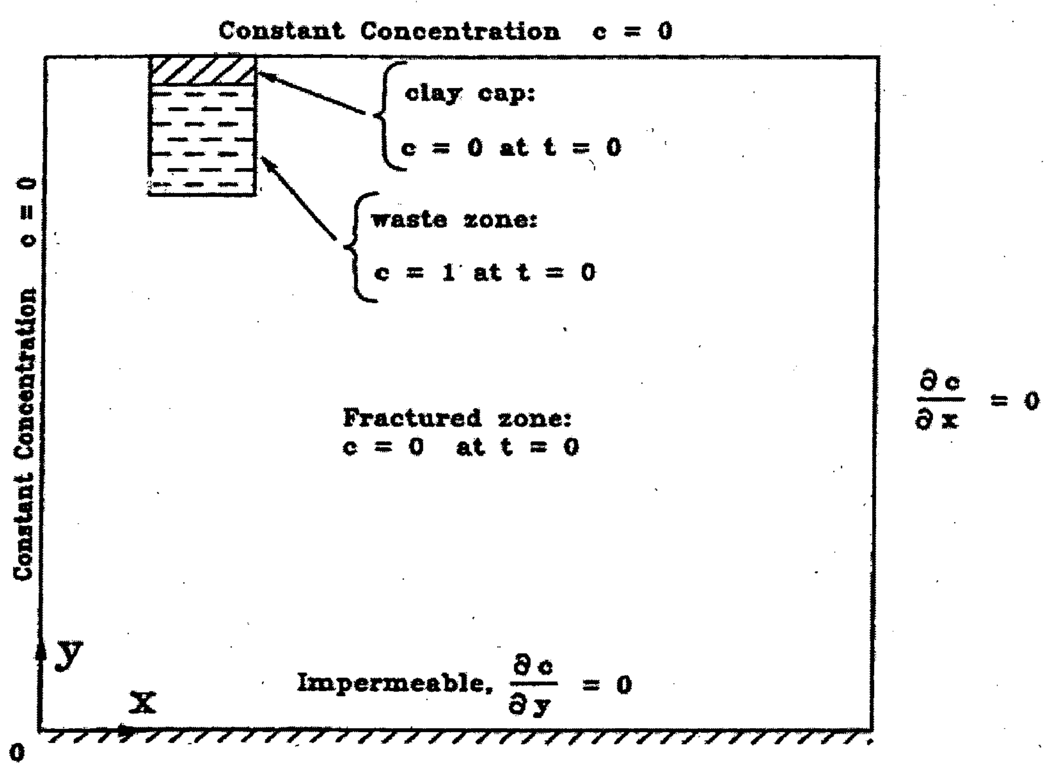
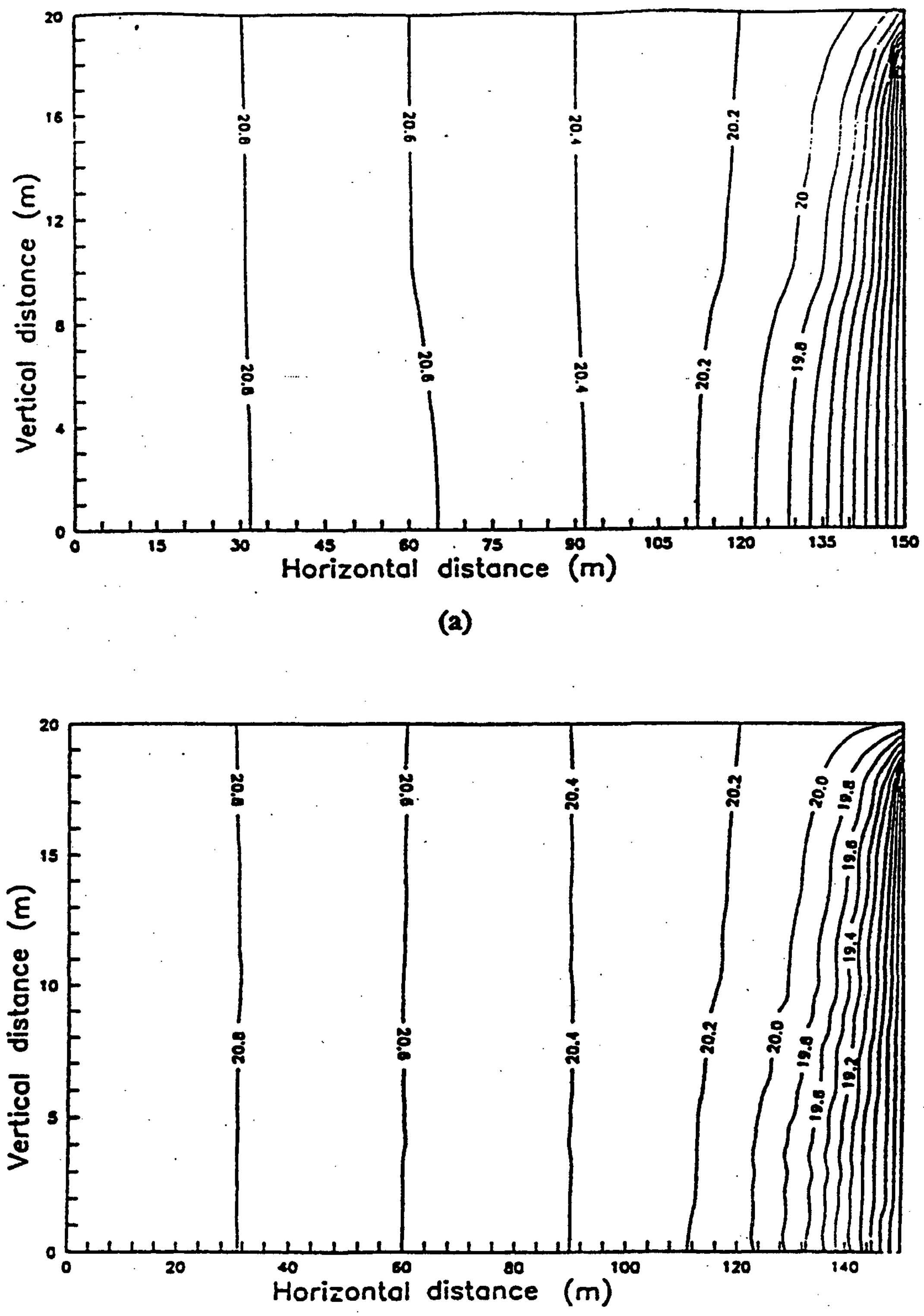


Figure 6. Boundary and initial conditions used in the simulation of conservative and reactive contaminant transport.



(b)

Figure 7. Steady-state hydraulic head distributions in the 2-D model domain simulated using the discrete fracture code (Sudicky and McLaren, 1992) and the ECM model (Huyakorn et al., 1991).

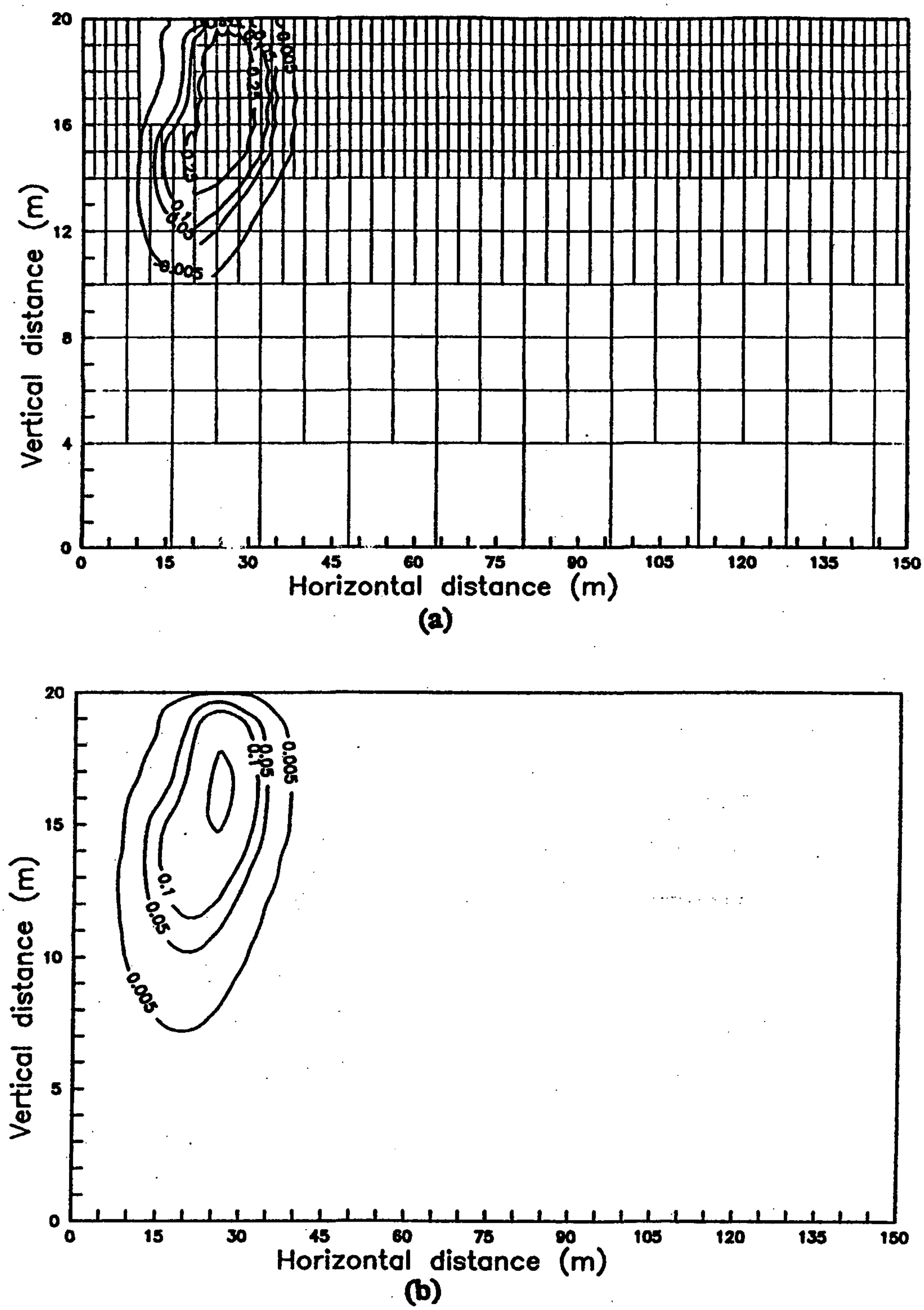


Figure 8. Concentration contours of conservative contaminant transport at t=50 years, simulated using the discrete fracture code (Sudicky and McLaren, 1992) and the ECM model (Huyakorn et al., 1991).

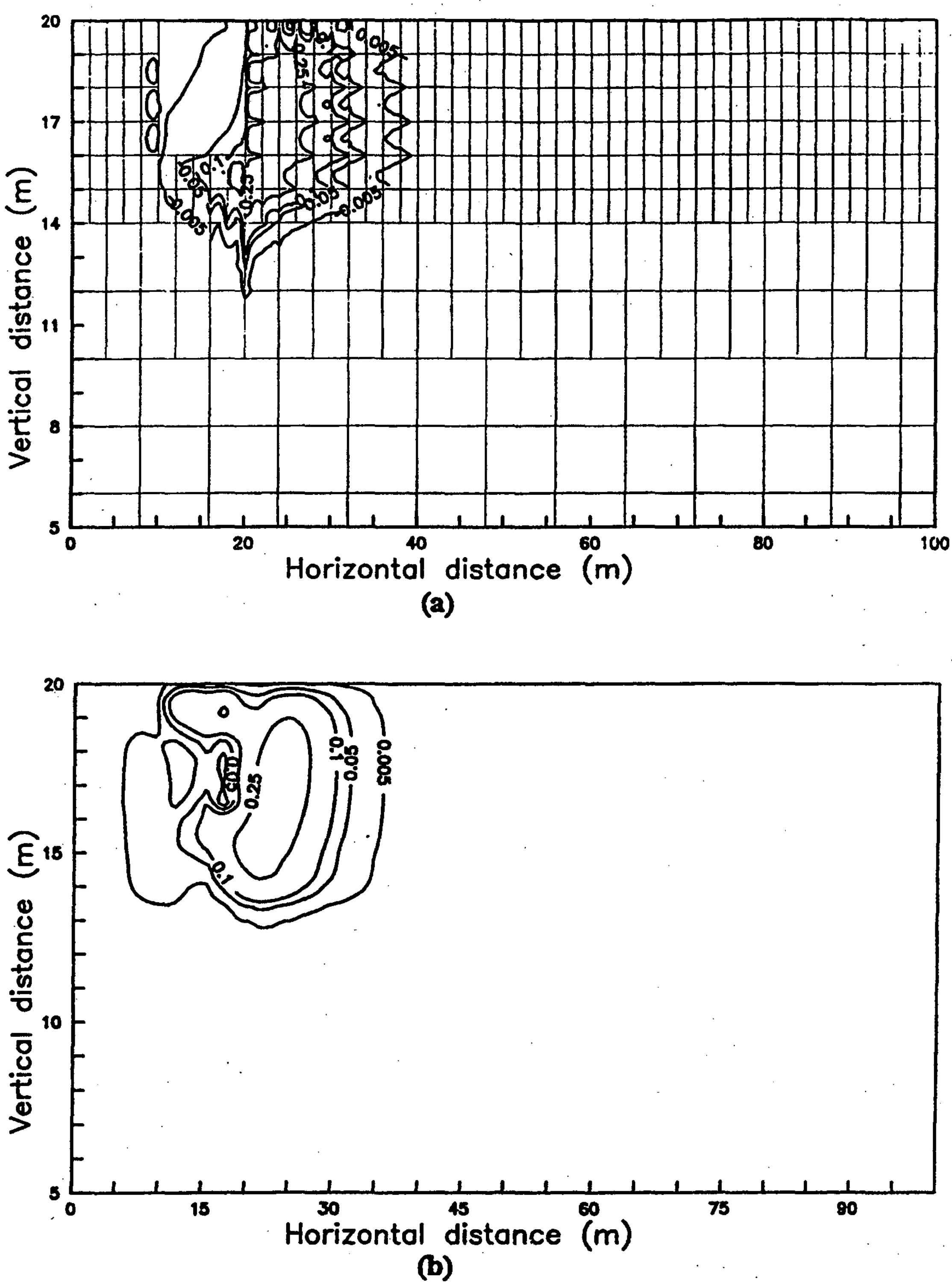


Figure 9. Concentration contours of reactive contaminant transport at t=2,500 years, simulated using the discrete fracture code (Sudicky and McLaren, 1992) and the ECM model (Huyakorn et al., 1991).

Figure Captions

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Figure 9. Concentration contours of reactive contaminant transport at t=2,500 years, simulated using the discrete fracture code (Sudicky and McLaren, 1992) and the ECM model (Huyakorn et al., 1991).

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Prepared for the U.S. Department of Energy under Contract No. DE-AC03-76SF00098