

MODFLOW/MT3DMS-BASED SIMULATION OF VARIABLE-DENSITY GROUNDWATER FLOW WITH SIMULTANEOUS HEAT AND SOLUTE TRANSPORT

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ABSTRACT

SEAWAT is a finite-difference computer code designed to simulate coupled variable-density ground water flow and solute transport. This paper describes a new version of SEAWAT that adds the ability to simultaneously model energy and solute transport. This is necessary for simulating the transport of heat and salinity in coastal aquifers for example. This work extends the equation of state for fluid density to vary as a function of temperature and/or solute concentration. The program has also been modified to represent the effects of variable fluid viscosity as a function of temperature and/or concentration. The classic Henry-Hilleke problem is solved with the new code.

1. INTRODUCTION

The density and viscosity of fluids vary with temperature. In computational hydrogeology such variations historically have been assumed to be minor and were largely ignored. However, there is now an increasing need to simulate the effects of direct manipulation of ground water systems where significant temperature differences might exist (e.g., aquifer storage and recovery, deep well waste injection, ground source heat pumps) and a need for more resolution in critical ground water studies where temperature is likely to play a role (e.g., sole source aquifers, coastal aquifer/ocean interactions). The increasing availability of adequate computational resources also has made such simulations accessible to a much broader set of potential users.

SEAWAT (Guo and Bennett, 1998; Guo and Langevin, 2002; Langevin et al, 2003), couples MODFLOW (Harbaugh et al, 2000) and MT3DMS (Zheng and Wang, 1999) to simulate variable density ground water flow. In previous SEAWAT versions, users could simulate transport of multiple chemical species, but fluid density was calculated as a function of solute concentration for only a single species (e.g., salinity, chloride, or relative seawater fraction). Furthermore, previous versions of SEAWAT did not represent the effects of fluid viscosity variations, which can be important for problems with large temperature or salinity variations.

This paper documents enhancements to the SEAWAT computer code, which allow it to represent the simultaneous transport of solutes and heat. To simulate heat transport within the context of the SEAWAT framework, one of the MT3DMS species is used to represent temperature. The effect of temperature variations on ground water flow is included in the

new program by modifying the density equation of state to vary with the temperature of the fluid as well as the concentration of a solute. In particular, the new equation of state is:

$$\rho(C,T) = \rho_f + \frac{\partial \rho}{\partial C} C + \frac{\partial \rho}{\partial T} T \quad (1)$$

where the density of freshwater ρ_f and the change in density with respect to concentration and temperature $\frac{\partial \rho}{\partial C}$ and $\frac{\partial \rho}{\partial T}$ are prescribed constants input by the user. The effect of viscosity variations on the resistance to ground water flow also was added through implementation of the relationship between permeability, viscosity, and hydraulic conductivity. Viscosity is incorporated into the flow equation as a function of both temperature and solute concentration (or just one or the other, as desired). A variety of published formulas for viscosity is supported by the new program (Holzbecher, 1998; Johannsen et al, 2002; Hughes and Sanford, 2004) but they are not described here. The paper culminates with our solution of the Henry-Hilleke problem, a seawater intrusion scenario involving the full equation of state, Equation (1).

2. MATHEMATICAL APPROACH

Two new capabilities are introduced to SEAWAT: (1) simultaneous transport of energy and solute, and (2) representation of fluid viscosity variations. MT3DMS was designed to simulate solute transport; however, the code also has been used to simulate heat transport (e.g. Martin et al., 2001). Here, we briefly introduce the analogy between solute and energy transport. Then we give a brief discussion of the role of variable viscosity in Darcy's law and its implementation.

2.1 Solute transport.

Among the forms of the advection-dispersion equation solved by MT3DMS is (Zheng and Wang, 1999):

$$\left(1 + \frac{\rho_b K_d}{\theta}\right) \frac{\partial(\theta C^k)}{\partial t} = \frac{\partial}{\partial x_i} \left(\theta D_{ij} \frac{\partial C^k}{\partial x_j} \right) - \frac{\partial}{\partial x_i} (\theta v_i C^k) + q_s C_s^k + \sum R_n \quad (2)$$

where ρ_b is porous medium bulk density, K_d is the linear sorption coefficient (distribution coefficient), θ is the volumetric water content, C^k is the concentration of species k , t is time, x_i is the i^{th} spatial coordinate, D_{ij} is the diffusion-dispersion tensor, v_i is the mean pore water velocity vector, q_s is a source or sink volumetric flow rate per unit volume, C_s^k is a source or sink concentration, and R_n is a reaction term considering first order production or decay. We wish to leverage this equation to solve energy transport, which is analogous to solute transport in several ways (e.g., Voss, 1984; Martin et al., 2001; Kim et al., 2005).

2.2 Energy transport.

Key parameters in energy transport processes are thermal conductivity, k_T , and specific heat capacity, c_p . In a way analogous to the hydraulic conductivity in Darcy's law or the diffusion coefficient in Fick's law, the thermal conductivity, k_T , is used in Fourier's law for heat transport:

$$q_T = -k_{T,i,j} \frac{\partial T}{\partial x_j} \quad (3)$$

The thermal conductivity has units of energy per unit time, length, and temperature (e.g., $\text{Wm}^{-1}\text{C}^{-1}$). Thus, the heat flux, q_T , has units of Wm^{-2} . Unlike solutes, where movement is essentially confined to fluid phases, energy also is transported through aquifer solids by conduction (controlled by the thermal conductivity of the solids). Hence, we have new parameters, k_{Tfluid} and k_{Tsolid} , to distinguish the thermal conductivities of the fluid and solid phases.

Heat is stored in the fluid and solid phases according to their specific heat capacities, c_{Pfluid} and c_{Psolid} , which relate the temperature to energy stored at constant pressure. Heat capacity has units of energy per unit mass and temperature (e.g., $\text{J kg}^{-1} \text{C}^{-1}$). For solutes, the prefactor of the time derivative in Equation (2) can account for both the dissolved and adsorbed solute. In the case of heat, the prefactor similarly accounts for the change in heat storage in both the fluid and solid phases. In the fluid phase, the energy stored is given by the temperature of the fluid multiplied by its volume, heat capacity, and density, which is $\theta c_{Pfluid} \rho T$, whereas the energy stored in the solids is given by the temperature multiplied by the solid volume, heat capacity, and density, which is $(1-\theta)c_{Psolid} \rho_s T$.

For solutes in water, the advective component is simply vC , but for heat we need to relate the temperature to the heat energy stored in the flowing fluid. Because v is the volumetric flux and c_P is on a unit mass basis, we need to multiply by density to convert volumetric flux to mass flux of liquid. Thus the advective heat flux in the moving water is $v \rho c_{Pfluid} T$. The dispersive heat flux involves the same factors and is $\frac{\partial}{\partial x_i} \rho c_{Pfluid} D_{ij} \frac{\partial T}{\partial x_j}$.

An equation that incorporates these processes is (Kipp, 1987; Voss and Provost, 2002; Hughes and Sanford, 2004):

$$\begin{aligned} \frac{\partial}{\partial t} \left(\left[\theta \rho c_{Pfluid} + (1-\theta) \rho_s c_{Psolid} \right] T \right) = \\ \frac{\partial}{\partial x_i} \left(\left\{ \left[\theta k_{Tfluid} + (1-\theta) k_{Tsolid} \right] \mathbf{I} + \theta \rho c_{Pfluid} D_{ij} \right\} \frac{\partial T}{\partial x_j} \right) \\ - \frac{\partial}{\partial x_i} \left(\theta \rho c_{Pfluid} v_i T \right) + q_s \rho c_{Pfluid} T_s + \theta \rho \gamma_{fluid} + (1-\theta) \rho_s \gamma_{solid} , \end{aligned} \quad (4)$$

where \mathbf{I} is the identity tensor, D_{ij} is now the dispersion tensor, and γ_{fluid} and γ_{solid} are zero-order rate constants for heat production or loss (energy per unit time and mass of fluid and solid respectively; e.g., W kg^{-1}). We write this equation so there is a one-to-one correspondence between its terms and the terms in Equation (2), although the reaction term has been split into two parts involving zero order production or loss in the fluid and solid phase, respectively.

Equation (4) makes it clear that it is energy being transported rather than just temperature. The first term describes the time rate of change of energy stored in both the fluid and solid phases. The second term describes both the conductive and dispersive energy fluxes. The conduction is assumed to be isotropic and hence involves the identity tensor \mathbf{I} . It is possible to consider the fluid and solid phase thermal conductivities, k_{Tfluid} and k_{Tsolid} , separately or combine them into a bulk value using one of several available ‘mixing’ models (e.g., Clauser and Huenges, 1995; Hughes and Sanford, 2004); the simplest of these is to weight the fluid thermal conductivity by the volumetric fluid content and add it to the solid conductivity weighted by the volumetric solids fraction. For a saturated porous medium, we then have $k_{Tbulk} = \theta k_{Tfluid} + (1-\theta) k_{Tsolid}$.

Like existing models that address energy transport (e.g., SUTRA, HST3D), dispersive energy transport is assumed here; as in solute transport, it accounts for the fact that the mean

ground water velocity used in Darcy's law is only an average of the detailed pore velocities. Thus, the treatment is that of anisotropic mechanical heat dispersion governed by a saturated aquifer thermal diffusivity tensor (D_{ij} in Equation (4)). Heat conduction is governed by the bulk thermal diffusivity, which is analogous to the solute diffusion coefficient. In the present formulation, the bulk thermal diffusivity is a combination of both the water and solid phases.

Finally, we utilize the Oberbeck-Boussinesq approximation (e.g., de Marsily, 1986; Holzbecher, 1998; Kolditz et al., 1998; Nield and Bejan, 1999) to assume constant fluid density, ρ , within the transport equation, which leads to considerable simplification. In each instance that this assumption is applied to the energy transport equation, it is in the context of the energy content and appears as $c_{pfluid}\rho T$. With this assumption, ρ (and c_{pfluid}) can be factored out of the derivatives and we can rewrite Equation (4) as

$$\left(\theta + (1 - \theta) \frac{\rho_s}{\rho} \frac{c_{psolid}}{c_{pfluid}} \right) \frac{\partial T}{\partial t} = \frac{\partial}{\partial x_i} \left(\theta [D^* + D_{ij}] \frac{\partial T}{\partial x_j} \right) - \frac{\partial}{\partial x_i} (\theta v_i T) + q_s T_s + \frac{\theta \gamma_{fluid}}{c_{pfluid}} + \frac{(1 - \theta) \gamma_{solid}}{c_{pfluid}} \frac{\rho_s}{\rho}, \quad (5)$$

which is basically Equation (2) with substitution of T for C^k . The coefficient on the time derivative represents heat stored in both the fluid and solid phases and corresponds to the retardation factor for sorbed solutes where the key equivalence that must be established is $K_d = \frac{\theta^2}{\rho_b} + (1 - \theta) \theta \frac{\rho_s}{\rho \rho_b} \frac{c_{psolid}}{c_{pfluid}} - \frac{\theta}{\rho_b}$, which further simplifies to $K_d = \frac{\theta^2}{\rho_b} + \frac{\theta}{\rho} \frac{c_{psolid}}{c_{pfluid}} - \frac{\theta}{\rho_b}$. This equation was determined by equating the prefactors of the time derivatives in Equations (2) and (5) and solving for K_d . The standard solute transport model diffusion coefficient, D^* , is replaced with the bulk thermal diffusivity, $D^* = \frac{k_{Tbulk}}{\rho c_{pfluid}}$.

Because the zero order heat production and decay are essentially distributed source/sinks, they can be combined with the preexisting source/sink term $q_s T_s$ by simply adding a $q'_s T'_s = \frac{\theta \gamma_{fluid}}{c_{pfluid}} + \frac{(1 - \theta) \gamma_{solid}}{c_{pfluid}} \frac{\rho_s}{\rho}$ term. Equation (5) and the equivalences noted here encapsulate the current SEAWAT implementation of energy transport based on an MT3DMS species.

2.3 Variable viscosity.

Darcy's law, as written in the MODFLOW user's guide (Harbaugh et al., 2000), is $Q = COND(h_A - h_B)$ where, for the extended SEAWAT, the conductance $COND$ is expanded as:

$$COND = \frac{\mu_f}{\mu} \frac{T^* W}{L}, \quad (6)$$

or in terms of hydraulic conductivity instead of transmissivity:

$$COND = \frac{\mu_f}{\mu} \frac{KWB}{L}, \quad (7)$$

where h is hydraulic head, T^* is transmissivity, W is width of the cell, L is length of the cell, K is hydraulic conductivity, and B is height of the cell. SEAWAT is formulated using "equivalent freshwater" hydraulic conductivity and transmissivity values (Guo and Langevin, 2002). Thus, the T^* and K values used in Equations (6) and (7) represent an aquifer that is

saturated with the reference fluid at the reference temperature (normally assumed to be freshwater at 25 degrees Celsius).

The ratio $\frac{\mu_f}{\mu}$ accounts for variation in viscosity $\mu = \mu(C,T)$ from some reference viscosity μ_f . When $\mu > \mu_f$, conductance $COND$ is lower than in the isoviscous case, and when $\mu < \mu_f$ the conductance $COND$ is higher than in the isoviscous case.

2.3.1 Horizontal conductance.

Horizontal conductance is conductance between adjacent cells across rows or columns. In the present version of SEAWAT, horizontal conductance is calculated using one of two methods for calculating the interblock transmissivity. The most common method is based on harmonic mean averaging, which assumes a piece-wise constant transmissivity distribution. The logarithmic mean also can be used for interblock averaging if it can be assumed that transmissivity varies linearly between cells. As an example, suppose cells 1 and 2 are adjacent across either rows or columns. To compute the conductance, $COND$, between two cells, Equation (6) is first used to calculate the conductance for each cell:

$$C_1 = \frac{\mu_f}{\mu_1} \frac{T_1^* W}{L_1} \text{ and } C_2 = \frac{\mu_f}{\mu_2} \frac{T_2^* W}{L_2} \quad (8)$$

If the harmonic mean method is selected, for example, then these conductances are substituted into $COND = \frac{C_1 C_2}{C_1 + C_2}$ (Equation 13 in the MODFLOW user's guide (Harbaugh et al., 2000)) to obtain, with some simplification,

$$COND = \mu_f W \frac{2T_1^* T_2^*}{T_1^* \mu_2 L_2 + T_2^* \mu_1 L_1} \quad (9)$$

2.3.2 Vertical conductance.

Vertical conductance is calculated using the harmonic average between cells that are adjacent across layers. Suppose cells 1 and 2 are adjacent across layers. To compute the conductance, $COND$, between the cells, substitute the conductances, Equation (7), of the two cells:

$$C_1 = \frac{\mu_f}{\mu_1} \frac{K_1 W L}{B_1} \text{ and } C_2 = \frac{\mu_f}{\mu_2} \frac{K_2 W L}{B_2}, \quad (10)$$

into $COND = \frac{C_1 C_2}{C_1 + C_2}$. This gives, after some simplification,

$$COND = \mu_f W L \frac{2K_1 K_2}{K_1 \mu_2 B_2 + K_2 \mu_1 B_1}. \quad (11)$$

3. HENRY-HILLEKE PROBLEM

The Henry problem (Henry, 1964) is a classic variable density flow problem, which is of particular interest in the context of saltwater intrusion along coastal areas. SEAWAT results for the Henry problem have been previously published (Guo and Langevin, 2002). In 1972, Henry and Hilleke expanded Henry's earlier work to include the effects of temperature-dependent density on the Henry problem (Henry and Hilleke, 1972). Since that time, HST3D

and the recently developed SUTRA-MS have been tested using this problem (Hughes and Sanford, 2004), and we compare our results to the SUTRA-MS solution here.

The Henry-Hilleke problem domain is rectangular and the problem has been simulated at a variety of aspect ratios. We present results for a square 1m-by-1m domain. In keeping with previous literature (Henry and Hilleke, 1972; Hughes and Sanford, 2004), concentration and temperature contour plots are shown on a grid reduced by a factor of 3 in the vertical direction. We show our results overlying the SUTRA-MS results. HST3D results are very similar to the SUTRA-MS results as shown by Hughes and Sanford (2004).

Constant temperature boundary conditions surround the domain. The southwestern corner is hot at 50°C, while the eastern boundary is cool at 5°C. There is a linear gradient in temperature from the hot southwestern corner to the cool eastern boundary as shown in Figure 1b. This corresponds to warm subterranean freshwater and cool seawater.

The Henry-Hilleke problem is designed to evaluate the influence of this temperature gradient between the land side and the sea side on Henry's original isothermal seawater intrusion scenario (Henry, 1964), which we present below. For the Henry-Hilleke problem,

the equation of state for fluid density uses the following values: $\rho_f = 1000 \text{ kg m}^{-3}$, $\frac{d\rho}{dC} = 0.7$,

and $\frac{d\rho}{dT} = -0.375 \text{ kg m}^{-3} \text{ }^\circ\text{C}^{-1}$.

The grid is 41-by-41 cells with $dx = dy = 0.025 \text{ m}$. This actually gives a slightly larger than 1m-by-1m domain, but allows our cell-centered finite difference grid points to exactly overlay the SUTRA vertex-centered finite element grid points. We run the simulation for about 0.5 days with time steps of 0.00069444 days (=60 seconds), which is long enough for equilibration in all cases shown here. The full set of parameters is shown in TABLE 1.

TABLE 1. Henry-Hilleke parameters.

Parameter	Variable	Value
Equivalent Freshwater Hydraulic Conductivity	K	864 m d ⁻¹ (=0.01 m s ⁻¹)
Porosity	θ	0.35
Equivalent Freshwater Viscosity	μ	86.4 kg m ⁻¹ d ⁻¹ (=0.001 kg m ⁻¹ s ⁻¹)
Molecular Diffusion	D_m	2.0571 m ² d ⁻¹ (=2.381×10 ⁻⁵ m ² s ⁻¹)
Thermal Diffusivity	D^*	20.571 m ² d ⁻¹ (=2.381×10 ⁻⁴ m ² s ⁻¹)
Longitudinal Dispersivity	α_l	0 m
Transverse Dispersivity	α_t	0 m
Inflow	Q_m	7.2 m ³ d ⁻¹ =(41 nodes)(0.1756 m ³ d ⁻¹) (=8.333 × 10 ⁻⁵ m ³ s ⁻¹)
Salinity Concentration in Freshwater	C_f	0 kg m ⁻³
Salinity Concentration in Sea Water	C_s	35.7 kg m ⁻³
Density of Freshwater	ρ_f	1000 kg m ⁻³
Density of Sea Water	ρ_s	1025 kg m ⁻³
Density Change with Concentration	$\frac{d\rho}{dC}$	0.7
Density Change with Temperature	$\frac{d\rho}{dT}$	-0.375 kg m ⁻³ °C ⁻¹

Figures 1b and c shows the simulation results. Contours of constant salinity concentration (referred to as isochlors here) are plotted in Figure 1c and isotherms are plotted in Figure 1d. The new SEAWAT results are plotted as thick colored contours. The SUTRA-MS results are plotted as thin gray contours. There is a difference in the isochlors near the upper right corner, but it is relatively minor.

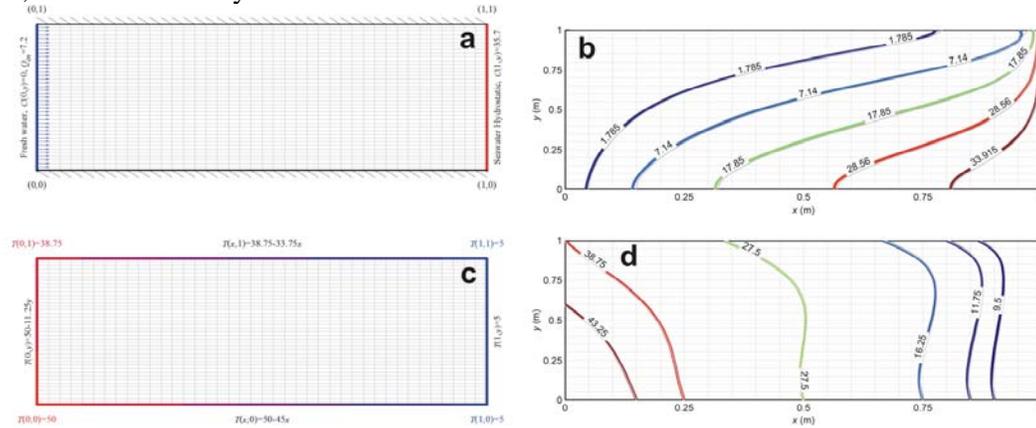


FIGURE 1. Domain with flow and concentration boundary conditions (a) and temperature boundary conditions (b). Flow in $\text{m}^3 \text{d}^{-1}$. Temperature in $^{\circ}\text{C}$. Simulation results are shown as isochlors (c) and isotherms (b). SEAWAT results in thick colored contours. SUTRA-MS results are plotted as thin gray contours

A possible explanation for the small differences between the SUTRA-MS and SEAWAT solutions may be the concentration units. SUTRA-MS uses mass fraction concentrations, whereas MT3DMS and hence SEAWAT use mass/volume concentrations.

4. CONCLUSIONS

The new version of SEAWAT introduced here is capable of simulating the simultaneous transport of heat and solute. The effect of temperature on fluid density is included through the addition of a new term to the equation of state. The new model also simulates the temperature and salinity dependence of viscosity. An initial test case verifies the new capabilities of the code. Comparison with the results of SUTRA-MS, which is capable of similar simulations, is good suggesting consistency with previous efforts. A key advantage of SEAWAT is that it is based on the widely used MODFLOW/MT3D packages and users of those models should find it straightforward to use.

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