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**On the Validity of a Fickian Diffusion Model for
the Spreading of Liquid Infiltration Plumes in
Partially Saturated Heterogeneous Media**

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ON THE VALIDITY OF A FICKIAN DIFFUSION MODEL FOR THE SPREADING OF LIQUID INFILTRATION PLUMES IN PARTIALLY SATURATED HETEROGENEOUS MEDIA

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ABSTRACT

Localized infiltration of aqueous and non-aqueous phase liquids (NAPLs) occurs in many circumstances. Examples include leaky underground pipelines and storage tanks, landfill and disposal sites, and surface spills. Because of ever-present heterogeneities on different scales such infiltration plumes are expected to disperse transversally and longitudinally.

This paper examines recent suggestions that liquid plumes are being dispersed from medium heterogeneities in a manner that is analogous to Fickian diffusion. Numerical simulation experiments on liquid infiltration in heterogeneous media are performed to study the dispersive effects of small-scale heterogeneity. It is found that plume spreading indeed tends to be diffusive. Our results suggest that, as far as infiltration of liquids is concerned, broad classes of heterogeneous media behave as dispersive media with locally homogeneous (albeit anisotropic) permeability.

INTRODUCTION

Figure 1. Schematic of liquid infiltration in an unsaturated heterogeneous medium. Regions of low permeability (shaded) divert flux sideways and cause a lateral spreading of the infiltration plume.

Liquids flowing downward through the unsaturated zone in coarse soils, or in large (sub-)vertical fractures, may encounter low-permeability obstacles, such as silt or clay lenses in soils, or asperity contacts between fracture walls. Water will pond atop the obstacles and be diverted sideways, until other predominantly vertical pathways are reached (Fig. 1). The conventional treatment of two-phase flow includes gravity, pressure, and capillary effects. Horizontal flow diversion from media heterogeneities can be represented only if such heterogeneity is modeled in full explicit detail. In practical applications, explicit numerical modeling of small-scale reservoir heterogeneities would require prohibitively large numbers of grid blocks, because heterogeneities occur on many different scales (small-scale laminations and layering in soils, low-permeability lenses, capillary barriers, fractures, fracture networks, lithologic units, etc.).

It has recently been suggested that plume spreading due to media heterogeneities may be approximated as a diffusive process (Espedal et al., 1991; Langlo and Espedal, 1992; Pruess, 1993, 1994). In this paper we briefly summarize our convection-dispersion model for infiltration of liquids in the vadose zone. The validity of the Fickian dispersion hypothesis is then examined by means of numerical simulation experiments in media with fully-resolved small-scale heterogeneity.

FICKIAN DISPERSION MODEL

In two-phase immiscible flow of liquid and gas, mass fluxes F_β (β = liquid, gas) are customarily written as a multiphase version of Darcy's law,

$$F_\beta = -k \frac{k_{r\beta}}{\mu_\beta} \rho_\beta (\nabla P_\beta - \rho_\beta g) \quad (1).$$

Here, k is the permeability tensor, $k_{r\beta}$ is relative permeability in phase β , μ is viscosity, ρ is fluid density, P_β is pressure in phase β , and g is acceleration of gravity. In the following we specialize to anisotropic media with principal axes of the permeability tensor in the horizontal and vertical directions.

$$k = k_h [e_x e_x + e_y e_y] + k_v e_z e_z \quad (2)$$

In Eq. (2) we have introduced unit vectors e in the x , y , and z -directions. k_h and k_v are the horizontal and vertical permeabilities, respectively. Our proposed Fickian-type diffusion model for phase dispersion involves adding a dispersive flux term for liquid phase to Eq. (1) which, in analogy to solute dispersion in miscible flow (de Marsily, 1986), is written as

$$F_{l,dis} = -\rho_l \phi D_{dis} \nabla S_l \quad (3).$$

Specializing to conditions where advective flow is dominated by gravity, we introduce the propagation velocity v of saturation disturbances in the absence of capillary effects (Pruess, 1991),

$$v = \frac{k_v}{\phi} \frac{\rho_l g}{\mu_l} \frac{dk_{rl}}{dS_l} \frac{g}{g} \quad (4),$$

The dispersion tensor D_{dis} is then written as (Pruess, 1993)

$$D_{dis} = v (\alpha_T [e_x e_x + e_y e_y] + \alpha_L e_z e_z) \quad (5).$$

Here we have introduced transverse (horizontal) and longitudinal (vertical) dispersivities α_T , α_L . g and v are the magnitude of the gravitational acceleration and velocity vectors, respectively. Note that the proposed phase-dispersive flux has the same structure as capillary flux. Indeed, the capillary-driven flux component of Eq. (1) can be written in a form like Eqs. (3-5), with transverse capillary dispersivity given by

$$\alpha_{\text{cap},T} = \frac{k_h}{k_v} \frac{1}{\rho_l g} \frac{dP_{\text{cap}}}{d \ln k_{rl}} \quad (6).$$

An analogous equation, without the anisotropy factor k_h/k_v , holds for the longitudinal capillary dispersivity. From the correspondence between phase-dispersive and capillary fluxes, we expect that phase dispersion effects from medium heterogeneities will be most important when capillary effects are weak, i.e., for non-wetting liquids, and for "coarse" heterogeneous media such as coarse-grained soils or large fractures. Longitudinal phase dispersion will modify the predominant downward advective flow. Transverse dispersion may lead to qualitatively new behavior, causing a lateral spreading of liquid plumes even when capillary pressures are weak. In the remainder of the paper we will focus mainly on transverse dispersion effects.

Numerical Simulation Experiments

To examine the validity of the proposed phase dispersion model we have performed numerical simulation experiments. The calculations were done with our multiphase flow code TOUGH2 (Pruess, 1991), enhanced with a set of preconditioned

Figure 2. Two-dimensional vertical section of a heterogeneous medium with a random distribution of impermeable obstacles (black segments). Length of obstacles is uniformly distributed in the range of 2-4 m.

conjugate gradient routines for efficient solution of multidimensional flow problems with 10,000 or more grid blocks (Moridis, private communication, 1993). The flow experiments involve placing a localized plume of liquid into an unsaturated heterogeneous medium, such as shown in Fig. 2, and then allowing the plume to migrate under the combined action of pressure, capillary, and gravity forces (Eq. 1). Small-scale medium heterogeneity is resolved in detail, and no explicit allowance for phase dispersion as in Eq. (3) is made. Many numerical experiments were carried out for media with different parameters and style of heterogeneity, both regular and random.

The spreading of the plumes is analyzed by evaluating spatial moments (Sahimi et al., 1986; Freyberg, 1986; Essaid et al., 1993). Specifically, an effective transverse diffusivity for a localized plume is calculated as

$$D_T = \frac{1}{2} \frac{d}{dt} (\sigma_T^2) \quad (7),$$

where σ_T^2 is the mean square plume size in the transverse (horizontal) direction. Dividing by the downward velocity $d\langle z \rangle/dt$ of plume movement yields the transverse dispersivity

$$\alpha_T = \frac{D_T}{(d\langle z \rangle / dt)} \quad (8).$$

Equations analogous to (7, 8) are used to calculate longitudinal dispersivities. Table 1 gives specifications for a test problem that involves infiltration of water at ambient

Table 1. Parameters for test problems with detailed explicit heterogeneity.

Permeability Porosity	$k = 10^{-11} \text{ m}^2$ $\phi = 0.35$
Relative Permeability	
van Genuchten function (1980) $k_{rl} = \sqrt{S^*} \left\{ 1 - \left(1 - [S^*]^{1/\lambda} \right)^\lambda \right\}^2$ irreducible water saturation exponent	$S^* = (S_l - S_{lr}) / (1 - S_{lr})$ $S_{lr} = 0.15$ $\lambda = 0.457$
Capillary Pressure	
van Genuchten function (1980) $P_{cap} = -(\rho_w g/a) \left([S^*]^{-1/\lambda} - 1 \right)^{1-\lambda}$ irreducible water saturation exponent strength coefficient	$S^* = (S_l - S_{lr}) / (1 - S_{lr})$ $S_{lr} = 0.0 \text{ or } 0.15$ $\lambda = 0.457$ $a = 5 \text{ m}^{-1}$
Geometry of Flow Domain	
2-D vertical (X-Z) section width (X) depth (Z) gridding	20 m 15 m 80 x 120 = 9600 blocks $\Delta X = .25 \text{ m}$ $\Delta Z = .125 \text{ m}$
heterogeneity: stochastic distribution of impermeable obstacles	
Initial Water Saturation	
for $6.5 \leq X \leq 13.5 \text{ m}$ and $-3.5 \leq Z \leq 0 \text{ m}$ remainder of domain	$S_l = 0.99$ $S_l = 0.15$

conditions ($T = 15 \text{ }^\circ\text{C}$) into a soil of 10^{-11} m^2 absolute permeability, with embedded impermeable obstacles. A simplified treatment with soil gas as passive bystander at constant pressure is used, corresponding to solving Richards' equation. Results are given in Figs. 3 and 4.

RESULTS

Water infiltration plumes for cases with and without capillary pressures show quite different structure (Fig. 3). When capillary pressures are neglected (or unimportant, as in coarse high-permeable media or large fractures), flow proceeds in the form of narrow fingers (Glass et al., 1989). Capillary suction pressures will tend to dampen out the narrower fingers. Overall, transverse spreading of plumes from medium heterogeneities increases when capillary pressures are included, while longitudinal spreading is seen to diminish (Fig. 4). Transverse dispersivities go through transient changes at early times, then stabilize at nearly constant values. Longitudinal dispersivities on the other hand are

Figure 3. Simulated infiltration plumes in the medium of Fig. 2 after 2×10^5 seconds. The plume on the left is for the case without capillary pressure, the one on the right has a capillary pressure as given in Table 1, with $S_{lr} = 0$. Initially, the plume has a uniform water saturation of $S_l = .99$ and occupies the region indicated by the white rectangle at the top of the figures.

Figure 4. Effective dispersivities for the liquid infiltration plumes of Fig. 3. Transverse (left) and longitudinal (right) dispersivities are shown for cases with increasingly strong capillary pressures: (1) no P_{cap} , (2) P_{cap} with $S_{lr} = 0$, (3) P_{cap} with $S_{lr} = .15$.

seen to stabilize only when capillary effects are included; otherwise they continue to increase with time. Fig. 4 shows that transverse dispersivities stabilize at approximately 1.2, 1.7, and 2 m, respectively, for the cases of (1) no capillary pressure, (2) weaker and (3) stronger capillary pressure.

DISCUSSION

The most important result is that transverse dispersivities stabilize, after a period of transient changes at early times, at nearly constant values. This stabilization occurs regardless of the strength of capillary pressure, and indicates that transverse plume spreading from the intrinsic heterogeneities of the medium indeed gives rise to a Fickian diffusion process. The changes at early times are numerical artefacts, caused by the extreme discontinuity of the initial saturation distribution. For the large initial water saturation of $S_i = .99$ in the plume water flow rates are large, leading to rapid saturation changes which are poorly resolved with the space and time discretization used in our simulation. From the results presented here as well as from many additional simulations we conclude that broad classes of heterogeneous media disperse infiltrating liquid plumes transversally in a Fickian manner.

It should be emphasized that Fickian-type dispersive behavior from medium heterogeneities is by no means inevitable or universal. In fact, for certain heterogeneity conditions and spatial scales infiltration plumes may show "anti-dispersive" behavior, becoming more narrowly focussed with depth (Kung, 1990). Flow behavior depends on the nature of the heterogeneities and the strength of capillary forces. When capillary effects are neglected, our simulations show "anomalous diffusion" behavior for longitudinal dispersion, with dispersivities growing with time.

To further elucidate the interplay between heterogeneity and capillarity, we have in Fig. 5 plotted transverse capillary dispersivities calculated from Eq. (6) for the medium of

Figure 5. Transverse capillary dispersivities for a typical soil with permeability $k = 10^{-11} \text{ m}^2$. Two curves are shown, for weaker ($S_{lr} = 0$) and stronger ($S_{lr} = .15$) capillary pressure. Dispersivity is proportional to the anisotropy ratio of horizontal to vertical permeability, which is here assumed as 6.41, appropriate for the medium in Fig. 2.

Fig. 2. The applicable anisotropy ratio was determined by running single-phase horizontal and vertical flow simulations to steady state. Effective horizontal and vertical permeabilities were found to be $k_h = 7.50 \times 10^{-12} \text{ m}^2$ and $k_v = 1.17 \times 10^{-12} \text{ m}^2$. Accordingly, the data in Fig. 5 are plotted for an anisotropy ratio of $k_h/k_v = 6.41$. For the function with $S_{lr} = 0$, transverse capillary dispersivity is seen to be approximately 0.5 m over a wide range of saturations. This value agrees closely with the difference between transverse dispersivities with (for $S_{lr} = 0$) and without capillary effects (Fig. 4), indicating that heterogeneity- and capillary-derived transverse dispersivities are additive.

Capillary dispersivities are expected to correlate inversely with permeability. For aqueous liquids, a rough estimate for the dependence of transverse capillary dispersivity on horizontal and

vertical soil permeabilities k_h , k_v may be given from the data shown in Fig. 5, using Leverett's scaling relationship $P_{cap} \propto k^{-1/2}$ in Eq. (6) (Scheidegger, 1974). We obtain

$$\alpha_{cap,T} \approx \frac{k_h}{k_v} \sqrt{\frac{10^{-11} \text{ m}^2}{k_h}} \times .08 \text{ m} \quad (9).$$

For nonaqueous phase liquids (NAPLs) capillary pressures are usually weaker. Dispersive effects of permeability heterogeneity are expected to be similar for aqueous and nonaqueous phase liquids. With capillary dispersivities being smaller for NAPLs, we expect that heterogeneity-derived dispersion would become relatively more important than it is for aqueous liquids.

CONCLUSIONS

Liquid phases infiltrating in the unsaturated zone disperse from capillary effects and from medium heterogeneities. Our high-resolution numerical simulation experiments suggest that for broad classes of medium heterogeneities transverse fluid phase dispersion tends to be Fickian. Further numerical and physical experiments, and field observations, are needed to determine the range of heterogeneity conditions under which the Fickian dispersion model is applicable.

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