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APPROACHES TO MODELING UNSTABLE FLOW AND MIXING OF VARIABLE OF DENSITY FLUIDS

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ABSTRACT

Density Variation of aqueous phase fluids flowing in a porous medium, resulting from spatial and temporal variation of solute concentration, often gives rise to unstable flow, and therefore has a significant effect on solute transport. Studies on simulating unstable flow and mixing of variable density fluids in seemingly homogeneous porous media are rare. In this study, one dimensional (1-D) model were developed to simulate unstable flow and mixing in a vertical, normally 1-D system. The 1-D numerical model was derived from a theoretical model to simulate the flow and the mixing of fluids with variable density and viscosity at the field scale. To evaluate the models, simulated results were compared with experimental data from displacement experiments in a vertical send column. The results show that the 1-D model provides fairly good prediction of breakthrough curves.

KEYWORDS: Groundwater, Gravitational Instability, Fingering, Variable Density Fluids

Mathematics Subject Classification: 76DXX

1. INTRODUCTION

While considerable advances have been made in understanding the influence of heterogeneity of porous media on solute transport, less attention has been given to the dependence of solute transport on the density variation of the fluid, especially when gravitational instabilities occur(Given et al . ,1992 ;Welty and Gelhar ,1991).Significant variation of aqueous phase fluid density may occur, e.g., in seawater intrusion into costal aquifers(Huyakorn et al. ,1987),transport of solute due to agricultural practies(Mulqeen and Kirkham, 1972),gravity sinking of contaminant plumes(Kimmel and Braid ,1980),and fluid fleow near salt domains and bedded salt deposits(Herbert et al.,1988).Based on the behaviour of some lechat eplumes in the Nrtherlands, van der Molen and van Ommen (1988) concluded that density effects probably more common than usually assumed.

While numerous laboratory studies have shown that density varations can result in significant flow and mixing in porous media (Wooding,1959,1962 Bachmat and Elrick,1970)Bigger and Nilesen,1964.Krupp and ELrick,1969, Rose and Passioura,1971 ; Oostrom et al,1992a,1992b;Schincariol and Schwartz,1990;Hayworth.1993; and Dane et al.,1994a), numerical model studies of unstable flow and mixing of variable density fluids are much scarer (Elder,1967;koch and Zhang, 1991;Schincariol et al ,1994; Dane et al.,1994b).In constrast, considerable attension has been given to numerical model studies of viscous fingering(instability), especially in the chemical and petroleum engineering literature(Chang and Slattery,1988,1990).Although the behaviour of gravitational instability is similar to that of viscous fingering, considerable differences exist, as will be discussed later.

In this study we will focus on two numerical approaches to simulate unstable flow and mixing of a variable density fluid in normally one-dimensional (1-D) homogeneous porous medium.

The approach is to simulate unstable flow and mixing in a normally 1-D system with a 1-D, coarse spatial discretization. In this approach, instabilities are considered as a larger scale dispersion process and flow and transport are viewed to be 1-D. The apparent dispersivity, therefore is afunction of the despersivity of an 'ideal' tracer, fluid properties and other related variables (Young, 1990). Since the fine spatial discretization approach is very computational intensive, and is difficult to be used in large scale problems, the coarse spatial discretization approach is more attractive for practical problems. The key to this approach is the development of an appropriate expression for the apparent dispersivity . Recently, an essentially 1-D theoretical model to simulate field scale flow and mixing of variable density and viscosity fluids, based on a stochastic analysis, was developed by Welty and Gelhar(1991,1992). The second objective of this research is, therefore, to develop an empirical 1-D model to simulate unstable flow and mixing due to the fluid density variation in a seemingly homogenous porous medium.

2.1-D SIMULATION MODEL

Before deriving the 1-D simulation model, we need to identity three length scales involved in the column displacements experiments, viz., the laboratory scale, the continuum scale and the pore scale.The laboratory scale is defined by the size of the column. The continuum scale is characterized by a REV (Bear,1972), while the pore scale is related to the size of the pore. Although the continuum approach, on which the governing equations for solute transport and fluid are based, widely accepted, the concept of a REV is still an issue of debate(Baveye and Sposito,1984). The dispersivity for a perfectly homogenous porous medium at the continuum scale is considered to result from pore scale heterogeneity (Gűven and Molz, 1988). The existence of a perfectly. Homogenous porous medium at the continuum scale can, however, be questioned. Welty and Gelhar(1991) pointed out that all sands exhibitsome degree of heterogeneity. Evidence of heterogeneity in a carefully packed sand column was given by Oostrom et al. (1992a). They employed a gamma radiation technique to determine *in situ* BTCs and a similar method as used in this study to determine effluent BTCs. For stable displacements, they showed that the logitudinal dispersivities, derived from *in situ* BTCs, were consistently smaller than those derived fronm effluent BTCs. Since the measuring scale of the gamma raditation technique is a scale betweem the continuum and the laboratory scale, the difference between measured dispersivities indicates the existence of continuum scale heterogeneity. The measured laboratory scale dispersivity, therefore, results from both pore scale and continuum scale heterogeneities.

Due to the complexity of interaction between the porous medium heterogeneities at several scales and the density variation of fluids, it is very difficult, if not impossible, to derive a theoretical expression for the apparent dispersivity in a seemingly homogenous porous medium. In this study we assumed that a similar relation as between the apparent and the 'ideal' tracer dispersivity at the field scale, developed by Welty and Gelhar(1991), can be applied to solute transport problems in a seemingly homogenous porous medium at the laboratory scale. In the derivation of this expression, we made no distinction between the notation of the field scale and the corresponding laboratory scale variables, except for the despervities. Following Welty and Gelhar (1991), the expression for apparent dispersivity at the field scale can be written as

$$\alpha_L = \alpha_L{}^0 e^{-2a_1} \quad (2.1)$$

Where

$$\beta = \frac{d\left(ln\frac{1}{\mu}\right)}{dc} \tag{2.2}$$

$$z^* = \frac{qt}{n}, \tag{2.3}$$

$$G_1 = -\frac{\partial c}{\partial z\prime} \tag{2.4}$$

Where α_L and $\alpha_L{}^0$ are the apparent longitudinal dispersivity and the longitudinal diapersivity for the ideal tracer at the field scale ,respectively,c is the mean contration at depth z' , z' is the vertical distance in the porous medium (porosity downward and z'= 0 at the top of the porous medium),t is the time,γ is the approximately constant flow factor (Wetly and Gelhar ,1991),ρ is the mean fluid density at depth z' ,μ is the mean liquid viscosity at depyh z' ,k is the mean permeability at depth z',g is the gravitational field strength ,q is the Darcy flux and n is the porosity .A detailed derivation of equation can be found in Welty and Gelhar (1991).It should be noted that several variables in the 1-D model are averaged ones over the horigental croos section of the vertical ,nominally 1-Dsystem.

Substituting the expressions for and into Equation yields:

$$a_1 = z^*\left[\frac{1}{\gamma\mu}\ \frac{\partial\mu}{\partial z'}\ + \frac{kg}{\mu q}\ \frac{\partial\mu}{\partial z'}\right] \tag{2.5}$$

If the viscosity gradient effect on solute transport is assumed to be negligible (Galeati et al., 1992), Equation can be rewritten as

$$a_1 = z^*\frac{kg}{\mu q}\ \frac{d\rho}{dc}\frac{\partial c}{\partial z'} \tag{2.6}$$

If we then approximate $\frac{d\rho}{dc}$ by

$$\frac{d\rho}{d\mu} \approx \frac{\rho_{max} - \rho_0}{c_{max}} = \frac{\Delta_\rho}{c_{nax}} \tag{2.7}$$

Where c_{max} and ρ_{max} are the concentration and the corresponding density of the solution introduced at the porous medium, and ρ_0 is the density of the background fluid (pure water), can be expressed as

$$a_1 = z^*\pi^* \frac{\partial\left(\frac{c}{c_{max}}\right)}{\partial z'} \tag{2.8}$$

Where

$$\pi^* = \frac{K\frac{\Delta_\rho}{\rho_0}}{q} \tag{2.9}$$

and

$$K = \frac{kg\rho_0}{\mu} \tag{2.10}$$

Combining Equation (2.1) and (2.8), we obtain

$$\frac{\alpha L}{\alpha L^0} = e^{-\frac{-2z^*\pi^*\left(\partial\left(\frac{c}{c_{max}}\right)\right)}{\partial z'}} \tag{2.11}$$

Based on the assumption about dispersivity relation at the field and the laboratory scale, we have

$$\frac{\alpha_1}{\alpha_1{}^0} = e^{-\frac{-2z^*\pi^*\left(\partial\left(\frac{c}{c_{max}}\right)\right)}{\partial z'}} \tag{2.12}$$

Where α_1 and $\alpha_1{}^0$ are the apparent longitudinal dispersivity and the longitudinal dispersivity for the ideal tracer at the laboratory scale, respectively.

The 1-D governing equation to modal solute transport at the laboratory scale is

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial z'^2} - \beta\frac{\partial c}{\partial z'} \tag{2.13}$$

Where D is the apparent dispersion coefficient for variable density fluid at the laboratory scale:

$$D = \alpha_1\frac{q}{n} + D_0 \tag{2.14}$$

$$\beta = \frac{q}{n} \tag{2.15}$$

$$D = \alpha_1 \beta + D_0 \tag{2.16}$$

Where D_0 is the molecular diffusion coefficient .Subject to the boundary and initial condition, Equation (2.13), coupled with the expression for the apperant dispersion coefficient, can be solved numerically by Ritz approximation method. With initial and boundary conditions are:

$$c(0,t) = c_0 \text{ at } z' = 0;\ t > 0 \tag{2.17}$$

$$c(1,t) = c_1 \quad \text{at } z' = 1;\ t > 0 \tag{2.18}$$

$$c(z', 0) = \theta\varepsilon << 1 \quad \text{at } z' > 0;\ t = 0 \tag{2.19}$$

$$\frac{\partial c}{\partial z'} = 0\ ;\ z' = 0 \text{ and } \frac{\partial c}{\partial z'} = 0\ ;\ z' = 1 \text{ at } t \geq 0 \tag{2.20}$$

3. SOLUTION BY RITZ APPROXIMATION METHOD

Step: 1 The weak form of the Equation is

$$\int V \frac{dc}{dt}\, dz' + D \int \frac{dV}{dz'} \frac{\partial c}{\partial z'}\, dz' + \beta \int V \frac{\partial c}{\partial z'}\, dz' - D.V.\frac{\partial c}{\partial z'} \Big|\, z' = 0 +$$

$$0 = D.V.\frac{\partial c}{\partial z'} \Big|\, z' = 1 \tag{3.1}$$

Putting V = $\emptyset_i$; i=1, 2 which satisfies the boundary conditions.

Step:2 We must select v = ϕi ; i = 1, 2 in the two-parameter Ritz approximation to satisfy the boundary conditions ϕi (0) = C_0, ϕi (1) = C_1 ; i = 1, 2. We choose the following functions as,

$$\emptyset_1\ (z') = (C_1 - C_0)\ z' + C_0$$

and

$$\emptyset_2\ (z') = (C_1 - C_0)\ z'^2 + C_0 \tag{3.2}$$

The Ritz method seeks an approximate solution to equation (2.5) in the form of a finite series

$$c\,(z', t) = a_1(t)\,\emptyset_1\ (z') + a_2(t)\,\emptyset_2\ (z') \tag{3.3}$$

Where the constants bj ; j = 1,2 called Ritz coefficients are chosen such that equation (3.1) holds for v = ϕi ; i = 1,2.

Step: 3 Substituting the values from equation (3.3) with v = ϕi ; i = 1,2 in the equation (3.1). We get Ritz equation as,

$$a_1' A_{11} + a_2' A_{12} + a_1 B_{11} + a_2 B_{12} + \beta\, a_1 E_{11} + \beta\, a_2 E_{12}$$

$$-D\,\phi_1 (a1\,\phi_1' + a_2\phi_2')\,\Big|_{z'=0} + D\,\phi_1 (a1\,\phi_1' + a_2\phi_2')\,\Big|_{z'=1} = 0 \tag{3.4}$$

and

$a_1' A_{21} + a_2' A_{22} + a_1 B_{21} + a_2 B_{22} + \beta a_1 E_{21} + \beta a_2 E_{22}$

$$-D \phi_2 (a_1 \phi_1' + a_2\phi_2') \Big|_{z'=0} + D \phi_2 (a_1 \phi_1' + a_2\phi_2') \Big|_{z'=1} = 0 \qquad (3.5)$$

Where

$$a_1' = \frac{\partial a_1}{\partial t} ; \qquad a_2' = \frac{\partial a_2}{\partial t}$$

$$\phi_1' = \frac{\partial \phi_1}{\partial z'} ; \qquad \phi_2' = \frac{\partial \phi_2}{\partial z'} \qquad (3.6)$$

$$Aij = \int_0^1 \phi i \cdot \phi j \, dz' ; \quad i, j = 1, 2 \qquad (3.7)$$

$$Bij = \int_0^1 \phi i' \cdot \phi j' \, dz' ; \quad i, j = 1, 2 \qquad (3.8)$$

$$Eij = \int_0^1 \phi i \cdot \phi j' \, dz' ; \quad i, j = 1,$$

Step: 4 Simplification of equation (3.4) and (3.5) with the help of Aij, Bij and Eij ; i, j = 1, 2 is given by

$$a_1'\left(\frac{c_1^2 + c_0c_1 + c_0^2}{3}\right) + a_2'\left(\frac{3c_1^2 + 4c_0c_1 + 5c_0^2}{12}\right) + a_1\left(\frac{c_1^2 - c_0^2}{2}\right)$$
$$+ a_2\left(c_0^2 - c_1^2 + \frac{(c_1 - c_0)(2c_1 + c_0)}{3}\right) = 0 \qquad (3.9)$$

and

$$a_1'\left(\frac{3c_1^2 + 4c_0c_1 + 5c_0^2}{12}\right) + a_2'\left(\frac{3c_1^2 + 4c_0c_1 + 8c_0^2}{15}\right) + a_1\left(\frac{(c_1 - c_0)(2c_0 + c_1)}{3}\right)$$
$$+ a_2\left(\frac{(c_1^2 - c_0^2)}{2} + \frac{4c_0^2 - 2c_0c_1 - 2c_1^2}{3}\right) = 0 \qquad (3.10)$$

Step: 5 the residual of the approximation in the initial condition is

$$y = C(z', 0) - \varepsilon \tag{3.11}$$

Using the Galerkin method, we have

$$\int_0^1 [C(z', 0) - \varepsilon]\,\phi i = 0;\quad i = 1, 2 \tag{3.12}$$

means

$$\frac{a_1(0)}{3}\left[C_1^2 + C_0C_1 + C_0^2\right] + \frac{a_2(0)}{12}\left[3C_1^2 + 4C_0C_1 + 5C_0^2\right] - \frac{\varepsilon C_1}{2} - \frac{\varepsilon C_0}{2} = 0 \tag{3.13}$$

and

$$\frac{a_1(0)}{12}\left[3C_1^2 + 4C_0C_1 + 5C_0^2\right] + \frac{a_2(0)}{15}\left[3C_1^2 + 4C_0C_1 + 8C_0^2\right] - \frac{\varepsilon C_1}{3} - \frac{2\varepsilon C_0}{3} = 0 \tag{3.14}$$

We obtain approximate initial conditions

$$a_1(0) \cong 0.0044 \quad \text{and} \quad a_2(0) \cong -0.0036 \tag{3.15}$$

Step: 6 We can solve the ordinary differential equation (3.9) and (3.10) subject to the initial condition (3.15) by exact means. Using Laplace transform method we obtain

$$L\{a_1\} = \frac{0.1667046}{(p+146.79459)^2 - 146^2}\; L\{a_2\} = \frac{0.000991}{(p-0.3557505)^2 - 1.2335^2}$$

Inverting and, we get

$$a_2 = (0.000991)e^{0.3557505.t}\, sinh(1.2335.t)$$

$$a_1 = (0.0011418)e^{-146.79459.t}\, sinh(146.t)$$

Step: 7 Required Solution of the problem is

$$C(z', t) = (0.001016202)e^{-146.79459.t}\, sinh(146.t)\,.\,z'$$

$$+(0.00088199)e^{0.3557505.t}\, sinh(1.2335.t)z'^2$$

The following values of the various parameters have been considered in the present analysis and for graphical representation

$C_0 = 0.01$, $C_1 = 0.9, \varepsilon = 0.001$

4. GRAPHICAL AND NUMERICAL REPRESENTATION

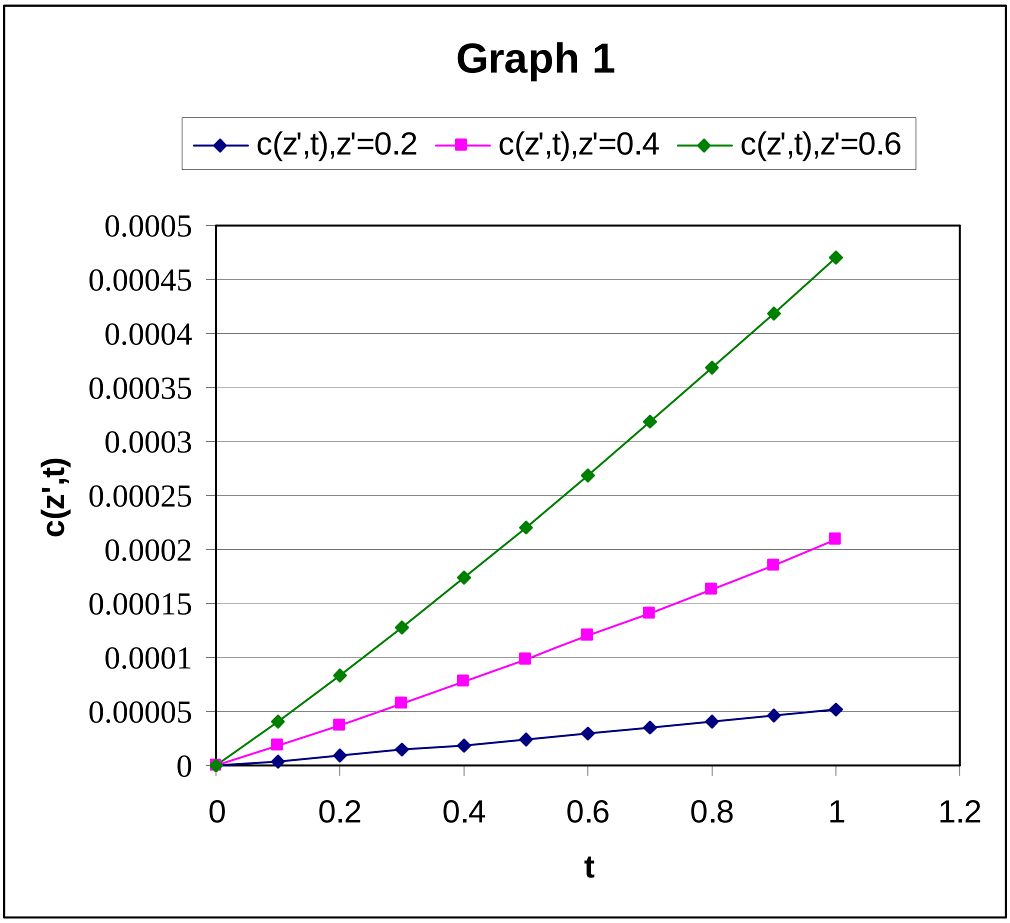

Table: 1

t	c(z',t),z'=0.2	c(z',t),z'=0.4	c(z',t),z'=0.6
0	0	0	0
0.1	4.49827E-06	1.79925E-05	4.04827E-05
0.2	9.253E-06	3.7012E-05	8.3277E-05
0.3	1.4213E-05	5.6852E-05	0.000127917
0.4	1.93327E-05	7.73308E-05	0.000173994
0.5	2.45778E-05	9.83112E-05	0.0002212
0.6	2.99259E-05	0.000119703	0.000269333
0.7	3.53652E-05	0.000141461	0.000318287
0.8	4.08926E-05	0.00016357	0.000368034
0.9	4.65112E-05	0.000186045	0.000418601
1	5.22282E-05	0.000208913	0.000470054

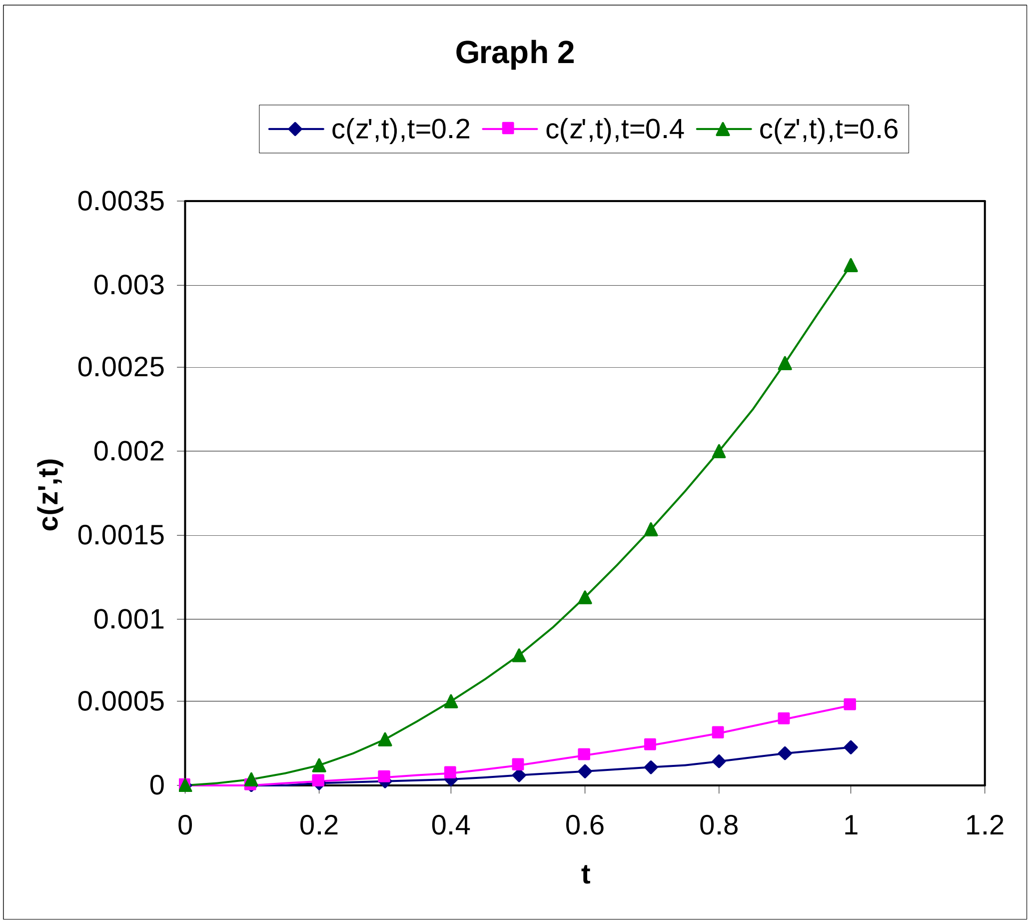

Table: 2

z'	c(z',t),t=0.2	c(z',t),t=0.4	c(z',t),t=0.6
0	0	0	0
0.1	2.31325E-06	4.83317E-06	3.12203E-05
0.2	9.253E-06	1.93327E-05	0.000124881
0.3	2.08193E-05	4.34986E-05	0.000280983
0.4	3.7012E-05	7.73308E-05	0.000499525
0.5	5.78313E-05	0.000120829	0.000780508
0.6	8.3277E-05	0.000173994	0.001123932
0.7	0.000113349	0.000236826	0.001529796
0.8	0.000148048	0.000309323	0.001998101
0.9	0.000187373	0.000391487	0.002528846
1	0.000231325	0.000483317	0.003122032

5. CONCLUSIONS

A 1-D modal to simulate unstable flow and mixing of variable density fluids in a vertical ,normaly 1-D system ,filed with a seemingly homogenous porous medium ,were developed .To evaluate theSimulation models ,displacement experiments were condected in a vertical column filled with either a fine or a medium sand.

- The experimental results demonstrated that the dispersion zone

- Increased with decreasing Darcy flux for a given input solute concentration.

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