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Systematic investigation of non-Boussinesq effects in variable-density groundwater flow simulations

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ABSTRACT

The validity of three mathematical models describing variable-density groundwater flow is systematically evaluated: (i) a model which invokes the Oberbeck–Boussinesq approximation (OB approximation), (ii) a model of intermediate complexity (NOB1) and (iii) a model which solves the full set of equations (NOB2). The NOB1 and NOB2 descriptions have been added to the HydroGeoSphere (HGS) model, which originally contained an implementation of the OB description. We define the Boussinesq parameter $\varepsilon_\rho = \beta_\omega \Delta\omega$ where β_ω is the solutal expansivity and $\Delta\omega$ is the characteristic difference in solute mass fraction. The Boussinesq parameter ε_ρ is used to systematically investigate three flow scenarios covering a range of free and mixed convection problems: 1) the low Rayleigh number Elder problem (Van Reeuwijk et al., 2009), 2) a convective fingering problem (Xie et al., 2011) and 3) a mixed convective problem (Schincariol et al., 1994). Results indicate that small density differences ($\varepsilon_\rho \leq 0.05$) produce no apparent changes in the total solute mass in the system, plume penetration depth, center of mass and mass flux independent of the mathematical model used. Deviations between OB, NOB1 and NOB2 occur for large density differences ($\varepsilon_\rho > 0.12$), where lower description levels will underestimate the vertical plume position and overestimate mass flux. Based on the cases considered here, we suggest the following guidelines for saline convection: the OB approximation is valid for cases with $\varepsilon_\rho < 0.05$, and the full NOB set of equations needs to be used for cases with $\varepsilon_\rho > 0.10$. Whether NOB effects are important in the intermediate region differ from case to case.

1. Introduction

Groundwater systems are potentially endangered by salt water intrusion in coastal aquifers, operation of saline water disposal basins and upconing of saline water from deep aquifers (Simmons et al., 2010). As a consequence, potentially unstable situations may exist where a dense fluid overlies a less dense fluid. This situation can produce instabilities that manifest as dense plume fingers that move vertically downwards counterbalanced by vertical upward flow of freshwater elsewhere (Simmons et al., 2002). Resulting free convection increases solute transport rates over large distances and times relative to constant-density flow. The importance of variable-density flow in groundwater hydrology has been reported by various authors (e.g. Oswald and Kinzelbach, 2004; Schincariol and Schwartz, 1990; Simmons et al., 2002). Diersch and Kolditz (2002) reviewed fundamental concepts, state equations, physical processes involved as well as problems used and relevant studies conducted in the field of variable-density flow and transport. Most recently, an extensive evaluation of advances in the field of variable-density flow was given by Simmons et al. (2010), in which physics, modeling approaches as well as future challenges are discussed.

Numerical models are useful tools to investigate variable-density flow and transport. Numerical modeling of variable-density flow and transport is described by the fluid and solute mass conservation equations that are coupled through Darcy's

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equation. A common mathematical assumption to solve the equations is to neglect the spatial and temporal density variations in the fluid and solute mass conservation equations and to only consider density variations in the buoyancy term of the Darcy equation (Frind, 1982; Holzbecher, 1998). This assumption is referred to as the Oberbeck–Boussinesq approximation (OB-approximation) (Boussinesq, 1903; Oberbeck, 1879). The validity of the OB-approximation has been questioned by several authors e.g. (Diersch and Kolditz, 2002; Holzbecher, 1998; Kolditz et al., 1998), who stated that the OB-approximation is not valid when high spatial density variations exist. Non-Boussinesq (NOB) effects can be studied when density variations are accounted for in one (or both) mass conservation equations. Accordingly, Kolditz et al. (1998) defined three physical description levels to represent density variations in the governing equations in order to evaluate the OB (low accuracy) and the NOB effects. Table 1 explains the definition of the OB and of the two NOB levels (NOB1 and NOB2), and gives the corresponding accuracy level for each physical description level. Here "✓" means that spatial and temporal density variations are accounted for in the regarded mass conservation equation and "∅" means that they are not.

Simulations of variable-density flow problems reported in the literature tend to use the various levels of description (OB, NOB1, NOB2) indiscriminately, a sample of which are presented in Table 2. Table 2 shows previously simulated variable-density flow and transport problems at different fluid density contrasts using different physical accuracy levels. Table 2 also shows the maximum fluid density $\rho_{\max}$ and the Boussinesq parameter $\varepsilon_\rho = \beta_\omega \Delta\omega$ used for each problem, where the β_ω is the solutal expansivity (see Section 2 and Eq. (6) for details) and $\Delta\omega$ is the characteristic difference in solute mass fraction. A large variety of cases have been simulated using a wide variety of models. However, a justification for the choice of the physical description level is often not given. OB is easier to include in a computational code but it may not adequately represent large density contrasts. Conversely, NOB1 and NOB2 are more challenging to program but they may not be necessary at low density contrasts. It is still not clear whether one should use OB, NOB1 or NOB2. Therefore a systematic evaluation that studies under what conditions the OB is no longer valid and when higher mathematical accuracy levels (NOB1 or NOB2) have to be applied is necessary.

The main objective of this study is to systematically analyze the validity of the OB and the non-Boussinesq effects (NOB1 and NOB2) used to describe spatial and temporal density variations in variable-density simulations of flow and transport. In order to do so, the HGS numerical model, originally capable of simulating OB conditions, was further developed here to include higher mathematical accuracy levels (NOB1 and NOB2) in the simulation of variable-density flow and transport. A recently obtained pseudospectral solution of a frequently used variable-density flow benchmark problem (Van Reeuwijk et al., 2009) will be used for model verification and testing. A range of density contrasts will be tested in order to determine at which density contrast the non-Boussinesq effects may have to be considered. Resulting differences between the models will be quantified. We will use the problem presented by Van Reeuwijk et al. (2009) defined as the low Rayleigh number Elder problem, the free convection problem presented by Xie et al. (2011) defined as the modified Xie problem and the mixed convection problem presented by Schincariol et al. (1994) defined as the modified Schincariol problem.

This paper is structured as follows. Section 2 describes the governing equations. A description of the HGS numerical model as well as the finite element formulation of the governing equations at NOB2 level implemented in HGS is given. Section 3 explains the nondimensionalization of the governing equations in order to quantify the impact of the non-Boussinesq effects using the ε_ρ. Section 4 focuses on a description of the flow scenarios used for verification of the implementations made to the HGS code and the flow scenarios used for the assessment of the OB, NOB1 and NOB2 models. The OB, NOB1 and NOB2 are diagnosed using the total solute mass in the system, center of mass, penetration depth and mass fluxes at different density contrasts. A mass error (Δ_m) and an L $_2$ norm are defined to asses the differences between the OB, NOB1 and NOB2 diagnostics. A discussion of the results obtained is presented. Finally, in Section 5, conclusions and a summary are given.

Table 1
Oberbeck and non Oberbeck–Boussinesq effects.

	Fluid mass conservation	Solute mass conservation	Accuracy
OB	∅	∅	Low
NOB1	✓	∅	Medium
NOB2	✓	✓	High

2. Mathematical formulation and discretization

2.1. Governing equations

Variable-density flow in aquifers under saturated flow conditions is described by the Darcy equation (Frind, 1982; Kolditz et al., 1998):

$$\mathbf{q} = -\frac{\mu_0}{\mu}\mathbf{K}_0 \cdot \left(\nabla h_f + \frac{\rho - \rho_0}{\rho_0}\mathbf{e}_z\right) \tag{1}$$

where $\mathbf{q}$ [L T^{-1}] is the specific discharge vector, $\mathbf{K}_0 = \rho_0 g \mathbf{k}/\mu_0$ [L T^{-1}] is the equivalent freshwater conductivity, ρ_0 [M L^{-3}] is the reference fluid density, g [L T^{-2}] is the gravitational acceleration, $\mathbf{k}$ [L^2] is the permeability tensor, μ [M L^{-1} T^{-1}] is the dynamic viscosity, μ_0 [M L^{-1} T^{-1}] is the reference dynamic viscosity, ρ [M L^{-3}] is the fluid density, $\mathbf{e_z}$ [−] is a unit vector in the vertical direction and h_f [L] is the equivalent freshwater head (Frind, 1982):

$$h_f = \frac{p}{\rho_0 g} + z \tag{2}$$

where p [M L^{-1} T^{-2}] is the pressure and z [L] is the elevation above datum. The mass conservation equations for the fluid and solute mass fraction ω [−] are given by (Bear, 1988):

$$\frac{\partial \phi\rho}{\partial t} + \nabla \cdot (\rho\mathbf{q}) = 0 \tag{3}$$

$$\frac{\partial \phi\rho\omega}{\partial t} + \nabla \cdot (\rho\omega\mathbf{q}) = \nabla \cdot (\phi\rho\mathbf{D} \cdot \nabla\omega). \tag{4}$$