TESTING NUMERICAL MODELS OF VARIABLE DENSITY GROUND WATER FLOW: CURRENT TRENDS AND THE RENAISSANCE OF THE HENRY PROBLEM

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Abstract

Current trends in the testing of numerical models for variable density flow by simulating benchmark problems are reviewed. Historical patterns in the establishment of benchmark standards and the subsequent attempts to refine and improve these standards over time seem to be ubiquitous. At the present time, the state-of-the-art benchmark problems involve simulating complicated multi-dimensional problems that rely upon a high degree of computing power and modeling sophistication. In contrast to these newer complex problems, progress is still being made in further understanding the simpler classical test cases. Simpson and Clement (2003, 2004) have made recent contributions to the classical Henry salt-water intrusion test case where the traditional Henry problem was shown to be almost insensitive to density coupling. This limitation was overcome by modifying the problem to decrease the influence of forced convection process. The overlap in the development of newer sophisticated benchmarks together with the improvement of classical benchmarks has resulted in a rich choice of test cases to be considered for model development. The time scale between development and improvement of benchmark standards (~ 40 years for the Henry problem) implies that the science of developing and improving benchmark standards is set to continue well into the future as the controversies associated with the newer test cases are discovered, explored and resolved.

Keywords: Variable density, Henry problem, salt-water intrusion, ground water, numerical modeling

Introduction and review

From the 1960's, the development of benchmark problems for variable density flow algorithms has been pioneered largely through physical and numerical modeling. Recently, the newer benchmark problems have become extremely sophisticated compared to the classical test cases. Within the framework of

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proving numerical models through developing benchmark test cases, certain long-term trends can be identified. Almost without exception, each of the popular benchmark problems devised to date has had some scientific controversy associated regarding the suitability of that problem for model testing. Thus such controversy has led to a continuous series of developments where both new benchmarks have been identified and tested, and, there has been a continual interest in the improvement of the established benchmarks. Although there are several benchmarks available for model testing, discussion here will be limited to the most popular cases.

The classic Henry problem considers steady-state salt-water intrusion, and the problem was solved by the semi-analytical method proposed by Henry (1964). The Henry problem involves intrusion of seawater into a fresh water aquifer forming stable density stratification (Figure 1). Henry's problem has been used as the fundamental test case for many numerical codes and has undergone several revisions that have included the use of different dispersion coefficients, both constant (Voss and Souza, 1987) and spatially variable (Frind, 1982), different outflow boundary conditions (Segol *et al.*, 1975), and most-recently different freshwater recharge rates (Simpson and Clement, 2004). Henry's problem was considered controversial until Segol (1994) re-evaluated the semi-analytical solution and updated several issues associated with the original semi-analytical work of Henry. Since this time, numerical analysts have been able to match the numerical and semi-analytical results with the standard problem (Ackerer *et al.*, 1999, Simpson and Clement, 2004).

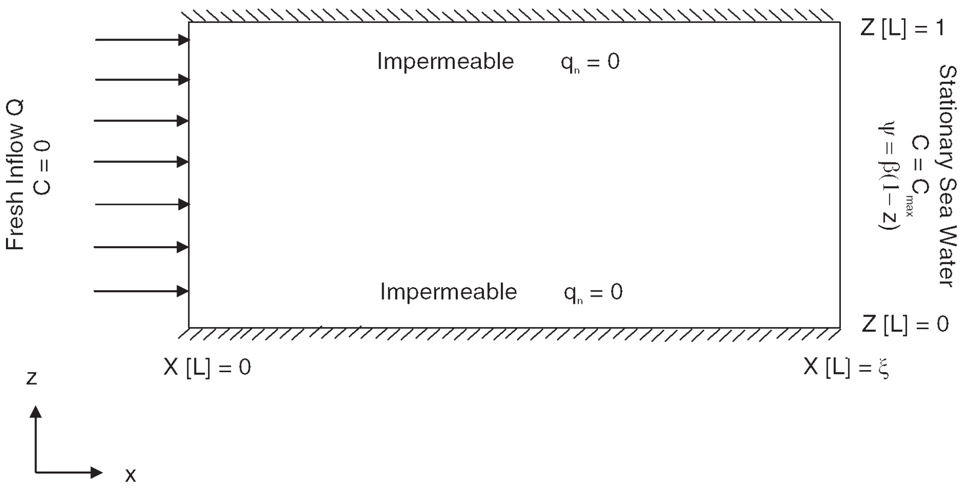

Figure 1. Domain and Boundary Conditions for the Henry salt-water intrusion problem.

Elder's short heater problem, also known as the Elder salt convection problem, is a well-established benchmark that was motivated by laboratory work completed in a Hele-Shaw cell (Elder, 1967). The Elder problem is a two-dimensional, transient, purely free convective driven problem with unstable density stratification. Elder's problem receives a great deal of attention in the literature due to the extreme sensitivity of numerical results (Diersch and Kolditz, 2002). The controversies associated with the Elder problem include the extreme grid sensitivity (Woods *et al.*, 2003), the question of the number of upwelling and down welling lobes (Kolditz *et al.*, 1998) as well discussion concerning the uniqueness of the steady state solution (Frolkovic and De Schepper, 2000). Although the Elder problem has received considerable attention in the variable density ground water modeling arena for a long period of time, new concepts are still being explored using the basic problem as a foundation upon which modifications are proposed. For example, recent advances concerning modifications of the Elder problem include the influence of variably saturated conditions, the influence of variable viscosity (Boudafel *et al.*, 1999) and also the importance of domain heterogeneity upon the generation of and stability of fingering patterns (Prasad and Simmons, 2003). All of these recent advances have been made using the Elder problem as a fundamental basis and subsequent improvements were possible by proposing carefully chosen modifications to the system.

The HYDROCOIN salt-dome problem is also a standard test case for variable density flow algorithms (OECD, 1988). This test case was devised as a theoretical case of brine flow similar to the Elder problem, except that the stratification is stable. The salt-dome problem involves simulating a transient two-dimensional flow regime associated with high-density conditions and a stable density stratification. After the popularization of the salt-dome problem certain controversies were reported regarding the number of overturning cells present in the aquifer. As a result of these controversies, various aspects of simulating this kind of problem were improved through a process of reflecting upon the successes and failures of the previous modeling efforts (Konikow *et al.*, 1997).

The salt-lake problem is a more recent test case that involved laboratory simulation using a Hele-Shaw cell to represent the complex generation of unstable fingers of dense fluid in the presence of a source of salt and evaporation (Simmons *et al.*, 1999). The salt-lake problem provides a nice alternative to the Elder salt-convection problem for simulating a two-dimensional unstable stratification and the problem has been replicated using different numerical algorithms (Simmons *et al.*, 1999). The salt-lake problem, similar to the Henry, Elder and salt-dome problems is not without controversy (Diersch and Kolditz, 2002). At the current time, there is a paradoxical situation reported in the literature where simulations performed upon coarse grids yield improved comparisons with the laboratory observations than those numerical simulations generated upon finer grids (Mazzia *et al.*, 2001).

The salt-pool problem was also recently presented with laboratory data to supplement the numerical testing process (Johannsen *et al.*, 2002). The salt-pool problem is a three-dimensional brine flow set-up with a stable density stratification. Fluid is pumped from the aquifer and the resulting breakthrough curves are identified and compared to resulting laboratory breakthrough curves. Simulating the salt-pool problem requires high computing power to replicate the three-dimensional dynamics and this is the main limitation of the problem.

This summary of the currently available benchmark cases indicates that there is a sophisticated suite of modeling test cases available from which the performance of numerical models can be assessed and measured. The purpose of this communication is to review the relative advantages of the more recent developments and explore how alternative developments through revising the classical test cases, such as the Henry problem, can also provide convenient model testing options together with the newer emerging test cases. One of the limitations associated with the recent test cases is their extreme numerical complexity. For example, finite element and finite volume grids with up to one million nodes have been used to solve the Elder salt-convection problem (Diersch and Kolditz, 2002); similarly the salt-pool problem has been simulated using extremely fine grids with almost seventeen million nodes (Diersch and Kolditz, 2002). This extremely fine resolution makes simulation very difficult to conduct due to the limitation of computing power. In contrast to this extreme numerical sophistication, the recent advancements of Simpson and Clement (2003, 2004) for the Henry problem are very simple to implement as the suggested improvements can be made using standard computing resources that are widely available.

Methods

Comparative advantages and disadvantages of some of the standard test cases can be assessed by solving the following model for two-dimensional saturated variable density flow:

$$\frac{\partial(\beta\varphi)}{\partial t} + S_s\beta\frac{\partial\psi}{\partial t} = \frac{\partial}{\partial x}\left(\beta K\frac{\partial\psi}{\partial x}\right) + \frac{\partial}{\partial z}\left(\beta K\frac{\partial\psi}{\partial z}\right) + \frac{\partial(\beta^2 K)}{\partial z} \tag{1}$$

$$\varphi\frac{\partial C}{\partial t} = \beta\frac{\partial}{\partial x}\left(D_x\varphi\frac{\partial C}{\partial x}\right) + \beta\frac{\partial}{\partial z}\left(D_z\varphi\frac{\partial C}{\partial z}\right) - V_x\varphi\frac{\partial C}{\partial x} - V_z\varphi\frac{\partial C}{\partial z} \tag{2}$$

where φ is the porosity of the porous medium, β is the ratio of the fluid density to a reference freshwater density, K [LT^{-1}] is the hydraulic conductivity of the porous medium, ψ [L] is the freshwater pressure head of the fluid, S_s [L^{-1}] is the specific storage coefficient for the porous medium, C [ML^{-3}] is the concentration of the solute which contributes to the density variation, D_i [L^2T^{-1}] is the total dispersion coefficient in the i^{th} Cartesian direction and V_i [LT^{-1}] is the fluid velocity in the i^{th} Cartesian direction. The fluid density is assumed to vary as a linear function of the solute concentration. Further details of the numerical model including a rigorous description of the Galerkin finite element numerical solution procedure are given in Simpson and Clement (2003).

To compare the effectiveness of benchmark problems, a coupled simulation (Equation 1 and 2) can be compared with an uncoupled simulation where Equation 1 and 2 are solved but the value of β is fixed at 1 so that the solute concentration portion of the algorithm represents the movement of a passive weightless tracer. Simulations made with $\beta = 1$ can be interpreted as situations where the process of free convection involving buoyancy forces are ignored. Comparisons made by Simpson and Clement (2003) focused upon the Elder salt-convection and Henry salt-water intrusion problems. The Elder problem, which involves an initial condition representing a quiescent aquifer with no-flow boundary conditions, relies totally upon free convection and therefore the coupled and uncoupled simulations were completely distinct (Simpson and Clement, 2003). This implies that a numerical model that does not properly describes the coupling of the flow and transport processes would not be able to replicate the dynamics of the Elder problem. The Henry problem, which depends upon a forced convection from the fresh water boundary, showed that the position of the 50% isochlor was similar for coupled and uncoupled simulations. Therefore, Simpson and Clement (2003) concluded that the Henry problem might not be a good test case for determining the ability of a variable density code to replicate density-coupled flow conditions. This coupled-uncoupled strategy, proposed in the work, was useful in distinguishing the differences between forced and free convection processes.

Quantitatively improving the Henry problem was the focus of the recent study by Simpson and Clement (2004). The improvement was possible by noting through Henry's semi-analytical solution that one of the significant parameters reflected a competition between the forced boundary convection and the internal free convection. Henry (1964) showed that the three significant dimensionless parameters for the problem were the aspect ratio of the domain, $\xi = \frac{w}{d}$, $a = \frac{Q}{k_1 d}$ and $b = \frac{d}{b}$. Here, Q [L^2T^{-1}] is the freshwater recharge per unit width of coast, w [L] is the horizontal length of the domain, d [L] is the depth of the domain, $k_1 = K\left(\frac{\rho_s - \rho_0}{\rho_0}\right)$ where K [LT^{-1}] is the saturated hydraulic conductivity, ρ_0 [ML^{-3}] is the freshwater density, ρ_s [ML^{-3}] is the salt-water density and D [L^2T^{-1}] is the coefficient of dispersion. The form of the dimensionless group *a* implies that a decrease in the influence of forced convection is possible by reducing the value of the dimensionless number *a*. Numerical tests presented by Simpson and Clement (2004) indicated that reducing *a,* by halving the inflow rate Q, yielded results (Figure 2) which showed an increase in sensitivity to the density coupling effects. Therefore, Simpson and Clement (2004) suggested this modified problem as the basis of an improved test case for benchmarking numerical models within the original framework of the Henry problem but enabling a more rigorous test of density-coupled free convection features.

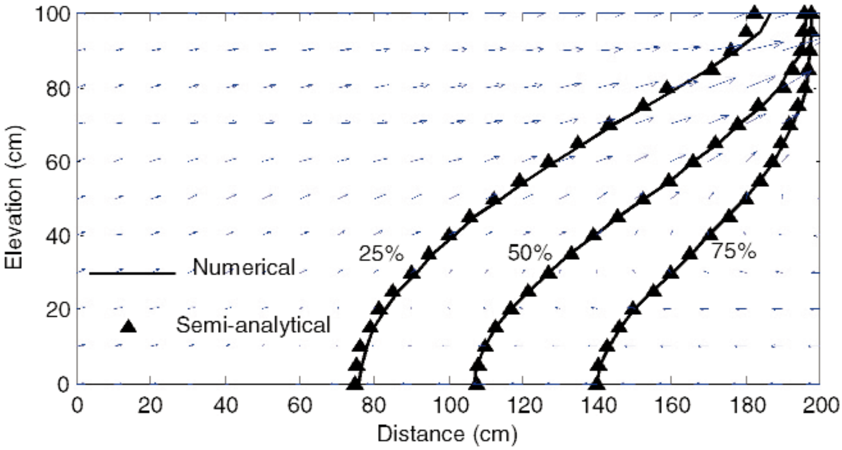

Figure 2. Numerical and semi-analytical results for the modified Henry salt-water intrusion problem a = 0.1315, b = 0.2 and ξ = 2.0. The velocity distribution is superimposed for completeness.

Reducing the value of Henry's non-dimensional parameter *a* implies that the relative importance of the forced convection (Q, the applied recharge through the boundary) was reduced compared to the internal free convection (k_1d, the internal free convection generated by density gradients). The physical argument that a reduction in *a* would lead to an improved test case through increasing the influence of free-convection is intuitive; however, the form of the non-dimensional parameter *a* reveals that there are several options for reducing *a*, these alternatives include increasing the density of the invading fluid, increasing the depth of the aquifer, or increasing the saturated hydraulic conductivity of the porous medium. Simpson and Clement (2004) chose to reduce the freshwater recharge, as this was the most intuitive means of increasing the importance of free convection processes relative to forced convection through the boundary. In addition, the reduction of recharge was a good option for conducting numerical simulations as the reduced recharge had the convenient effect of reducing the fluid velocities throughout the aquifer. The reduction in fluid velocity resulted in a reduced maximum grid Peclet number which is convenient for conducting numerical simulations of transport problems (Simpson and Clement, 2004).

The most useful feature of the modified Henry problem is that the simulation can be performed using standard numerical algorithms. The numerical algorithm presented by Simpson and Clement (2003, 2004) uses a standard finite element procedure where the spatial discretization is done using linear triangular elements. Temporal integration was done with a backward Euler scheme and iterative coupling between the flow and transport equations was invoked to simulate the density-coupled processes. The finite element discretization was a simple 861-node, 5 cm $\times$ 5 cm uniform grid. These standard numerical procedures enabled the finite element algorithm to be executed very efficiently. The resulting numerical profiles compare extremely well with the re-computed semi-analytical solution (Figure 2) and therefore the numerical algorithm used to solve the modified Henry problem is not limited by any of the grid dependence issues associated with the other popular benchmarks.

The improvements made to the standard Henry salt-water intrusion problem reveal that the classic Henry problem can still play a role in algorithm development. By demonstrating that the standard Henry problem is almost insensitive to density coupling, it seems that the standard problem which has dominated the model testing procedure for 40 years is not well-suited for testing the density-coupling ability of new algorithms. However, the proposed modified Henry problem permits a more rigorous of the algorithms ability to replicate density-coupled flow conditions. Unlike many of the alternative benchmark problems, the modified Henry problem does not show extreme sensitivity to grid resolution and it permits a semi-analytical solution that gives great confidence in the numerical results.

Discussion and conclusion

The proposition of a modified Henry salt-water intrusion problem, 40 years after it was first conceived, is an interesting new development. The revised Henry problem enables an improved model testing procedure as the original limitations of the problem have been addressed. In addition, the revised Henry problem shows certain advantages over the current suite of alternative benchmarks as the Henry problem enables a semi-analytical solution and does not show the extreme grid sensitivity that many of the other benchmarks are renown for. Although the Henry problem is unable to account for certain phenomena associated with variable density flow, such as unstable finger development, the revised problem retains the advantage of simplicity which will ensure that the Henry problem, and its variants, will remain one of the most popular benchmark test cases for demonstrating improvements in variable density algorithms.

In addition to comparing the relative advantages of the revised Henry problem, the recent advances imply that further fundamental insight into the dynamics of variable density flow problems can be made through additional exploration of the Henry problem. Simpson and Clement (2004) recomputed the Henry solution after reducing the recharge value by a factor of two; however, the physical arguments provided through the dimensionless parameters indicate that further improvements can be made by alteration of the dimensionless groups. Re-visiting the semi-analytical solution to test numerical results implies that using the semi-analytical method of Henry is an excellent means of testing numerical algorithms. More detailed understanding of intrusion processes seem likely with further evaluations of the semi-analytical solution, which has to date, only been evaluated for three conditions. Segol (1994) evaluated the standard case (a = 0.263, b = 0.1) and a second case for reduced dispersion (a = 0.263, b = 0.05). Simpson and Clement (2004) evaluated the standard case (a = 0.263, b = 0.1) and the proposed modified problem (a = 0.1315, b = 0.2). Therefore, while the Henry problem is thought of as a classical test case of variable density flow algorithms, it appears that the Henry problem still has a role to play in the improvement of our understanding of variable density problems and is likely to remain as a point of discussion in the scientific arena for some time to come.

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