Numerical implementation of a consistent velocity approximation for variable-density flow and transport in porous media

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Density-driven flows play a major role in various natural and engineering systems. Among other areas of application, variable density flows in permeable solids (porous media) are of central interest in subsurface hydrology, where the effects of variable density are key for the prediction of a series of flow phenomena of technological and environmental impact. Examples include the intrusion of saltwater in exploited coastal aquifers, the upconing of saline waters from deep aquifers, the flow around salt domes used as repositories, the brine transport of pollutants released in rock salt formations, the infiltration of industrial waste disposals, the modeling of flow near pollutant sources where high densities are encountered, the design of geothermal energy extraction systems, the permafrost of magma chambers (Diersch and Kolditz, 2002), and others.

An important issue afflicting the numerical simulation of systems involving variable density flow in porous media is the consistency of the velocity approximation [1]. Most attempts to devise consistent discretization rely on finite elements formulations and involve a considerable computational overhead. For example, Younes et al. [2] and Ackerer and Younes [3] have used a mixed finite element (MFE) method together with Discontinuous Galerkin (DG) and Multipoint Flux Approximation methods (MPFA) to address this issue in heterogeneous flows. The MFE method is locally conservative and produces accurate and consistent velocity fields even for highly heterogeneous domains. However, a MFE naturally results in a directly coupled matrix system with fluxes as primary variables, which increases significantly the number of unknowns [1]. Moreover, the implementation of MFE is generally grid-geometry-dependent, e.g. Ackerer and Younes [3] presented their methodology for triangles, a limitation that implies the use of qualitatively homogeneous cell geometries.

In this work, we present a new finite-volume based consistent discretization method for approximating the Darcy velocity in variable density flow in porous media. The advantages of the proposed descritization when compared to existing consistent schemes are its computational efficiency and the relatively insignificant extra computational complexity that needs to be introduced in existing finite-volume codes.

Here we will show the details of implementing the new scheme in a finite volume unstructured code that uses a collocated discretization of the equations in a node-based formulation. The aim is to show how the new consistent velocity approximation is related to other numerical terms and operators used within the code. This discussion will serve to underline the simplicity with which the new consistent scheme can be implemented, since most of the required numerical operators are already defined and applied throughout the code. This is significant because it shows that a whole class of similar general-use finite volume methodologies could also be easily adapted for consistent porous media computations.

Finally, we validate the new formulation against two benchmark problems where the consistency of the velocity approximation becomes critical: the hydrostatic case and the salt-pool problem [4]. The numerical results are furthermore assessed against an alternative non-consistent formulation (also implemented in the current in-house code for comparison) and against other independent numerical solutions for both test cases. In the case of the salt-pool problem (see Figure 1a), computations using the new consistent formulation reproduce the experimental data, providing the closest agreement with experiments so date. For example, in Figure 1b we show the evolution with time of salt mass fraction (smf) at the outlet of the cubical box for an initial smf=10%. The experimental data are shown as symbols and the current computations as a solid line. Computational results from various other attempts are shown in dashed lines. We will show that the improved agreement with experimental data is obtained primarily due to the new consistent velocity approximation. Still, the effects of grid-refinement and of mathematical model choice also play an important role and will devote part of the presentation to a discussion of these aspects.



Fig[1]: The last-pool problem: (a) experimental configuration [4]; (b) time evolution of the salt mass fraction (smf) at the outlet for an initial smf=10%.

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