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MOVEMENT OF DENSE PLUMES IN VARIABLY SATURATED POROUS MEDIA: NUMERICAL MODEL AND RESULTS

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Summary. Accidentally spilled leachate from sanitary landfills can have total dissolved solid concentrations up to 40,000 mg/L. As a result, leachate fluids have a significantly higher density than water found in both the unsaturated and saturated subsurface. Leachate spilled on the soil or released at the bottom of disposal sites will therefore be transported by variable-density flow through the unsaturated soil zone, and eventually reach the saturated groundwater zone. To better understand plume transport in the subsurface, Simmons et al. (2002) have performed laboratory experiments in a sand-filled glass tank under both fully saturated and variably-saturated flow conditions. In the present study, a new numerical model is developed to simulate the movement of dense fluid under variably saturated conditions. The new model is based on the existing HydroGeoSphere model, and it is verified for two-dimensional unsaturated-saturated variable-density flow and transport in porous media using the unsaturated flow version of the Elder (1967) problem defined by Boufadel et al. (1999). The new model can alternatively apply the first or second level of the Oberbeck-Boussinesq (OB) assumptions for variable-density flow. Numerical simulations are performed that focus on the usefulness of the OB assumptions when simulating the laboratory experiments done by Simmons et al. (2002). Simulations suggest that salt fingers tend to coalesce earlier when applying OB2, and that OB1 is more suitable to simulate variable-density flow.

1 INTRODUCTION

Understanding variable-density flow and transport under unsaturated-saturated conditions is important, and there are a number of examples where these processes are significant, including: (i) spilled leachate from sanitary landfills, (ii) agricultural activities, (iii) flooding of coastal areas by saltwater, (iv) dense fluid flow below salt lakes, and (v) hazardous waste injection. Comprehensive review articles by Diersch and Kolditz (2002) and Simmons (2005) clearly illustrate the widespread importance, diversity and interest in applications of variable-density flow phenomena in groundwater hydrology.

Mathematical groundwater models have become useful tools to study complex physical processes. Even though fluid density can greatly vary, a common modeling assumption is to neglect spatial density differences in the continuum equations and to only account for density effects in the buoyancy term of Darcy's equation. This simplification is called the first level of the Oberbeck-Boussinesq (OB) assumption (Oberbeck, 1879; Boussinesq, 1903), and the more general formulation that accounts for spatial density differences is called the second level of the OB assumption. Although the OB assumption "has not been completely justified" (Joseph, 1976), it has been adapted in a number of variable-density flow studies (e.g. Evans and Raffensperger (1992), Graf and Therrien (2005), Kolditz et al. (1998)). Referring to the OB assumption 1, Joseph (1976) also states "that there is no special reason besides our lack of proofs to doubt the validity of the nonlinear OB-equations".

The usefulness of the OB assumptions has previously been tested numerically (Kolditz et al., 1998). However, numerical results of variable-density flow are known to be a function of the computer code that solves the density-problem (Simpson and Clement, 2003). As high-quality laboratory results of variable-density flow are available (Simmons et al., 2002), this paper examines the usefulness of the OB assumptions by comparing numerical modeling results with experimental results. This is the first study that discusses the usefulness of OB assumptions based on laboratory modeling results. The HydroGeoSphere model is further developed to apply and test OB1 and OB2.

2 NUMERICAL MODEL

2.1 Model Development

HydroGeoSphere is a numerical variable-density, variably saturated flow and solute transport model for fractured porous media, and is based on the FRAC3DVS model (Therrien and Sudicky, 1996; Graf and Therrien, 2005). Because the unchanged HydroGeoSphere model only accounts for OB assumption 1, it is further developed here to simulate with OB assumption 2. Thus, emphasis is put on the ability of the new model to simulate high-density fluid flow.

2.2 Governing equations

The enhanced model employs the freshwater pressure head ψ_0 [L] as flow variable, and fluid flow velocity is calculated using an unsaturated version of Darcy's law given by (Bear, 1988)

$$\mathbf{q} = -\mathbf{K}_0 k_{rw} \frac{\mu_0}{\mu} \cdot \left(\nabla \psi_0 + \frac{\rho}{\rho_0} \nabla z \right) \tag{1}$$

where

$\mathbf{q}$	[L T^{-1}]	Darcy flux vector
$\mathbf{K}_0$	[L T^{-1}]	Reference hydraulic conductivity of rock matrix; $\mathbf{K}_0 = \mathbf{k}\rho_0 g/\mu_0$
$\mathbf{k}$	[L^2]	Intrinsic permeability
k_{rw}	[–]	Relative permeability
μ_0	[M L^{-1} T^{-1}]	Reference fluid viscosity
μ	[M L^{-1} T^{-1}]	Fluid viscosity
∇	[L^{-1}]	Nabla operator
ρ_0	[M L^{-3}]	Reference fluid density
ρ	[M L^{-3}]	Fluid density
g	[L T^{-2}]	Gravitational acceleration
z	[L]	Gravitational head

In the enhanced HydroGeoSphere model, fluid flow is described by two different flow equations (2) and (3). The continuity equation is used to formulate the conservation of fluid mass (water mass and solute mass), and it fully accounts for spatial and temporal density variations, which is known as the second level of the OB assumption:

$$\text{OB2:} \qquad -\nabla \bullet \{\rho \mathbf{q}\} = \frac{\partial(\rho \phi S_w)}{\partial t} \tag{2}$$

where

ϕ	[–]	Aquifer volumetric porosity
S_w	[–]	Degree of water saturation
t	[T]	Time

A common simplification of Eq. (2) is to neglect density variations in the flow equation, which is only correct when density variations are small (Evans and Raffensperger, 1992). This simplification leads to the first level of the OB assumption written as

$$\text{OB1:} \qquad -\nabla \bullet \{\mathbf{q}\} = \frac{\partial(\phi S_w)}{\partial t} \tag{3}$$

The unsaturated model to calculate S_w and k_{rw} is that presented by van Genuchten (1980). Fluid density is calculated using a linear function, and viscosity is calculated using a polynomial function of the form

$$\mu = \mu_0 \cdot \sum_{i=0}^{6} a_i c^i \tag{4}$$

Solute transport is described by the solute mass conservation equation (Bear, 1988)

$$\nabla \bullet \{\phi S_w \mathbf{D} \nabla c - \mathbf{q} c\} = \frac{\partial(\phi S_w c)}{\partial t} \tag{5}$$

which is independent of fluid density variations for both OB assumptions 1 and 2. The hydrodynamic dispersion tensor is given by $\mathbf{D}$ [L^2 T^{-1}].

2.3 Model Verification

The new model was verified using the unsaturated version of the Elder problem (Elder, 1967) presented by Boufadel et al. (1999), where the water table is kept constant at half domain height (z=75 m), and where the conceptual model is shown in Fig. 1. Simulation parameters are given in Boufadel et al. (1999). That test case has been used here to verify both OB assumptions as well as both viscosity assumptions (constant: $\mu = \mu_0$; variable: Eq. 4) of the new HydroGeoSphere model presented here.

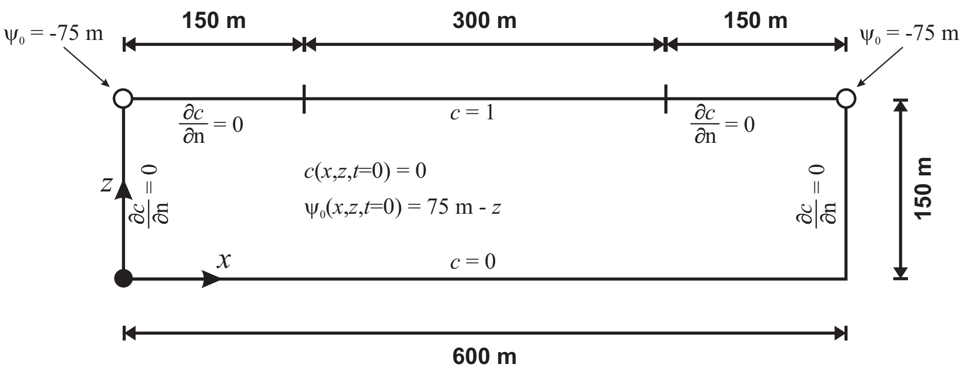

Figure 1: Conceptual model for the Elder problem (Voss and Souza, 1967; Boufadel et al., 1999).

Results of HydroGeoSphere and Boufadel et al. (1999) for the test case are shown in Fig. 2. The figure indicates that convective patterns, number of fingers and central flow directions are identical, and that concentration contours and saturation contours are mostly identical.

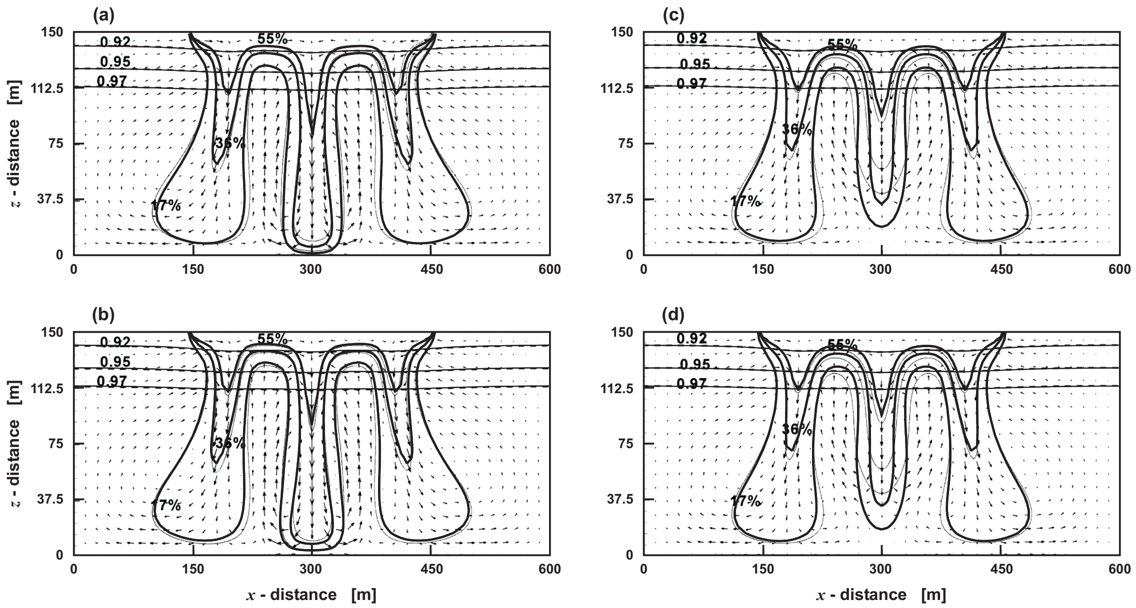

Figure 2: Results of the unsaturated-saturated Elder problem after 10 years using different Oberbeck-Boussinesq (OB) assumptions and different viscosity functions: (a) OB1-constant-viscosity, (b) OB2-constant-viscosity, (c) OB1-variable-viscosity, (d) OB2-variable-viscosity. Bold concentration contours and solid saturation contours are from HydroGeoSphere; thin concentration contours and dashed saturation contours are from Boufadel et al. (1999).

3 PHYSICAL MODEL

3.1 Definition of the Physical Model

Simmons et al. (2002) have performed experiments in a sand-filled 2-D glass tank under both fully saturated and variably-saturated flow conditions. The focus was put on the processes that occur at the capillary fringe and below the water table as dense contaminant plumes migrate through the unsaturated zone. Source fluids stained with Rhodamine-WT were introduced at the upper boundary of the tank at a wide range of fluid densities. The conceptual model is shown in Fig. 3.

3.2 Validity of OB Assumptions

Saturated plume transport of the experimental model is numerically simulated with HydroGeoSphere using OB1 and OB2. The model domain is discretized by 500×500 rectangular elements. The time domain is divided into adaptive time steps. Flow and transport equations are coupled through a Picard iteration scheme. Fig. 4 exhibits results of the laboratory experiment as well as of both numerical simulations. Clearly, the numerical model reproduces the experiments reasonably well for both OB assumptions. The number of fingers decrease with time, which is correctly simulated. Also, the depth of penetration of dense solute fingers into the sand tank corresponds to that simulated in the laboratory. Differences, however, can be observed when inspecting the width of the solute fingers. While OB1 (central panels) seems to adequately reproduce the finger width, OB2 appears to merge fingers faster than OB1. Therefore, OB2 generates fewer and wider fingers, which corresponds to reduced density- and concentration gradients. Reduced concentration gradients can be explained by expanding the left hand side of Eq. (2) to $-\mathbf{q} \bullet \nabla \{\rho\} - \rho \nabla \bullet \{\mathbf{q}\}$ and by recognizing that the spatial density difference $\nabla \{\rho\}$ in the first term of the expanded form reduces density gradients and, therefore, reduces concentration gradients and widens solute fingers. Another difference between OB1 and OB2 is the ability to split an existing solute finger into multiple fingers. As reported by Simmons et al. (2002), the tip of solute fingers tends to split as the plume migrates downwards. Clearly, Fig. 4f indicates that OB1 is suitable to simulate finger splitting while OB2 is not.

The new findings are counterintuitive because it could be expected that a more general formulation of the fluid mass balance equation (OB2) leads to more accurate results. It could be speculated that the numerical error inherent to OB1 generates numerical artifacts that are equivalent to pore-scale heterogeneities inherent to the sand body within the tank. Results presented here suggest that the widely used and never rigorously justified OB assumption 1 may indeed be superior when simulating high-density fluid flow. Future studies will also examine the validity of OB1 and OB2 in the simulation of unsaturated variable-density flow.

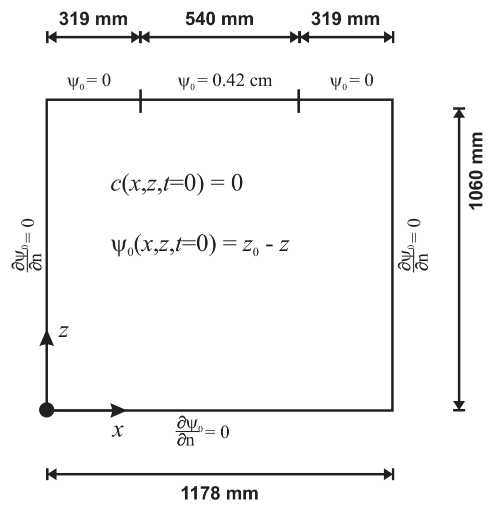

Figure 3: Conceptual model for the laboratory experiment by Simmons et al. (2002). The groundwater table is located at $z_0 = 1060$ mm.

4 CONCLUSIONS

- The HydroGeoSphere model has been expanded here to simulate variable-density flow using both Oberbeck-Boussinesq (OB) assumptions 1 and 2.

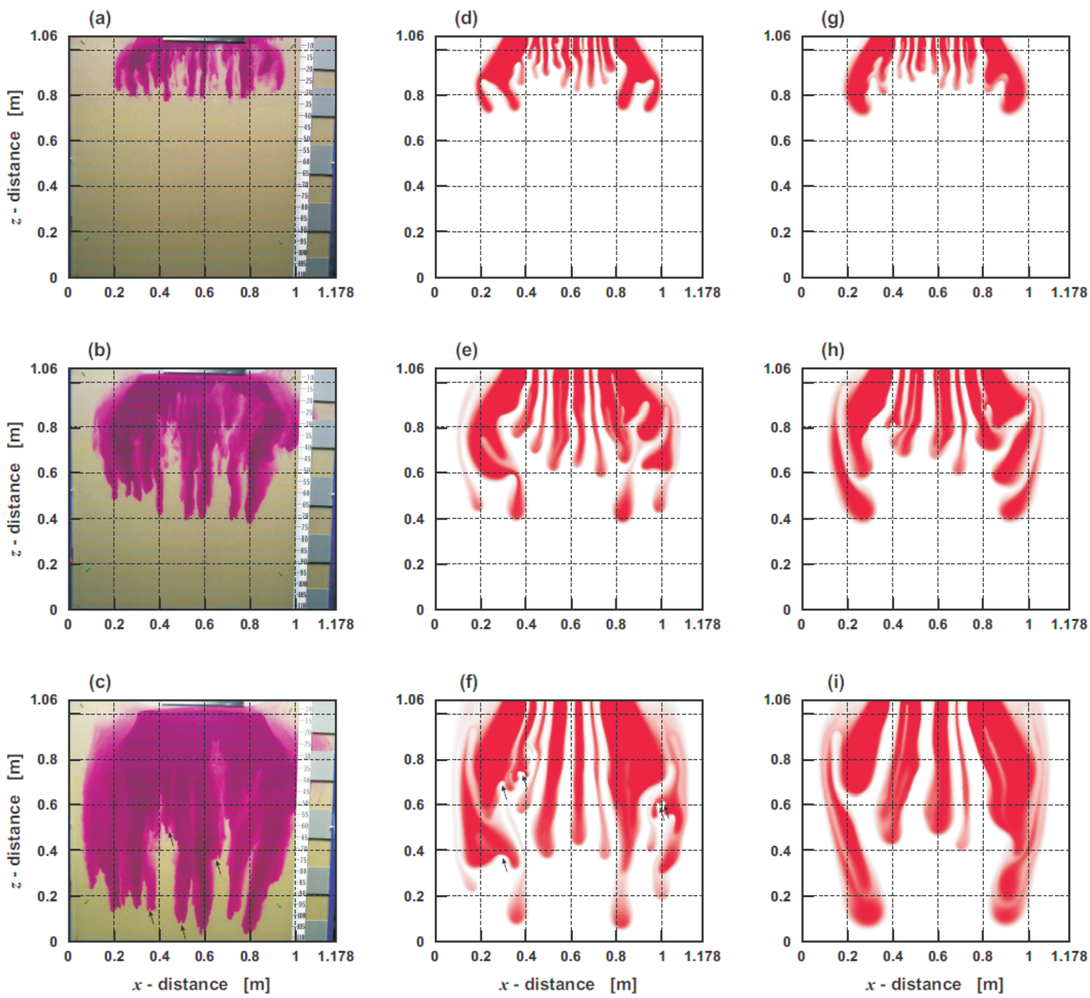

Figure 4: Saturated high-density (SHD) flow: Unstable plume behavior in (a-c) the sand tank laboratory experiment, and (d-i) the unsaturated-saturated transport (HydroGeoSphere) model. Central panels (d-e) are simulated with OB1, right panels (f-i) are simulated with OB2. Elapsed times in (a,d,g), (b,e,h), (c,f,i) are 20, 40, 60 min, respectively, measured from simulation start. Black arrows at 60 min indicate the occurrence of finger splitting.

- A laboratory experiment has been simulated using OB1 and OB2.
- Downwards migration of dense solute fingers is adequately reproduced with OB1 and OB2.
- OB1 adequately reproduces both finger thickness and finger splitting.
- OB2 does not adequately reproduce neither finger thickness nor finger splitting.

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