ground water

MODFLOW/MT3DMS–Based Simulation of Variable-Density Ground Water Flow and Transport

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Abstract

This paper presents an approach for coupling MODFLOW and MT3DMS for the simulation of variable-density ground water flow. MODFLOW routines were modified to solve a variable-density form of the ground water flow equation in which the density terms are calculated using an equation of state and the simulated MT3DMS solute concentrations. Changes to the MODFLOW and MT3DMS input files were kept to a minimum, and thus existing data files and data files created with most pre- and postprocessors can be used directly with the SEAWAT code. The approach was tested by simulating the Henry problem and two of the saltpool laboratory experiments (low- and high-density cases). For the Henry problem, the simulated results compared well with the steady-state semianalytic solution and also the transient isochlor movement as simulated by a finite-element model. For the saltpool problem, the simulated breakthrough curves compared better with the laboratory measurements for the low-density case than for the high-density case but showed good agreement with the measured salinity isosurfaces for both cases. Results from the test cases presented here indicate that the MODFLOW/MT3DMS approach provides accurate solutions for problems involving variable-density ground water flow and solute transport.

Introduction

For many ground water problems, fluid density variations are not large enough to warrant the use of a variable-density model. These problems may be solved with a model in which the density is approximated as constant, such as MODFLOW (McDonald and Harbaugh 1988; Harbaugh et al. 2000), which is based on an assumption of constant fluid density. For a number of ground water problems, however, spatial variations in fluid density can markedly affect ground water flow patterns. For example, ground water flow near the coast is often influenced by density variations, and more complicated density-dependent models are required to accurately simulate processes such as salt water intrusion and submarine ground water discharge. Other types of ground water problems where fluid density may be important include aquifer storage and recovery, deep-well injection, brine transport, and ground water flow near salt domes. Sorek and Pinder (1999) provided a survey of 15 computer codes that can be used to simulate density-dependent ground water flow. Two commonly used examples are the USGS finite-element SUTRA code (Voss 1984; Voss and Provost 2002) and the finite-difference HST3D code (Kipp 1986, 1997). Approaches and challenges for studying variable-density ground water flow are summarized by Simmons et al. (2001), Diersch and Kolditz (2002), Post (2005), and Simmons (2005).

Efforts to simulate density-dependent flow with a MODFLOW-based code coupled with an advective and dispersive transport program were first reported by Guo and Bennett (1998a, 1998b), Oude Essink (1998), and van Gerven and Schaars (1998). Two of these early programs, SEAWAT (Guo and Bennett 1998a, 1998b) and MOCDENS3D (Oude Essink 1998), have been continuously updated with recent MODFLOW developments, including the incorporation of MODFLOW-2000 (Harbaugh et al. 2000). SEAWAT and MOCDENS3D follow similar approaches; the main functional difference is that MT3DMS (Zheng and Wang 1999) is used to represent solute transport in SEAWAT and the Ground Water Transport Process (previously referred to as MOC3D; Konikow et al. 1996)

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is used to represent solute transport in MOCDENS3D. Two other MODFLOW-based programs are currently available for simulation of density-dependent flow: MODHMS (HydroGeoLogic Inc. 2002) and the SWI Package for MODFLOW (Bakker 2003; Bakker and Schaars 2003). MODHMS is similar to SEAWAT and MOCDENS3D in that it simulates dispersive solute transport, whereas the SWI package uses a nondispersive, continuity-of-flow approach to simulate movement of multiple-density isosurfaces. Langevin et al. (2004a) provide a summary of these four MODFLOW-based density-dependent codes.

MODFLOW-based codes designed to simulate variable-density flow typically solve a formulation of the ground water flow equation in terms of equivalent fresh water head. Weiss (1982) was one of the first to recast the ground water flow equation in this form. With the equivalent fresh water head formulation, density effects can be incorporated into a constant-density flow model as "pseudosources." Lebbe (1983) also implemented an equivalent fresh water head formulation of the flow equation by modifying the method of characteristics program (Konikow and Bredehoeft 1978) to simulate variable-density flow. Maas and Emke (1988) and Olsthoorn (1996) described the approach for calculating pseudosources that could be entered into MODFLOW through the well package. Olsthoorn (2000) presented an approach for incorporating density effects into the source term of a numerical model based on stream functions. With the exception of the approaches by Lebbe (1983) and Olsthoorn (2000), which represented two-dimensional systems, a limitation with these previous approaches was that a known density field was required prior to the simulation in order to calculate the pseudosource values, and the density field was assumed to remain constant during the simulation.

The purpose of this paper is to present a concise description of the underlying methodology for coupling a constant-density ground water flow code with a solute transport code to simulate variable-density ground water flow and solute transport in three dimensions. The methodology is presented in the context of the MODFLOW/MT3DMS–based SEAWAT computer program. SEAWAT has been tested with many of the commonly used benchmark problems (Guo and Langevin 2002; Langevin et al. 2003; Bakker et al. 2004). In this paper, the results from two additional tests—the modified Henry problem (Simpson and Clement 2004) and the saltpool problem (Johannsen et al. 2002; Oswald and Kinzelbach 2004)—are presented to demonstrate the level of accuracy that can be obtained with a MODFLOW/MT3DMS–based approach.

Model Description

This section describes the mathematical model, finite-difference form of the variable-density flow equation, coupling procedure, and program structure. In this paper, the SEAWAT name generally refers to all versions of the code, including the most recent SEAWAT-2000 version, because the underlying mathematical formulations are the same, except where noted.

Mathematical Model

A general form of the continuity equation based on mass conservation for variable-density conditions is:

$$\frac{\partial(n\rho)}{\partial t} + \nabla \cdot (\rho \mathbf{q}) = \rho_s q'_s \tag{1}$$

where n is porosity [−], $\boldsymbol{\rho}$ is fluid density [ML^{-3}], t is time [T], $\mathbf{q}$ is specific discharge [LT^{-1}], and q'_s is a source or sink [T^{-1}] of fluid with density $\boldsymbol{\rho}_s$. The general form of Darcy's law for variable-density conditions is (Bear 1979):

$$\mathbf{q} = -\frac{\mathbf{k}}{\mu}(\nabla p + \rho g \nabla z) \tag{2}$$

where $\mathbf{k}$ is the permeability tensor [L^2], μ is dynamic viscosity [$ML^{-1}T^{-1}$], p is pressure [$ML^{-1}T^{-2}$], g is gravity [LT^{-2}], and z is the upward coordinate direction aligned with gravity. The Oberbeck-Boussinesq approximation is sometimes used to simplify Equation 1 by conserving volume as opposed to mass (e.g., Holzbecher 1998; Kolditz et al. 1998; Nield and Bejan 1999). Although this approximation eliminates the density terms in Equation 1, the density term in Equation 2 (second term within the parentheses) can still be included to account for buoyancy effects (e.g., Senger and Fogg 1990; Holzbecher 1998; Oude Essink 1998). For many problems with weak density variations, such as those encountered in most shallow coastal aquifers, the Oberbeck-Boussinesq approximation is valid, but Kolditz et al. (1998) do not recommend using this approximation for problems involving large density variations.

Many existing codes used for density-dependent ground water simulation formulate the equations in terms of pressure. To facilitate the use of MODFLOW routines to solve for flow, the equations presented here are formulated in terms of the head of a reference fluid. This reference fluid is commonly taken to be fresh water (denoted with a subscript f). Using fresh water as the reference fluid, Lusczynski (1961) defined the equivalent fresh water head, h_f [L], as:

$$h_f = \frac{p}{\rho_f g} + z \tag{3}$$

Oberlander (1989) and Bachu (1995) described the use of equivalent fresh water head for deep aquifer systems, and Juster (1995) described the use of pressure, equivalent fresh water head, reduced pressure, and environmental head for analysis of variable-density ground water flow systems. Any one of these measures can be used in studies of variable-density ground water flow, provided the associated governing equations correctly account for density differences. The equivalent fresh water head formulation, however, leads to a system of equations that can be solved relatively easily using the existing MODFLOW structure.

By solving Equation 3 for p and introducing the fresh water hydraulic conductivity tensor as $\mathbf{K}_f = \mathbf{k}\rho_f g/\boldsymbol{\mu}_f$ [LT^{-1}] (Senger and Fogg 1990), Equation 2 may be rewritten as:

$$\mathbf{q} = -\mathbf{K}_\mathrm{f}\frac{\mu_\mathrm{f}}{\mu}\left(\nabla h_f + \frac{\rho - \rho_\mathrm{f}}{\rho_\mathrm{f}}\nabla z\right) \quad (4)$$

The form of Equation 4 indicates that horizontal flow components can be evaluated directly from the gradient in fresh water head under variable-density conditions. For flow with a vertical component, the second term within the parentheses of Equation 4, referred to as a buoyancy term (Holzbecher 1998; Oude Essink 1998) or relative density difference term (Guo and Langevin 2002), can be similar in magnitude to the fresh water head gradient term, and must be considered. Dynamic viscosity is a weak function of solute concentration, typically varying by ~8% over the range between fresh water and sea water, and some codes, including SEAWAT and MOCDENS3D, neglect viscosity differences by approximating μ_f/μ to be 1. Holzbecher (1998) argues that for practical applications, local variations in viscosity are often much less than the unknown local variations in permeability, and thus the effects of variable viscosity are important only in rare cases.

The final form of the flow equation solved by SEAWAT is obtained by substituting Equation 4 into Equation 1 and expanding the time derivative into a familiar storage term and a term that accounts for the volumetric expansion due to solute concentration changes (Guo and Langevin 2002):

$$\nabla\cdot\left[\rho\mathbf{K}_\mathrm{f}\left(\nabla h_\mathrm{f} + \frac{\rho - \rho_\mathrm{f}}{\rho_\mathrm{f}}\nabla z\right)\right] = \rho S_\mathrm{sf}\frac{\partial h_\mathrm{f}}{\partial t} + n\frac{\partial\rho}{\partial C}\frac{\partial C}{\partial t} - \rho_\mathrm{s}q'_\mathrm{s} \quad (5)$$

where S_sf is the fresh water specific storage [L^{-1}] defined as the volume of water released from storage per unit volume per unit decline of fresh water head, and C is the concentration of solute mass per unit volume of fluid [ML^{-3}]. For a constant-density system, Equation 5 reduces to the flow equation solved by MODFLOW.

The MT3DMS computer program is used in SEAWAT to solve the following general form of the solute-transport equation (Zheng and Wang 1999):

$$\frac{\partial(nC)}{\partial t} = \nabla\cdot(n\mathbf{D}\cdot\nabla C) - \nabla\cdot(\mathbf{q}C) - q'_\mathrm{s}C_\mathrm{s} \quad (6)$$

where $\mathbf{D}$ is the hydrodynamic dispersion coefficient tensor [$\mathrm{L}^2\mathrm{T}^{-1}$] and C_s is the source or sink concentration [ML^{-3}]. Concentrations resulting from the solution of Equation 6 are used by an equation of state to calculate fluid density. Although Equation 6 is presented here for only a single chemical species, MT3DMS is capable of simulating transport for multiple dissolved species. Thus, in addition to simulating the species used in the equation of state to calculate fluid density, SEAWAT can also simulate the simultaneous transport of other species, such as contaminants.

For conditions with large spatial density gradients, which may be encountered in studies of dense connate brines, the ∇C term in Equation 6 should be formulated as $\rho\nabla(C/\rho)$ (Fried 1975; de Marsily 1986; Zheng and Bennett 2002). To further complicate the matter, laboratory column experiments involving high-concentration brines have shown that a nonlinear dispersion law is required to describe brine transport (Hassanizadeh and Leijnse 1995; Schotting et al. 1999). Interestingly, Diersch and Kolditz (2002) noted that a numerical simulation by Johannsen et al. (2002) of the high-density salt-pool experiment (described later) successfully matched the observed concentration breakthrough curve using a Fickian dispersion model. For most practical applications with moderate density variations, Zheng and Bennett (2002) suggest that Equation 6 represents a suitable approximation.

Equations 5 and 6 are coupled in variable-density ground water systems. Fluid density is a function of solute concentration, transport is dependent on the flow field, and the storage term in the transient flow equation incorporates changes in concentration. The relation between fluid density and solute concentration is represented by an equation of state, which can be approximated with the following linearized form developed by Baxter and Wallace (1916):

$$\rho = \rho_\mathrm{f} + \frac{\partial\rho}{\partial C}C \quad (7)$$

The present equation of state does not include the dependence of fluid density on temperature or pressure, and thus Equation 7 is valid for isothermal systems with an incompressible fluid. For deep aquifer systems and for aquifers with large temperature variations, an equation of state based on pressure, temperature, and solute concentration is required. Diersch and Kolditz (2002) provide a summary of more rigorous forms of the equations of state.

Variable-Density Flow Approximation

MODFLOW is based on the formulation of a generalized block-centered finite-difference approximation that includes flexibility for adding various types of sources and sinks. In SEAWAT, the generalized formulation was modified to include the effects of a three-dimensional density field calculated from solute concentrations. The full form of the variable-density finite-difference approximation is presented in Guo and Langevin (2002). Guo and Bennett (1998a, 1998b) and Oude Essink (1998) present the finite-difference equation based on the Oberbeck-Boussinesq approximation. The equations solved by SEAWAT are different from the Oberbeck-Boussinesq form in that the full-continuity equation is used, and thus, each flux term is multiplied by fluid density in order to conserve fluid mass instead of fluid volume. The finite-difference equation also includes the solutal volumetric expansion term, which is commonly eliminated as part of the Oberbeck-Boussinesq approximation.

MODFLOW contains approximations for water table conditions, downward leakage to a partially saturated layer, and the conversion between unconfined and confined conditions. To ensure that these approximations function under variable-density conditions, modifications

were required to ensure accurate representation of the intended approximation. For example, heads in terms of the native aquifer water, as opposed to equivalent fresh water heads, are used in the evapotranspiration algorithm and in the calculation of saturated thicknesses for flow conductances. Descriptions of the variable-density approximations for these special conditions and for many of the MODFLOW boundary packages are described in Guo and Langevin (2002) and Langevin et al. (2003).

Coupling Procedure

SEAWAT provides an explicit solution method and an iterative Picard method for coupling the flow and solute-transport equations. In the explicit method, solute concentrations from the previous transport time step are used to update the fluid densities used in the flow equation for the current time step. Advective fluxes from the flow solution are then used in the solution of the transport equation. With this iterative coupling method, solutions to the flow and transport equations are repeated within each time step until the largest change in fluid density at a single cell for consecutive iterations is less than a user-specified value (provided convergence was achieved in the solutions for both head and concentration).

The time discretization in SEAWAT is a combination of the approaches used by MODFLOW and MT3DMS. Simulations are divided into stress periods and transport time steps. The concept of a MODFLOW time step (called a flow time step) is also retained in SEAWAT but only for the purpose of saving model output. The lengths of transport time steps are determined by stability criteria but may be specified by the user if the implicit finite-difference option is used to solve the solute-transport equation. A limitation of the current version of SEAWAT is that flow and transport are solved for each transport time step.

Program Structure

The first two versions of SEAWAT (Guo and Bennett 1998a, 1998b; Guo and Langevin 2002) were developed by incorporating calls to MT3D or MT3DMS routines directly into the main program of MODFLOW-88 (McDonald and Harbaugh 1988). With the release of MODFLOW-2000, Harbaugh et al. (2000) introduced the concept of a process, which is a set of routines that solve an equation. For example, the constant-density ground water flow equation is solved using the Ground Water Flow (GWF) Process. The process concept was introduced to support other capabilities that require solving an equation, such as solute transport, sensitivity analysis, and parameter estimation (McDonald and Harbaugh 2003). One purpose for developing SEAWAT-2000 (Langevin et al. 2003) was to restructure the code using the process concept. SEAWAT-2000 contains the original GWF Process, which solves the constant-density flow equation and additionally contains the Variable-Density Flow (VDF) Process that solves Equation 5. In SEAWAT-2000, solute transport is solved using the Integrated MT3DMS Transport (IMT) Process. An advantage for incorporating this feature in SEAWAT-2000 is that processes can be combined in different ways as needed. For example, the IMT Process can be used with either the GWF or the VDF Processes. Also, the VDF Process can be used without the IMT Process, which allows for fast variable-density simulations, but only if it can be assumed that fluid density remains constant during the simulation. This type of variable-density simulation would be similar to those represented by Weiss (1982), Maas and Emke (1988), and Olsthoorn (1996). Langevin et al. (2003) provide a description of the processes and their compatibility in SEAWAT-2000.

One major objective in the development of SEAWAT and SEAWAT-2000 was to maintain the original structure of MODFLOW and MT3DMS and to minimize changes to the input and output files. This allows for new or updated versions of MODFLOW and MT3DMS to be incorporated with only modest effort. This design element is also beneficial for pre- and postprocessing because SEAWAT reads and writes standard MODFLOW and MT3DMS input and output files. SEAWAT-2000, however, requires a simple additional input file that contains coefficients for the equation of state and several other variables specific to the VDF Process.

Code Evaluation

SEAWAT has been tested with many of the common variable-density benchmark problems, such as the Henry, Elder, HYDROCOIN, and salt lake problems, among others. In general, the results from SEAWAT compare well with the results from other codes and analytic solutions (Guo and Langevin 2002; Langevin et al. 2003; Bakker et al. 2004). In this section, SEAWAT is tested with two of the more recent variable-density benchmark problems: the modified Henry problem, and the saltpool problem. The simulations described here were made using SEAWAT-2000 (version 3.11), which consists of MODFLOW-2000 (version 1.15.00) and MT3DMS (version 5.0).

Henry Problem

The Henry problem (Henry 1964) is commonly used as a benchmark problem for variable-density ground water simulation codes (Frind 1982; Voss and Souza 1987; Segol 1993; Simpson and Clement 2003, 2004) because it is one of the few problems that have a semi-analytic solution. The SEAWAT program was tested against the two cases of the Henry problem, referred to here as the original and modified Henry problems. For the first test, results from SEAWAT were compared with the semianalytic solution to the original Henry problem as recalculated by Simpson and Clement (2004). This semi-analytic solution is improved over the one presented by Segol (1993) in that it is valid for the entire problem domain. For the second test, results from SEAWAT were compared with a semianalytic solution to a modified version of the Henry problem that is more sensitive to density-dependent effects (Simpson and Clement 2003, 2004). The only difference between the original and modified Henry problems is that the inflow rate for the

modified problem is one-half the inflow rate for the original problem. The Henry problem is also used here to demonstrate the flexible time-step options in SEAWAT, which can be used to improve computer runtimes by substantially reducing the number of transport time steps required to reach a steady-state solution.

The basic design of the Henry problem is shown in Figure 1; parameter values are given in Table 1. A constant flux of fresh water is applied to the left boundary at rates of 5.702 m^2/d for the Henry problem and 2.851 m^2/d for the modified Henry problem. Sea water hydrostatic conditions were applied to the right boundary with a constant concentration of 35 kg/m^3. The problem was discretized with a finite-difference grid consisting of one row with 21 columns and 10 layers. A 0.1- by 0.1-m cell size was used for each column with the exception of the cells in column 21. A 0.01-m horizontal by 0.1-m vertical cell size was used in column 21 to more precisely locate the sea water hydrostatic boundary at a distance of 2 m.

For both the Henry and modified Henry problems, the implicit finite-difference solver was used for the dispersion and source terms in Equation 6, and the explicit third-order total variation diminishing (TVD) scheme was used to solve the advection term. The lengths of transport time steps were calculated using a specified Courant number of 0.1. For both Henry problems, the box was initially filled with fresh water, and the simulations were run until steady-state conditions were achieved. For the original Henry problem, the simulation reached steady state after 0.12 d, which required 1090 time steps. The average time-step length for the simulation was ~9.5 s.

A comparison between the numerical results of SEAWAT and the semianalytic solution that was recalculated by Simpson and Clement (2004) is shown in Figure 2. In general, the SEAWAT results are in good agreement with the results of the analytic solution, with the exception that the results deviate slightly near the outflow part of the constant-head boundary. This discrepancy is likely due to the relatively large velocities near the outflow region, which complicate solution of the transport equation. Simpson and Clement (2004) also reported difficulties in obtaining accurate solutions near the upper right boundary due to a relatively high grid Peclet number of 4.1. They used this difficulty as further support for their modified Henry problem, which had a maximum grid Peclet number of 2.8.

For the modified Henry problem, steady state was reached after 0.5 d, requiring a total of 3473 time steps. The average time-step length was ~12.4 s. SEAWAT results are compared with the semianalytic solution for the modified Henry problem in Figure 3. For the modified Henry problem, which is more controlled by density-dependent effects than the original Henry problem, the numerical results of SEAWAT are in good agreement with the semianalytic solution. Simpson and Clement (2004) also suggested that an additional test can be performed by making intercode comparisons on the transient movement of the 25%, 50%, and 75% isochlors at the base of the box; no analytic or semianalytic solutions exist for the transient isochlor movement. The comparison is made here between SEAWAT and the finite-element model of Simpson and Clement (2003, 2004). As shown in Figure 4, the two codes are in good agreement for the transient movement of the three isochlors along the base of the box.

Simulation of the steady-state position of the transition zone between fresh water and salt water is commonly performed as part of a salt water intrusion modeling study. SEAWAT has been shown to give accurate results, both in terms of the steady-state position and the transient isochlor movement, for the original and modified Henry problems. For the two problems, the TVD method was used with relatively short time steps. MT3DMS (and thus SEAWAT) has an option to implicitly solve all the transport terms, which means that the number of time steps can be reduced for certain problems. In some instances, substantial improvements in computer runtimes can be obtained if the value of the transport time-step multiplier (TTSMULT) is set to a value larger than 1. An analysis was performed with the modified Henry problem to evaluate the effects of using longer time steps in SEAWAT. Because the TVD method in MT3DMS cannot be solved implicitly, the analysis was performed using the implicit finite-difference method in MT3MDS with central-in-space weighting. The central-in-space weighting method reduced numerical dispersion for the simulations, but

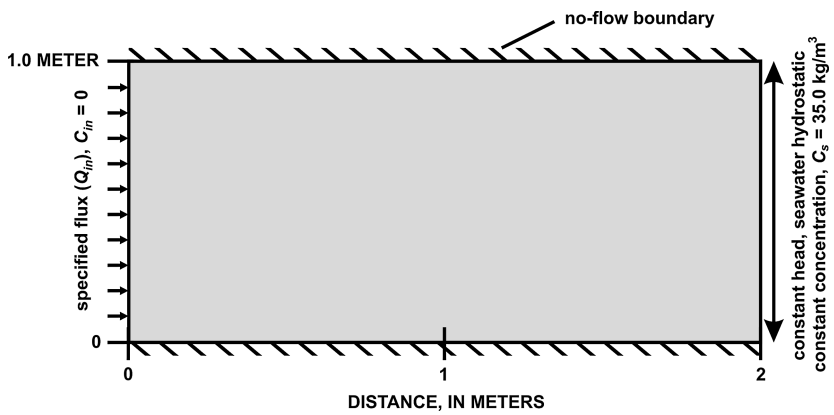

Figure 1. Boundary conditions and dimensions for the Henry problem. Variables are defined in Table 1.

Table 1
Input and Numerical Solution Parameters for the Henry Problem

	Value
Input parameters	
Q_{in} (Henry)	5.702 m^2/d
Q_{in} (modified Henry)	2.851 m^2/d
C_{in}	0.0 kg/m^3
K_f	864 m/d
n	0.35
α_L, α_T	0 m
D_m	1.62925 m^2/d
C_s	35 kg/m^3
ρ_s	1025 kg/m^3
ρ_f	1000 kg/m^3
Numerical solution parameters	
Cell size (columns 1 to 20); dx, dz	0.1 × 0.1 m
Cell size (column 21); dx, dz	0.01 × 0.1 m
Solution of flow equation	
Matrix solution technique	PCG
Head convergence value	1×10^{-7} m
Flow convergence value	1×10^{-7} kg/d
Solution of transport equation	
Advection term	TVD
Dispersion and source terms	Implicit finite difference; generalized conjugate gradient
Time-step length	Calculated during simulation using Courant value of 0.1
Concentration convergence value	1×10^{-6}

a negative concentration at the outflow cell indicated a problem with artificial oscillation due to the relatively high grid Peclet number at this cell. For many practical simulations, it may be preferable to use the upstream weighting in MT3DMS (and accept some numerical dispersion) as a method for reducing the potentially large negative concentrations associated with artificial oscillation (Huyakorn 1977, 1979).

Four simulations were performed with the implicit finite-difference method used for all of the transport terms (including advection). The iterative Picard method for coupling flow and transport was used for several preliminary simulations but did not significantly improve model results. Thus, flow and transport were explicitly coupled for the simulations reported here. For the first simulation, the time step was held constant at 1×10^{-4} d. For the remaining three simulations, TTSMULT values of 1.1, 1.5, and 1.9 were used to increase the transport time-step lengths during the simulation. Results for the four simulations are shown as plots of the transient isochlor movement at the base of the aquifer (Figure 5). The total number of time steps for each of the four simulations (TSMULT = 1.0, 1.1, 1.5, and 1.9) was 5001, 66, 20, and 14. The fourth simulation (TTSMULT = 1.9) ran ~180 times faster than the first (TTSMULT = 1.0). It is evident from Figure 5 that the increases in time-step lengths resulted in less accurate movement of the isochlors. The initial isochlor movement was too slow with the longer time steps. The isochlors also overshot their steady-state positions before finally converging on accurate distances

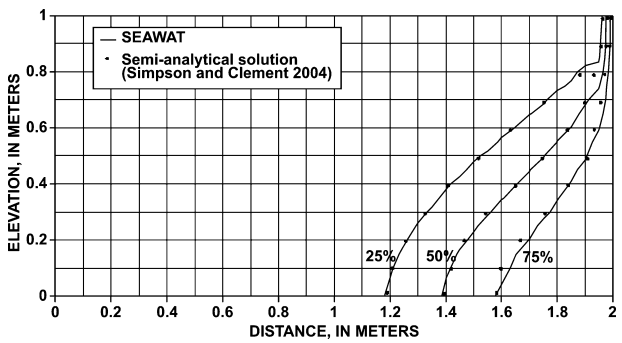

Figure 2. Comparison of SEAWAT results with the semi-analytic solution to the original Henry problem. Values represent relative concentration (in %).

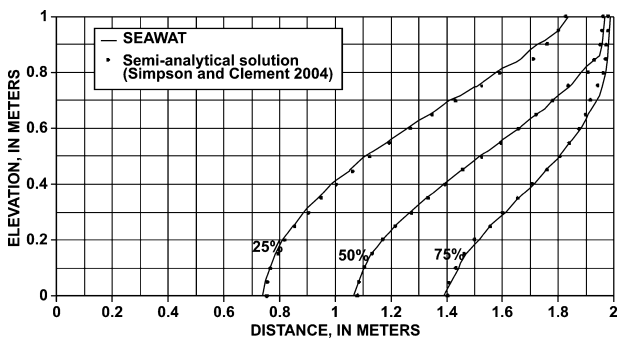

Figure 3. Comparison of SEAWAT results with the semi-analytic results for the modified Henry problem. Values represent relative concentration (in %).

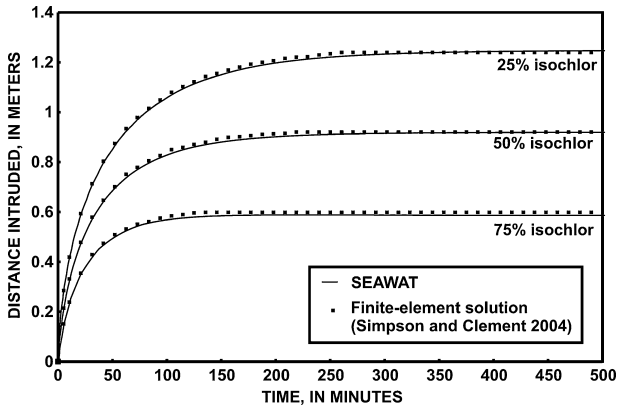

Figure 4. Transient position of the intersection of the 25%, 50%, and 75% isochlors with the base of the aquifer for the modified Henry salt water intrusion problem.

from the boundary. For this particular problem, the simulation with TTSMULT = 1.1 appears to give reasonable transient results with a significant reduction in the number of time steps. This analysis also suggests that if the steady-state position of the isochlors is the only result of interest, computer runtimes may be substantially reduced through the use of relatively large time-step multipliers.

Based on this analysis with the Henry problem, the implicit finite-difference solution scheme with relatively large time steps can be used to quickly solve the transport terms, including advection. Although the transient interface movement may be inaccurate due to the long time steps, the resulting steady-state salinity distribution will likely be reasonable. Whether or not this conclusion holds for field-based applications can be determined through a simple sensitivity analysis on time-step lengths. There remains some question regarding the appropriate weighting scheme to use with the implicit finite-difference solution. In the simulations described here, negative concentrations and concentrations greater than sea water were encountered during simulations in which the advection term was solved using the finite-difference method with central-in-space weighting. An alternative approach that also would have allowed relatively long time steps would have been to accept a higher level of numerical dispersion and use the upstream weighting option.

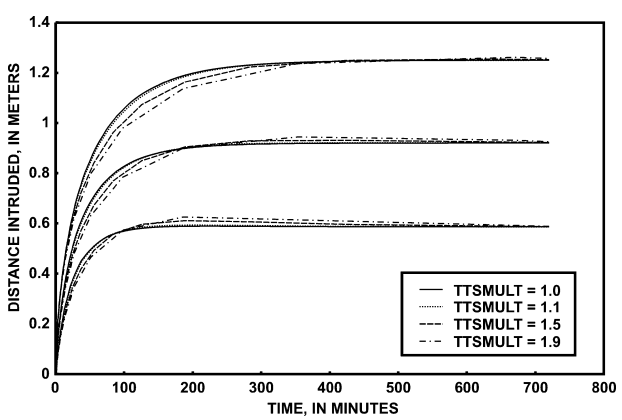

Figure 5. Effect of time-step length on the movement of the intersection of the 25%, 50%, and 75% isochlors with the base of the aquifer for the modified Henry salt water intrusion problem.

Saltpool Problem

Oswald and Kinzelbach (2004) describe the results from a series a laboratory experiments involving salt water upconing within a clear acrylic box filled with spherical glass beads (average diameter is 1.2 mm). Nuclear Magnetic Resonance Imaging (NMRI) was used during the experiment to noninvasively obtain high-resolution three-dimensional concentration distributions at selected times (Oswald et al. 2002). These saltpool experiments provide a unique test for variable-density codes because of the three-dimensional nature of the problem; most benchmark problems used to test variable-density codes are for two-dimensional flow. Results of variable-density numerical simulations of the saltpool experiments have been reported with varying degrees of success by Diersch and Kolditz (2002), Johannsen et al. (2002), and Oswald and Kinzelbach (2004). Johannsen et al. (2002) seem to have had the best success, which was obtained by adjusting several of the input parameters (hydraulic conductivity, porosity, and transverse dispersivity) within a reasonable range using parameter estimation techniques. The values estimated by Johannsen et al. (2002) were used for the SEAWAT simulations reported here.

The design of the saltpool experiment is shown in Figure 6, and the input parameters and parameters for the numerical representation are listed in Table 2. The initial fluid distribution consisted of 14 cm of fresh water overlying 6 cm of salt water. This stable configuration was obtained by injecting salt water though a centralized port at the bottom of the cube and then allowing the salt water to settle as a flat layer with a minimal mixing zone. After stable equilibrium was reached, fresh water was injected into a corner port at the top of the cube, and discharge was allowed through a separate outflow port. During the experiment, the outflow concentration was measured, and NMRI snapshots of the three-dimensional concentration field were taken at various times. Oswald and Kinzelbach (2004) describe six different laboratory experiments, each with a different initial salt water concentration; however,

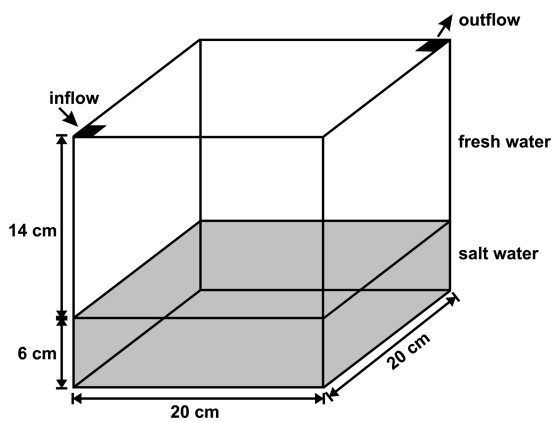

Figure 6. Diagram of the saltpool experiment.

Table 2
Input and Numerical Solution Parameters for the Saltpool Problem

	Value
Input parameters	
Inflow/outflow (saltpool_1)	0.163 m^3/d
Inflow/outflow (saltpool_10)	0.158 m^3/d
K_f	1010 m/d
n	0.3578
α_L	0.0012 m
α_T	4.32×10^{-5} m
D_m	8.64×10^{-5} m^2/d
C_{fresh}	0
C_{salt}	1
ρ_{fresh}	998.23 kg/m^3
ρ_{salt} (saltpool_1)	1005.82 kg/m^3
ρ_{salt} (saltpool_10)	1071.6 kg/m^3
Numerical solution parameters	
$G_{(1)}$ grid	
Cell size	1 cm
Nodes	8000
$G_{(2)}$ grid	
Cell size	0.5 cm
Nodes	64,000
$G_{(3)}$ grid	
Cell size	0.25 cm
Nodes	512,000
$G_{(4)}$ grid (irregular; created from $G_{(3)}$)	
Cell size	0.25 and 0.125 cm
Nodes	704,400
Solution of flow equation	
Matrix solution technique	PCG
Head convergence value	1.00×10^{-5} m
Flow convergence value	0.001 kg/d
Solution of transport equation	
Advection term	TVD or implicit finite difference
Dispersion and source terms	Implicit finite difference; generalized conjugate gradient
Time-step length	Calculated during simulation using Courant value of 0.5 (TVD); initially specified as 1×10^{-9} d and increased during simulation using multiplier of 1.001 (implicit finite difference)
Concentration convergence value	1.00×10^{-8}

the NMRI analysis was performed on only two of the laboratory experiments: one with an initial concentration for the salt water of 1% salt mass fraction (smf) and one with an initial concentration of 10% smf. The analysis described here focuses on only these two experiments, referred to as saltpool_1 and saltpool_10. For the saltpool_1 experiment, the salt water density was ~1005.82 kg/m^3, whereas for the saltpool_10 experiment, the salt water density was ~1071.60 kg/m^3. The density difference between the two experiments leads to very different flow patterns. In saltpool_1, the fresh water depresses the interface beneath the inflow port, forcing the salt water upward and out toward the outflow face. In saltpool_10, there is a dispersive flux of salt into the fresh water as it flows over the interface and toward the outlet, but much of the dense salt water remains at the bottom of the cube for the duration of the experiment.

SEAWAT was used with four different finite-difference grids to simulate the saltpool experiments. The grids are referred to as $G_{(L)}$, where L denotes the grid level. Higher values of L indicate a more refined grid. Details of the grids are listed in Table 2. Two different options were tested for solving the advection term of the transport equation: TVD and implicit finite difference with central-in-space weighting. For the TVD simulations, the time-step lengths were calculated during the simulation using a Courant number of 0.5. For the implicit finite-difference simulations, the initial time-step length was specified as 1×10^{-9} d, and increased during the simulation using a time-step multiplier of 1.001. Flow and transport were explicitly coupled for all the simulations.

A comparison between the SEAWAT TVD simulations (using $G_{(1)}$ and $G_{(2)}$) and the laboratory experiment is shown in Figure 7. Following the comparisons of Johannsen et al. (2002) and Oswald and Kinzelbach (2004), the plots in Figure 7 are for a vertical cross section along a diagonal line from the inflow port to the outflow port. The isolines represent 10% and 50% of the maximum salt

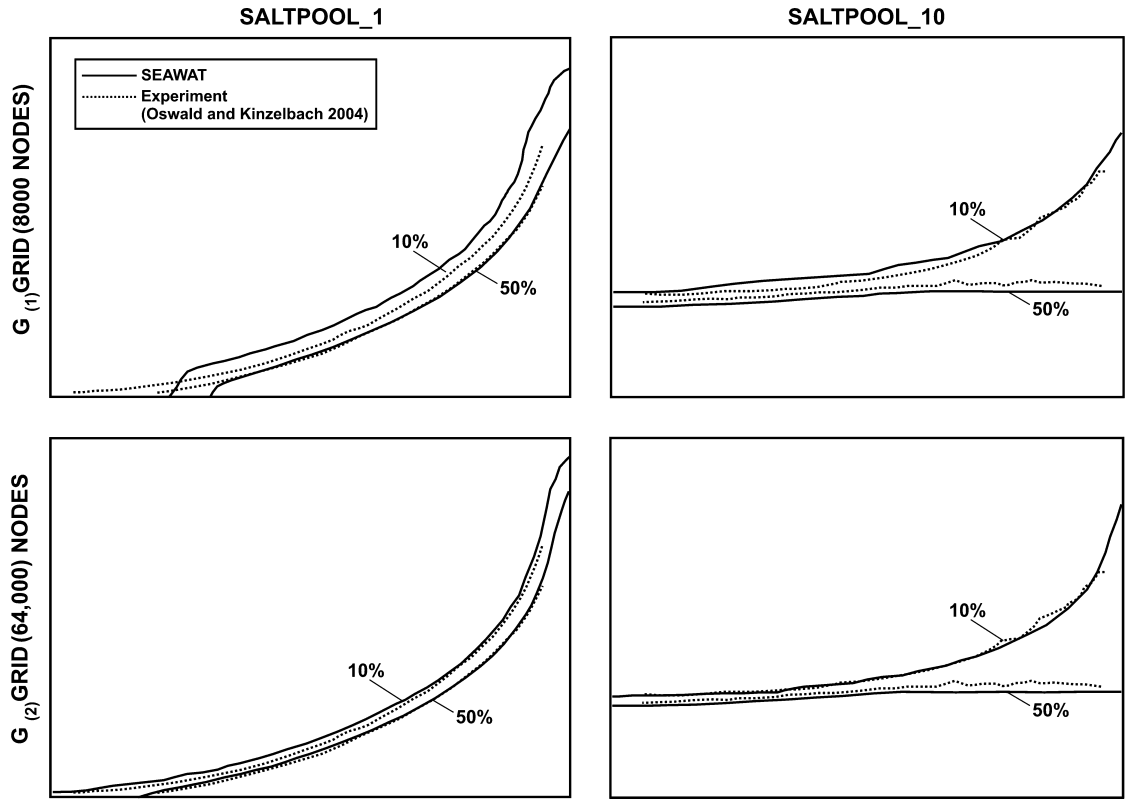

Figure 7. Comparison of SEAWAT results with the results of the laboratory experiment for the saltpool_1 and saltpool_10 experiments. For saltpool_1 and saltpool_10, the elapsed times are 140.2 and 160 min, respectively. Isolines represent salt concentration relative to the initial salt water concentration. For all plots, the vertical section is along the diagonal between the inflow and outflow points.

water concentrations. In general, the model seems to adequately capture the flow and transport processes for both saltpool experiments. Simulation results obtained with $G_{(2)}$ have less numerical dispersion and better replicate the experiment than simulations with $G_{(1)}$. The effects of numerical dispersion are clearly apparent in the $G_{(1)}$ results for saltpool_1. In this simulation, numerical dispersion has artificially widened the transition zone between the 10% and 50% isolines and has also resulted in inaccurate positions of the isolines at the base of the box. With $G_{(2)}$, the simulated transition zone and isoline positions at the base of the box compare well with the experimental results.

A comparison of the concentration breakthrough curves for the SEAWAT TVD simulations and the laboratory experiment is shown in Figure 8. For saltpool_1, simulated results with $G_{(1)}$ and $G_{(2)}$ compare well with the measured concentrations, although the concentration peak is better represented with $G_{(2)}$. For saltpool_10, however, there is only modest agreement between simulated results and the laboratory experiment. $G_{(1)}$ results match slightly better than results from $G_{(2)}$ in terms of the

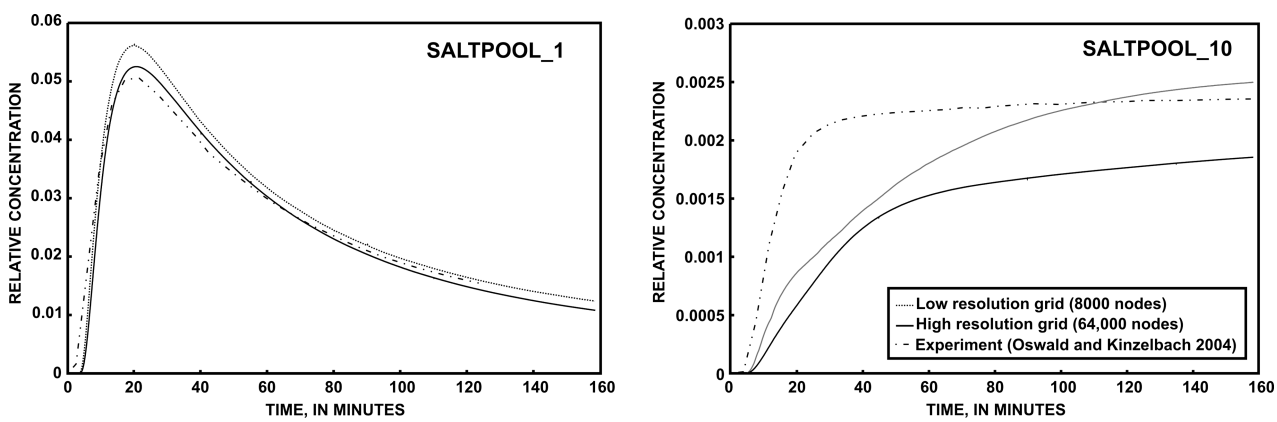

Figure 8. Experimental and simulated concentration breakthrough curves for saltpool_1 and saltpool_10.

relative concentration values, but the shape of the breakthrough curve does not match well with the experiment. Results from the $G_{(2)}$ simulation have an improved shape for the breakthrough curve, but the concentration increase at the beginning of the experiment is not sharp enough, and the curve levels off at a concentration value that is too low.

The discrepancy between the SEAWAT TVD simulations and the laboratory results for the saltpool_10 breakthrough curve prompted the following sensitivity analysis of grid resolution. TVD simulations with large grids and small model cells were impractical due to a Courant restriction with the explicit method, and thus the implicit finite-difference scheme was used with central-in-space weighting. Results from simulations using grids $G_{(1)}$ through $G_{(4)}$ are shown in Figure 9. Even with over 700,000 nodes, grid convergence has not been met for this problem, which is consistent with Johannsen et al. (2002) who concluded that an extremely fine mesh with as many as 17 million nodes was required to accurately simulate the saltpool_10 experiment. Results from $G_{(1)}$ and $G_{(2)}$ show numerical oscillations in concentration and an overall concentration decrease for the second half of the simulation. This gradual decrease in concentration is likely the result of overshoot caused by the central weighting scheme and clearly is not supported by the measurements. Simulated breakthrough curves from $G_{(3)}$ and $G_{(4)}$ match better with the overall shape of the measured breakthrough curve, and concentrations increase during the entire simulation, which is consistent with the experiment. Results from $G_{(3)}$ and $G_{(4)}$ at early times, however, do not match well with the experiment. Curiously, results from $G_{(1)}$ and $G_{(2)}$ show rapid increases in concentration at the beginning of the simulation, which is actually in better agreement with the experiment. These rapid concentration increases at early times are likely due to numerical dispersion, and the close match (particularly for $G_{(2)}$) does not necessarily indicate that the physical processes of the experiment are being represented.

Results from the SEAWAT simulations demonstrate the level of accuracy that one can expect when using a MODFLOW/MT3MS–based code to represent complex variable-density ground water flow and solute transport problems. Overall, the simulations provided a reasonable representation of the physical experiment. Some concerns remain regarding the discrepancy between the simulated and observed concentration breakthrough curves for saltpool_10. A possible explanation for the discrepancy is that higher grid resolution is required for the model to accurately represent the dispersive mixing that occurs in the experiment. Although further increases in grid resolution would improve numerical accuracy, the grid convergence analysis suggests that the early time concentrations would further deviate from the experiment. The effect of variable fluid viscosity was also investigated using a research version of the SEAWAT code, which was developed to simulate simultaneous heat and solute transport. Results showed very slight decreases in the simulated concentrations (<2%), and thus the effect of variable viscosity does not explain the discrepancy between the simulations and the experiment.

The saltpool experiments provide a challenging test for variable-density ground water models. Initial FEFLOW simulations completely failed for saltpool_10 because of an inconsistent velocity approximation (Oswald and Kinzelbach 2004), which was subsequently corrected. The SEAWAT results reported here are similar to the results obtained with the corrected version of FEFLOW (Diersch and Kolditz 2002). Further improvement of the SEAWAT simulation for saltpool_10 could likely be obtained by following the example of Johannsen et al. (2002) and adjusting one or more of the model input parameters.

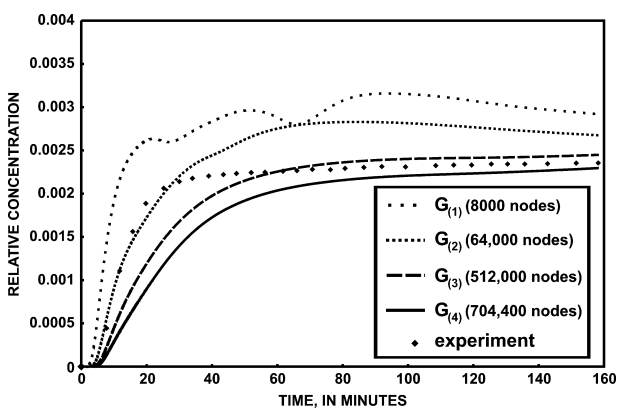

Figure 9. Results from four SEAWAT simulations with different levels of grid resolution for the saltpool_10 experiment.

Summary

This paper presents the approach for coupling MODFLOW and MT3DMS into a single computer program (SEAWAT) for the simulation of variable-density ground water flow. The approach consists of formulating the ground water flow equation in terms of equivalent fresh water head and fluid density, which is calculated from solute concentrations using a linear equation of state. To demonstrate the accuracy of the MODFLOW/MT3DMS–based approach, the code was tested using the modified Henry problem and the saltpool problem. For the Henry problem, the simulated steady-state results compared well with the semianalytic solution and the simulated transient results compared well with results of the finite-element model. For the saltpool problem, which is based on a three-dimensional laboratory experiment, the simulated results compared well with the measured results from the experiment. The results from these tests demonstrate that the MODFLOW/MT3DMS–based approach is capable of representing complex variable-density ground water flow and solute transport.

One of the main advantages of SEAWAT is that it is based on MODFLOW and MT3DMS—two popular and widely accepted computer programs with many options for representing boundaries and for simulating solute transport. SEAWAT is routinely updated with new versions of MODFLOW and MT3DMS, and thus

improvements and new features in these programs are available for variable-density simulations. The modular design of the code also allows for coupling with other processes, such as hydrodynamic surface water flow (Langevin et al. 2004b) and geochemical reactions (Mao et al. in press).

Although real world applications are not described here, the program has been applied to issues related to submarine ground water discharge (Langevin 2001, 2003), salt water intrusion (Shoemaker and Edwards 2003; Rao et al. 2004; Shoemaker 2004; Masterson 2004; Dausman and Langevin 2005), coastal wetland hydrology (Langevin et al. 2004b, in press), and island hydrology (Schneider and Kruse 2003).

SEAWAT is a public domain computer program with published documentation and is freely distributed by the USGS (http://water.usgs.gov/ogw/seawat/). A review of SEAWAT-2000 was reported by Simpson (2004) in the Software Spotlight column of *Ground Water.*

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