SEAWAT Version 4: A Computer Program for Simulation of Multi-Species Solute and Heat Transport
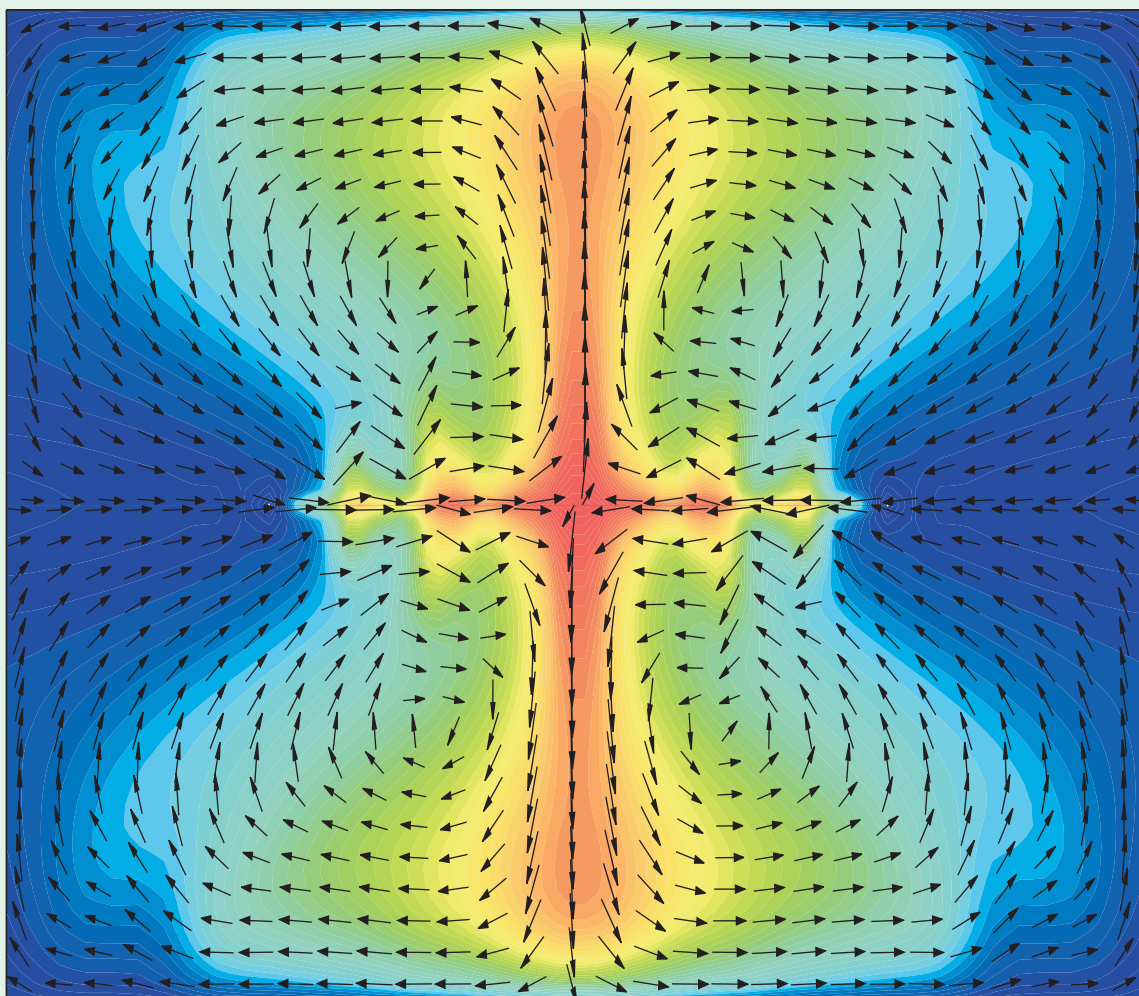

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SEAWAT Version 4: A Computer Program for Simulation of Multi-Species Solute and Heat Transport

Christian D. Langevin[1], Daniel T. Thorne, Jr.[2], Alyssa M. Dausman[1], Michael C. Sukop[3], and Weixing Guo[4]

[1] Florida Integrated Science Center, U.S. Geological Survey, Fort Lauderdale, Florida.
[2] Department of Mathematics, Physics, and Computer Science, Georgetown College, Georgetown, Kentucky.
[3] Department of Earth Sciences, Florida International University, Miami, Florida.
[4] Schlumberger Water Services, Fort Myers, Florida.

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Preface

This report describes an enhanced version of the SEAWAT computer program that can be obtained on the Internet as follows: *http://water.usgs.gov/software/ground_water.html/*

The performance of the program has been tested in a variety of applications. Future applications, however, might reveal errors that were not detected in the test simulations. Users are requested to send notification of any errors found in this User Guide or the model program to the contact listed on the SEAWAT website. Updates might be made to both the report and to the model program. Users can check for updates at the Internet address shown above.

SEAWAT Version 4 is a replacement for SEAWAT-2000. SEAWAT-2000 users are encouraged to use this new version, even if the features documented in this report are not required for a particular application. SEAWAT Version 4 is backward compatible with datasets created for SEAWAT-2000 and, therefore, SEAWAT-2000 is no longer supported or maintained.

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Conversion Factors

Multiply	By	To obtain
meter (m)	3.281	foot (ft)
kilogram per day (kg/d)	2.205	pound per day (lb/d)
kilogram per cubic meter (kg/m^3)	0.06242	pound per cubic foot (lb/ft^3)
square meter per day (m^2/d)	10.7636	square foot per day (ft^2/d)
square meter per second (m^2/s)	10.7636	square foot per second (ft^2/s)
Celsius (°C)	°F = (1.8 × °C) + 32	Fahrenheit (°F)

Acronyms and Abbreviations

BAS6	Basic	PCG2	Pre-Conditioned Conjugate Gradient
BCF	Block Centered Flow	RCT	Reactions
CHD	Time Variation Constant Head	SSM	Source and Sink Mixing
DSP	Dispersion	TDS	Total Dissolved Solids
GCG	Generalized Conjugate Gradient	VDF	Variable Density Flow
GWF	Ground Water Flow	VSC	Viscosity
HUF2	Hydrogeologic Unit Flow	g/L	gram per liter
IMT	Integrated MT3DMS Transport	J/kg°K	Joule per kilogram degrees Kelvin
LPF	Layer Property Flow		

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Abstract

The SEAWAT program is a coupled version of MODFLOW and MT3DMS designed to simulate three-dimensional, variable-density, saturated ground-water flow. Flexible equations were added to the program to allow fluid density to be calculated as a function of one or more MT3DMS species. Fluid density may also be calculated as a function of fluid pressure. The effect of fluid viscosity variations on ground-water flow was included as an option. Fluid viscosity can be calculated as a function of one or more MT3DMS species, and the program includes additional functions for representing the dependence on temperature. Although MT3DMS and SEAWAT are not explicitly designed to simulate heat transport, temperature can be simulated as one of the species by entering appropriate transport coefficients. For example, the process of heat conduction is mathematically analogous to Fickian diffusion. Heat conduction can be represented in SEAWAT by assigning a thermal diffusivity for the temperature species (instead of a molecular diffusion coefficient for a solute species). Heat exchange with the solid matrix can be treated in a similar manner by using the mathematically equivalent process of solute sorption. By combining flexible equations for fluid density and viscosity with multi-species transport, SEAWAT Version 4 represents variable-density ground-water flow coupled with multi-species solute and heat transport. SEAWAT Version 4 is based on MODFLOW-2000 and MT3DMS and retains all of the functionality of SEAWAT-2000.

SEAWAT Version 4 also supports new simulation options for coupling flow and transport, and for representing constant-head boundaries. In previous versions of SEAWAT, the flow equation was solved for every transport timestep, regardless of whether or not there was a large change in fluid density. A new option was implemented in SEAWAT Version 4 that allows users to control how often the flow field is updated. New options were also implemented for representing constant-head boundaries with the Time-Variant Constant-Head (CHD) Package. These options allow for increased flexibility when using CHD flow boundaries with the zero-dispersive flux solute boundaries implemented by MT3DMS at constant-head cells.

This report contains revised input instructions for the MT3DMS Dispersion (DSP) Package, Variable-Density Flow (VDF) Package, Viscosity (VSC) Package, and CHD Package. The report concludes with seven cases of an example problem designed to highlight many of the new features.

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[1] Florida Integrated Science Center, U.S. Geological Survey, Fort Lauderdale, Florida.
[2] Department of Mathematics, Physics, and Computer Science, Georgetown College, Georgetown, Kentucky.
[3] Department of Earth Sciences, Florida International University, Miami, Florida.
[4] Schlumberger Water Services, Fort Myers, Florida.

Introduction

SEAWAT is a coupled version of MODFLOW (Harbaugh and others, 2000) and MT3DMS (Zheng and Wang, 1999; Zheng, 2006) designed to simulate three-dimensional, variable-density ground-water flow and multi-species transport. The Variable-Density Flow (VDF) Process in SEAWAT is based on the constant-density Ground-Water Flow (GWF) Process of MODFLOW-2000. The VDF Process uses the familiar and well-established MODFLOW methodology to solve the variable-density ground-water flow equation (Langevin and others, 2003). The MT3DMS part of SEAWAT, referred to as the Integrated MT3DMS Transport (IMT) Process, solves the solute transport equation.

Previous versions of SEAWAT (Guo and Bennett, 1998; Guo and Langevin, 2002; Langevin and others, 2003) were developed for isothermal conditions, and thus, did not solve simultaneous solute and heat transport with the combined effects of concentration and temperature on variable-density flow. This restriction was due to the implementation of the equation of state for fluid density, which could be a function of only solute concentration. Furthermore, previous versions of SEAWAT did not represent the effects of fluid viscosity variations, which are most commonly caused by temperature variations. The updated version of SEAWAT described herein, called SEAWAT Version 4, or SEAWAT_V4, retains all of the capabilities of SEAWAT-2000, but is also able to simulate solute and heat transport simultaneously, as well as the effect that fluid viscosity variations have on resistance to ground-water flow.

Heat transport and solute transport contain many similarities (Anderson, 2005). Their mathematical representation is nearly identical when the terms describing heat transport are formulated in equivalent solute expressions. SEAWAT_V4 leverages these similarities by using MT3DMS to simulate heat transport. With this approach, temperature is one of the simulated species. Thorne and others (2006) provide a description of the approach and show how to assign appropriate thermal parameters for the temperature species.

Although SEAWAT_V4 was designed primarily to accommodate simultaneous solute and heat transport, the features that allow for this capability have been implemented in a general fashion that may be useful for other applications where temperature variations are not important. Other features have also been added to improve overall functionality. The new features are:

- The equation of state for fluid density can be a function of one or more MT3DMS species and, optionally, a pressure term.

- The effect of fluid viscosity on the internodal conductance terms can be included in a simulation by using the Viscosity (VSC) Package and the Layer Property Flow (LPF) Package. The equation for viscosity can be a function of one or more MT3DMS species. There is also an option to designate the temperature species, and to specify one of several non-linear equations to represent the dependence of viscosity on temperature.

- An option has been implemented to solve the VDF equation to update the flow field only if fluid densities have changed by some user-specified value. This option may substantially reduce runtimes for simulations in which a new flow solution is not necessarily required for each transport timestep.

- Auxiliary variables can now be used with the Time-Variant Constant-Head (CHD) Package to designate the fluid density value associated with the prescribed head. This option allows for more control of boundary heads specified with the CHD Package.

This user guide provides a brief description of new options available in SEAWAT_V4, describes the required input data files, and demonstrates the options with a simple example problem. This user guide describes only these new features, and does not provide all of the background material necessary for designing successful SEAWAT simulations. Background material is available in the published user guides for SEAWAT (Guo and Langevin, 2002), SEAWAT-2000 (Langevin and others, 2003), MODFLOW-2000 (Harbaugh and others, 2000), and MT3DMS (Zheng and Wang, 1999; Zheng, 2006).

Mathematical Formulation

This section presents the governing equations and the equations of state used to represent fluid density and viscosity as a function of state variables. The equations presented here do not explicitly allow for dissolution and precipitation of minerals that may likely result from large temperature changes and the heat lost or gained from those reactions. The formulation presented here is for water in the liquid phase only and does not represent the transition to ice or vapor.

Governing Equations for Flow and Transport

The VDF Process solves the following form of the variable-density ground-water flow equation (tensors and vectors shown in bold):

$$\nabla \cdot \left[\rho \frac{\mu_0}{\mu} \mathbf{K_0} \left(\nabla h_0 + \frac{\rho - \rho_0}{\rho_0} \nabla z \right) \right] = \rho S_{s,0} \frac{\partial h_0}{\partial t} + \theta \frac{\partial \rho}{\partial C} \frac{\partial C}{\partial t} - \rho_s q'_s, \tag{1}$$

where

ρ_0 is the fluid density [ML^{-3}] at the reference concentration and reference temperature;

μ is dynamic viscosity [ML^{-1}T^{-1}];

$\mathbf{K}_0$ is the hydraulic conductivity tensor of material saturated with the reference fluid [LT^{-1}];

h_0 is the hydraulic head [L] measured in terms of the reference fluid of a specified concentration and temperature (as the reference fluid is commonly freshwater). Note that h_0 was referred to as h_f in previous SEAWAT publications.

$S_{s,0}$ is the specific storage [L^{-1}], defined as the volume of water released from storage per unit volume per unit decline of h_0;

t is time [T];

θ is porosity [-];

C is salt concentration [ML^{-3}]; and

q'_s is a source or sink [T^{-1}] of fluid with density ρ_s.

The IMT Process solves the following form of the solute transport equation:

$$\left(1 + \frac{\rho_b K_d^k}{\theta} \right) \frac{\partial \left(\theta C^k \right)}{\partial t} = \nabla \cdot \left(\theta \mathbf{D} \cdot \nabla C^k \right) - \nabla \cdot \left(\mathbf{q} C^k \right) - q'_s C_s^k, \tag{2}$$

where

ρ_b is the bulk density (mass of the solids divided by the total volume) [ML^{-3}],

K_d^k is the distribution coefficient of species k [L^{3}M^{-1}],

C^k is the concentration of species k [ML^{-3}],

D is the hydrodynamic dispersion coefficient tensor [L^{2}T^{-1}],

q is specific discharge [LT^{-1}], and

C_s^k is the source or sink concentration [ML^{-3}] of species k.

In previous versions of SEAWAT, $\frac{\mu_0}{\mu}$ was approximated as one, and thus viscosity effects were neglected, and fluid density was treated as a simple linear function of only one solute species. In SEAWAT_V4, fluid density and viscosity can be calculated using concentrations from one or more solute species. These equations of state relate the density and viscosity terms in equation 1 to one or more of the MT3DMS species concentrations (C^k) in equation 2. As will be discussed later, equation 2 can also be used to represent heat transport. In this case, one of the MT3DMS solute species is used to represent temperature, and the mathematical terms describing heat transport are converted into forms analogous to those used in equation 2. By allowing one or more of the MT3DMS species to affect fluid density and viscosity, variable-density ground-water flow can be coupled with simultaneous solute and heat transport.

Fluid Density

The equation of state, which relates fluid density to solute concentration, temperature, and pressure, is typically written as a function of the volumetric expansion coefficient (Nield and Bejan, 1999). As presented in Diersch and Kolditz (2002), the volumetric expansion coefficients for solute concentration (β_C), temperature (β_T), and pressure (β_P) are:

$$\beta_C = \frac{1}{\rho}\left(\frac{\partial \rho}{\partial C}\right)_{T,P},$$
(3)

$$\beta_T = \frac{1}{\rho}\left(\frac{\partial \rho}{\partial T}\right)_{C,P}, \text{ and}$$
(4)

$$\beta_P = \frac{1}{\rho}\left(\frac{\partial \rho}{\partial P}\right)_{C,T},$$
(5)

where T is temperature [°K] and P is pressure [ML^{-1}T^{-2}]. Each expansion coefficient is expressed for one dependent variable (that is concentration, temperature or pressure) while holding the others fixed. If it also can be assumed that each volumetric expansion coefficient is constant over the range of expected values, a general equation of state for fluid density can be written as:

$$\rho = \rho_0 \exp\left[\beta_C\left(C - C_0\right) + \beta_T\left(T - T_0\right) + \beta_P\left(P - P_0\right)\right].$$
(6)

A linearized form of equation 6 is typically implemented in numerical flow and transport codes, such as SUTRA (Voss, 1984) and HST3D (Kipp, 1987), and is obtained using the first term of a series expansion (Bear, 1972). The linearized form is written as:

$$\rho = \rho_0 + \rho_0\beta_C\left(C - C_0\right) + \rho_0\beta_T\left(T - T_0\right) + \rho_0\beta_P\left(P - P_0\right),$$
(7)

or by expanding equation 7 around the reference density:

$$\rho = \rho_0 + \frac{\partial\rho}{\partial C}\left(C - C_0\right) + \frac{\partial\rho}{\partial T}\left(T - T_0\right) + \frac{\partial\rho}{\partial P}\left(P - P_0\right),$$
(8)

where:

$$\frac{\partial\rho}{\partial C} = \rho_0\beta_C,$$
(9)

$$\frac{\partial\rho}{\partial T} = \rho_0\beta_T, \text{ and}$$
(10)

$$\frac{\partial\rho}{\partial P} = \rho_0\beta_P.$$
(11)

For the transport of multiple solute species, where the concentration of each species can affect fluid density, Hughes and Sanford (2004) implemented the following equation of state (with the exception of the pressure term) in SUTRA-MS:

$$\rho = \rho_0 + \sum_{k=1}^{NS}\frac{\partial\rho}{\partial C^k}\left(C^k - C_0^k\right) + \frac{\partial\rho}{\partial T}\left(T - T_0\right) + \frac{\partial\rho}{\partial P}\left(P - P_0\right),$$
(12)

where NS is the number of solute species that affect fluid density. A difference between SEAWAT and SUTRA-MS is that SEAWAT is formulated in terms of a reference head, whereas SUTRA-MS is formulated in terms of pressure. For this reason, the third term on the right-hand side of equation 12 is reformulated here using the height of a water column ℓ [L] of density, ρ_0. This variable, which can be thought of as the pressure head in terms of the reference density, is related to pressure by:

$$P = \ell\rho_0 g,$$
(13)

where $\ell = h_0 - z$. With some simple rearrangement, the final form of the equation of state used and implemented in the program is:

$$\rho = \rho_0 + \sum_{k=1}^{NS}\frac{\partial\rho}{\partial C^k}\left(C^k - C_0^k\right) + \frac{\partial\rho}{\partial T}\left(T - T_0\right) + \frac{\partial\rho}{\partial\ell}\left(\ell - \ell_0\right),$$
(14)

where $\frac{\partial\rho}{\partial\ell}$ can be calculated from the volumetric expansion coefficient for pressure, β_P, using:

$$\frac{\partial\rho}{\partial\ell} = \rho_0^2 g\beta_P.$$
(15)

Fluid Viscosity

Dynamic viscosity is considered here to be a function of only temperature and solute concentration, which is the typical approach (Diersch and Kolditz, 2002), and neglects the weak dependence of viscosity on fluid pressure. This approach is also used in other ground-water modeling codes such as HST3D (Kipp, 1987) and SUTRA-MS (Hughes and Sanford, 2004). A general equation for representing fluid viscosity as a function of concentration and temperature is:

$$\mu = \mu_0 + \sum_{k=1}^{NS} \frac{\partial \mu}{\partial C^k}\left(C^k - C_0^k\right) + \frac{\partial \mu}{\partial T}\left(T - T_0\right). \tag{16}$$

This linear equation is one of the options available in SEAWAT_V4.

Over many temperature ranges, the linear approximation does not adequately represent the effect of temperature on dynamic viscosity. For this reason, an alternative equation for dynamic viscosity has been implemented:

$$\mu = \mu_T(T) + \sum_{k=1}^{NS} \frac{\partial \mu}{\partial C^k}\left(C^k - C_0^k\right). \tag{17}$$

When using equation 17, users have several options for representing dynamic viscosity as a function of temperature. These options include:

$$\mu_T(T) = A_1 \cdot A_2^{\left(\frac{A_3}{T+A_4}\right)}, \tag{18}$$

$$\mu_T(T) = A_1 \cdot \left[A_2 + A_3(T + A_4)\right]^{A_5}, \text{ and} \tag{19}$$

$$\mu_T(T) = A_1 \cdot T^{A_2}. \tag{20}$$

Values for the *A* constants are specified by the user. These three equations are based on viscosity and temperature relations encountered in the literature. For example, SUTRA (Voss, 1984) uses the following viscosity and temperature relation:

$$\mu(T) = 239.4x10^{-7} \cdot 10^{\left(\frac{248.37}{T+133.15}\right)}, \tag{21}$$

where *T* is expressed in degrees Celsius. To use this same relation in SEAWAT_V4, the user would select equation 18 and specify values of 239.4 x 10⁻⁷, 10, 248.37, and 133.15 for A_1, A_2, A_3, and A_4, respectively. Values for *A* can be found in table 1.

Table 1. Values used in equations that relate dynamic viscosity to temperature in degrees Celsius.

[--, not applicable for this equation]

A_1	A_2	A_3	A_4	A_5	Equation (in report)	Reference
2.394 x 10⁻⁵	10	248.37	133.15	--	18	Voss (1984)
1 x 10⁻³	1	1.5512 x 10⁻²	-20	-1.572	19	Pawlowski (1991)
0.168	-1.0868	--	--	--	20	Guo and Zhao (2005)[*]

*Relation is for oil viscosity as a function of temperature (between 5 and 170 degrees Celsius). Relation is not applicable to water.

Implementation of Fluid Viscosity Effects on Ground-Water Flow

The variable-density form of Darcy's Law used in previous versions of SEAWAT was modified to include the effects of viscosity variations. The equations for including the viscosity terms in the finite-difference representation are given in Thorne and others (2006). The following are some general considerations for including viscosity effects in a SEAWAT simulation:

- The effects of viscosity variations are activated by using the Viscosity (VSC) Package;

- The effects of these viscosity variations are implemented only for the Layer-Property Flow (LPF) Package; the Block-Centered Flow (BCF) and Hydrogeologic Unit Flow (HUF2) Packages cannot be used with the VSC Package;

- Flows to or from boundaries (for example, river or general-head boundaries) are not adjusted for the effects of viscosity variations; and

- The VSC Package was designed specifically for the VDF Process, which means that the "VDF" file type must be included in the name file.

The LPF Package was modified to include the effects of viscosity variations for each of the different horizontal conductance weighting options. The LPF Package includes three weighting options for calculating the horizontal internodal conductances: harmonic, logarithmic, and a mixed method that uses the arithmetic mean for saturated thickness and the logarithmic mean for hydraulic conductivity. The LPF package supports only harmonic weighting for internodal conductances in the vertical direction.

Including the effects of viscosity, variations on ground-water flow required two programming modifications. First, the hydraulic conductivity of each cell is multiplied by $\dfrac{\mu_0}{\mu}$ (where μ represents the cell viscosity) before the internodal conductance is calculated using one of the weighting options. Second, the LPF Package was modified to ensure that the internodal conductances are recalculated each time the flow equation is solved; in a standard MODFLOW simulation, internodal conductances for a confined layer are calculated once at the start of a simulation and remain constant for the entire simulation. Thorne and others (2006) verified the viscosity implementation through a match with results from an equivalent analytical solution.

Use of MT3DMS to Simulate Heat Transport

The standard stand-alone version of MT3DMS can be used in its present form to approximate heat transport in porous media. For example, Martin and others (2001) used MT3DMS to simulate heat transport on Grand Cayman Island. A key assumption in using the standard stand-alone version of MT3DMS to represent heat transport is that temperature does not affect fluid density and viscosity, and thus, it is not necessary to couple flow and transport. Another limitation prior to MT3DMS version 5.2 was that simultaneous solute and heat transport during the same simulation could not be performed because only a single molecular diffusion coefficient (representative of all species) could be entered. Similarly, previous versions of SEAWAT could be used to approximate heat transport, provided that: (1) temperature was the only species included in the simulation; and (2) the effect of temperature variation on fluid density was the only feedback on ground-water flow (that is viscosity did not affect ground-water flow).

In SEAWAT_V4, both heat and multi-species solute transport can be performed in the same simulation, and as shown in the previous section, concentration and temperature affect ground-water flow through the density and viscosity terms. Simulation of simultaneous solute and heat transport is performed by simply treating temperature as a species in MT3DMS. The ability to enter different molecular diffusion coefficients for each species was implemented in MT3DMS version 5.2. This MT3DMS version has been implemented in SEAWAT_V4, thereby eliminating an important limitation to representing simultaneous solute and heat transport.

Analogous forms of the solute and heat transport equations highlight similarities between the two processes. These similarities are used to calculate the correct input values required by MT3DMS when representing heat transport. The following is a general form of the solute transport equation solved by MT3DMS:

$$\left(1 + \frac{\rho_b K_d^k}{\theta}\right)\frac{\partial\left(\theta C^k\right)}{\partial t} = \nabla \cdot \left[\theta\left(D_m^k + \boldsymbol{\alpha}\frac{\mathbf{q}}{\theta}\right) \cdot \nabla C^k\right] - \nabla \cdot \left(\mathbf{q}C^k\right) - q'_s C_s^k,\tag{22}$$

where $D_m^{\ k}$ is the molecular diffusion coefficient [$L^2 T^{-1}$] for species k, and $\boldsymbol{\alpha}$ is the dispersivity tensor [L]. The following is a form of the heat transport equation, which was manipulated by Thorne and others (2006) to highlight the similarity with the solute transport equation:

$$\left(1 + \frac{1-\theta}{\theta}\frac{\rho_s}{\rho}\frac{c_{Psolid}}{c_{Pfluid}}\right)\frac{\partial\left(\theta T\right)}{\partial t} = \nabla \cdot \left[\theta\left(\frac{k_{Tbulk}}{\theta\rho c_{Pfluid}} + \boldsymbol{\alpha}\frac{\mathbf{q}}{\theta}\right) \cdot \nabla T\right] - \nabla \cdot \left(\mathbf{q}T\right) - q'_s T_s,\tag{23}$$

where

ρ_s is the density of the solid (mass of the solid divided by the volume of the solid) [ML^{-3}],

c_{Psolid} is the specific heat capacity of the solid [$L^2 T^{-2}\,{}^{\circ}K^{-1}$],

c_{Pfluid} is the specific heat capacity of the fluid [$L^2 T^{-2}\,{}^{\circ}K^{-1}$],

k_{Tbulk} is the bulk thermal conductivity of the aquifer material [$ML^3 T^{-2}\,{}^{\circ}K^{-1}$], and

T_s is the source temperature [°K].

Note that ρ_b, ρ_s, and θ are related by: $\rho_b = \rho_s (1-\theta)$.

Specific relations are required when using MT3DMS to represent thermal equilibration between the fluid and solid, heat conduction, and a specified heat flux. There are no special considerations for representing advective heat transport (convection).

Thermal Equilibration between Fluid and Solid

The analogy between solute and heat transport is evident in equations 22 and 23. In equation 22, the factor preceding the time derivative on the left-hand side of the equation represents solute sorption. A similar term is shown in equation 23 and represents an equilibration of temperature between the fluid and solid. For solute and heat transport, this term acts as a "retardation coefficient" and causes a concentration or temperature front to move slower than the average linear flow velocity. To represent thermal equilibrium between the fluid and solid using MT3DMS, the thermal distribution factor, K_{d_temp} [$M^{-1}L^3$], can be calculated for the temperature species using the following equation:

$$K_{d\_temp} = \frac{c_{Psolid}}{\rho c_{Pfluid}}.\tag{24}$$

This expression contains the fluid density, which means that the user must assume a fluid density value prior to running the simulation. This is a limitation with the present implementation in SEAWAT_V4. It is unlikely, however, that model results will be highly sensitive to errors in this term, so use of a representative fluid density in the calculation of K_{d_temp} should provide satisfactory results for most simulations. Another limitation is that the specific heat capacity of water, and perhaps other substances, may not be constant over large temperature ranges. For example, Holzbecher (1998) reports that although the specific heat capacity for water remains constant at a value of about 4,200 J/kg °K for temperatures less than 100 °C, the value increases by about 40 percent over the range from 100 °C to 300 °C. Table 2 provides a list of specific heat capacity values for a variety of substances.

The linear sorption isotherm should be selected to represent the thermal exchange between the water and the solid. By using the linear isotherm, the thermal exchange between the fluid and solid is constant for different temperatures (that is, the exchange is not a function of temperature). For solute sorption (which is used here to represent thermal exchange), other isotherms are sometimes required to express the relation between the sorbed and dissolved solute.

Table 2. Values of specific heat capacity (c_p) and density for selected substances and materials.

[All values are at 25 °C unless otherwise noted. The rock densities listed here represent ρ_s. J/kg°K, joules per kilogram degrees Kelvin; kg/m^3, kilogram per cubic meter]

Substance	c_p (J/kg°K)*	ρ (kg/m^3)
Freshwater (liquid)	4.186×10^3	1.00×10^3
Freshwater (ice)	2.108×10^3 (at 0 °C)	0.92×10^3
Seawater	3.93×10^3 (at 2.2 °C)	1.025×10^3
Air	1.005×10^3	1.205 (at 20 °C)
Granite	7.9×10^2	**2.75×10^3
Marble	8.8×10^2	**2.80×10^3
Sandstone	9.2×10^2	**2.80×10^3
Limestone	8.4×10^2	**2.70×10^3
Dolostone	9.2×10^2	**2.90×10^3
Clay	9.2×10^2	*1.8×10^3 - 2.6×10^3
Quartz	7.1×10^2 (at 0 °C)	**2.64×10^3
Calcite	8.4×10^2 (average over 0–100 °C)	**2.71×10^3

*Engineering Tool Box (2007).

**Cote and Konrad (2005).

Heat Conduction

The solute transport process of molecular diffusion is mathematically similar to the heat transport process of thermal conduction. In both processes, transport occurs in response to a gradient (Fick's law for molecular diffusion and Fourier's law for heat conduction). The relation between equations 22 and 23 indicates that the molecular diffusion coefficient entered for the temperature species (D_{m_temp}) is:

$$D_{m\_temp} = \frac{k_{Tbulk}}{\theta \rho c_{Pfluid}} .$$

(25)

This thermal conduction term, D_{m_temp} [$L^2 T^{-1}$], is referred to here as the bulk thermal diffusivity. Hughes and Sanford (2004) present two equations for calculating the bulk thermal conductivity from the solid and fluid thermal conductivities (k_{Tfluid} and k_{Tsolid}, respectively). A simple arithmetic mean that is weighted by volume can be calculated using:

$$k_{Tbulk} = \theta k_{Tfluid} + (1 - \theta) k_{Tsolid} .$$

(26)

Evidence indicates that the geometric mean may also be appropriate for calculating the bulk thermal conductivity (Ingebritsen and Sanford, 1998). The bulk thermal conductivity can be calculated using the following geometric mean equation:

$$k_{Tbulk} = k_{Tfluid}^{\theta} k_{Tsolid}^{(1-\theta)} .$$

(27)

Whether using the arithmetic mean or the geometric mean, the value for D_{m_temp} entered into MT3DMS (as a molecular diffusion coefficient) to represent heat conduction could be calculated using equation 25 and either equation 26 or 27. Table 3 provides a list of thermal conductivity values for a variety of substances. Note that many of the thermal conductivity values in table 3 are for dry rock; bulk thermal conductivity values for saturated rock may be higher.

Table 3. Values of thermal conductivity (k_T) for selected substances and materials.

[All values are at 25 degrees Celsius, except for freshwater (ice), which is at 0 degrees Celsius]

Substance	k_T (W/[m °K])	Reference
Freshwater (liquid)	0.58	Engineering Tool Box (2007)
Freshwater (ice)	2.18	Engineering Tool Box (2007)
Air	0.024	Engineering Tool Box (2007)
Granite	1.73 - 3.98	Marble Institute of America (2007)
Quartzite	5.38	Marble Institute of America (2007)
Marble	2.07 - 2.94	Marble Institute of America (2007)
Sandstone	1.83 - 2.90	Marble Institute of America (2007)
Limestone	1.26 - 2.15	Marble Institute of America (2007)
Dolostone	3.8	Cote and Konrad (2005)
Clay	1	Ingebritsen and Sanford (1998)
Quartz	3	Engineering Tool Box (2007)
Calcite	3.59	Horai (1971)

    In MT3DMS versions prior to 5.2, the molecular diffusion coefficient was entered as a single value for each model layer. When using molecular diffusion to represent heat conduction, it may be necessary to enter variations of D_m within a model layer to characterize heterogeneity patterns. In version 5.2, MT3DMS was modified to allow D_m to be entered as a three-dimensional array. Thus, heat conduction can be represented using a heterogeneous distribution for thermal conductivity, porosity, and fluid density. Although it is possible that the thermal conductivity can be anisotropic—for example, where strong grain alignments characterize the aquifer fabric—this is not expected to be an important factor in most cases and only isotropic thermal conductivities can be entered into the model.

    There are several limitations with using the present implementation of the molecular diffusion process in MT3DMS to represent heat conduction:

  • The approach requires an isotropic representation of thermal conductivity;

  • A representative fluid density must be used to calculate D_{m_temp}, which is fixed for the entire simulation regardless of whether or not the fluid density changes; and

  • Over large temperature ranges, thermal conductivity (and therefore D_{m_temp}) is a function of temperature (Holzbecher, 1998).

These limitations are not considered to be overly restrictive; however, users are encouraged to evaluate their effects. For example, to quantify the limitation of having a fluid density term in equations 24 and 25, the user could recalculate the three-dimensional K_d and D_m input arrays using fluid densities calculated from a previous simulation.

Specified Heat Flux

    A heat flux expressed as energy per unit time, $\dot{E}$ [ML^{2}T^{-3}], may be specified for any model cell by using the "mass-loading source" option (ITYPE = 15) in the MT3DMS Source and Sink Mixing (SSM) Package. The appropriate "solute equivalent," denoted here as $\dot{M}_T$ [°KL^{3}T^{-1}] to enter in the SSM Package can be calculated using the following relation:

$$\dot{M}_T = \frac{\dot{E}}{\rho c_{Pfluid}} .$$

(28)

This calculated input value for $\dot{M}_T$ can be entered on a cell-by-cell basis in the SSM input file.

Additional Simulation Options in SEAWAT_V4

Two new simulation options have been added in SEAWAT_V4. The first option allows the user to control whether or not the flow field is recalculated based on a user-specified tolerance for the maximum change in fluid density at any cell. The second option allows for more flexibility in specifying heads with the CHD Package.

Flow-Field Update Control

In previous versions of SEAWAT, the flow and transport equations are solved for each transport timestep. For most problems that require the use of a variable-density code, such as SEAWAT, this is a conservative and reasonable approach. For some problems, however, it may not be necessary to solve the flow equation during each transport timestep. This is the case for standard applications of MT3DMS, where it is assumed that the dilute solute has no affect on fluid density.

To reduce computer runtimes, a new option was added to SEAWAT_V4 that allows the user to control how often the flow field is updated. Because this option cannot be used with the iterative coupling option in SEAWAT (NSWTCPL is assigned a value greater than 1), the flow-field update control is activated by assigning a -1 to NSWTCPL in the VDF Package input file. The user also specifies a value for the maximum change in fluid density (DNSCRIT). If the maximum change in fluid density (between the present transport timestep and the last transport timestep for which the flow field was updated) is less than DNSCRIT, then SEAWAT_V4 does not update the flow field. Once the maximum change in fluid density exceeds DNSCRIT, then SEAWAT_V4 updates the flow field by solving the flow equation. Sanford and Konikow (1985) implemented a similar option in the MOCDENSE computer code. Under the present implementation, SEAWAT_V4 will always solve for the flow field:

- If the density change since the last flow field update exceeds DNSCRIT at one or more cells,
- For the first transport timestep of the flow timestep, or
- For the last transport timestep of a flow timestep.

Users can evaluate the loss of accuracy that will result from using the flow-field update control. For a seawater intrusion problem, where the fluid density may vary between freshwater (1,000 kg/m^3) and seawater (1,025 kg/m^3), users may want to assess the compromise between shorter computer runtimes and loss of accuracy for different percentages of the density range. To update the flow field if the density changes by more than 10 percent of the freshwater-seawater range, users would specify a value of 2.5 kg/m^3 for DNSCRIT.

As a cautionary note, parameter estimation programs may require extremely precise sensitivities for accurate identification of an optimal parameter set. Because the flow-field update control can reduce accuracy, in perhaps a non-linear manner, use of the flow-field update control is not recommended when precise sensitivities are required by a parameter estimation program.

Options for Constant-Head Boundaries

Assignment and proper use of constant-head boundaries in MODFLOW is relatively straightforward. There are some widely recognized problems in that a constant-head boundary can provide or remove unrealistic quantities of water, but in general, measured heads from the field can be assigned directly to constant-head boundaries without problem. For variable-density systems, assignment of heads to model boundaries is less straightforward. The complication arises from the dependence of heads on fluid density. This complication can be avoided, provided the user recognizes that head values (whether observed in the field or simulated by a model) have an associated density to which that head is referenced.

SEAWAT-2000 reads and writes heads in terms of the density at the point where the head is measured (or simulated). These head values are called "point-water heads," "actual heads," "heads in terms of the native aquifer water," or just, "heads." After the point-water heads are read, SEAWAT converts them into heads in terms of the reference fluid density (ρ_0). Because ρ_0 is normally set to the density of freshwater, these reference heads are commonly referred to as equivalent freshwater heads. For heat and solute transport simulations or multi-species simulations where fluid density is dependent upon more than one species, the term "equivalent freshwater head" does not provide enough information and requires an additional qualifier, such as "at the reference temperature." The term "reference head," therefore, more clearly states the intended meaning. SEAWAT solves the flow equation in terms of the reference head; however, SEAWAT writes point-water heads to the output files. These point-water heads are referenced to the simulated density at that location and time.

The dependence of head on fluid density has important implications for assigning boundary heads, particularly when the density of the boundary head changes during the simulation. This commonly occurs when using the MT3DMS constant-head boundary condition (ITYPE = 1 in the SSM Package) to represent the ocean or other coastal water body. When this solute boundary type is applied, the concentration at the cell is calculated as part of the simulation, subject to the condition that there is no dispersive flux across the cell boundary. Additionally, any fluid entering the aquifer from the boundary cell is assigned a concentration equal to that specified by the user in the SSM input file. When a constant-concentration boundary condition is used (ITYPE = -1), the following issues do not apply.

As described in the SEAWAT-2000 documentation (Langevin and others, 2003), simulation results may vary slightly depending on whether the Basic (BAS6) or the CHD Package is used to assign constant-head boundaries. If the BAS6 Package is used to specify constant-head cells, the initial head is converted to a reference head using the initial fluid density array, and this reference head value remains constant during the simulation. If the CHD Package is used, the reference head value assigned to the boundary cell is updated prior to each transport timestep using the fluid density from the previous transport timestep. Thus, if the density changes in a constant-head cell, SEAWAT may produce different results depending on the method used to simulate the constant-head cell.

Previous implementations of the BAS6 and CHD methods for simulating constant-head cells in SEAWAT did not provide a robust approach for assigning boundary head values. Consider the model section shown in figure 1A where a constant-head boundary is assigned to the last column of cells to represent the ocean. The solute boundary assigned in the SSM input file (using ITYPE = 1) specifies that any flow into the model from the boundary is assigned seawater salinities. When flow is reversed, however, from the aquifer into the boundary, the salinity value calculated at the boundary cell may not necessarily equal the salinity value specified in the SSM input file. If seawater salinities were assigned everywhere as the initial condition for this simulation, the BAS6 approach would provide a reasonable representation of the head boundary; the reference head value at the boundary would be calculated using seawater densities (the initial densities), and the reference head value would be held constant for the duration of the simulation.

The BAS6 approach has two potential limitations: (1) the constant head (ocean level) cannot be changed during the simulation, and (2) this condition may not be appropriate for estuaries or boundaries in which the discharge can change the salinity of the boundary feature. In such cases, it is necessary to reference the specified point-water head to the calculated density at the boundary cell, rather than the initial density. Both of these limitations are avoided by using the CHD Package to simulate constant-head cells. With the CHD Package, the boundary head can change during the simulation, and the head value used for each transport timestep is referenced to the calculated density value at that cell. Although this method was appropriate for shallow estuaries or other features where ground-water discharge could change the surface water salinity, it was not appropriate for deep ocean boundaries, where it can reasonably be assumed that ocean salinity is not affected by fresh ground-water discharge.
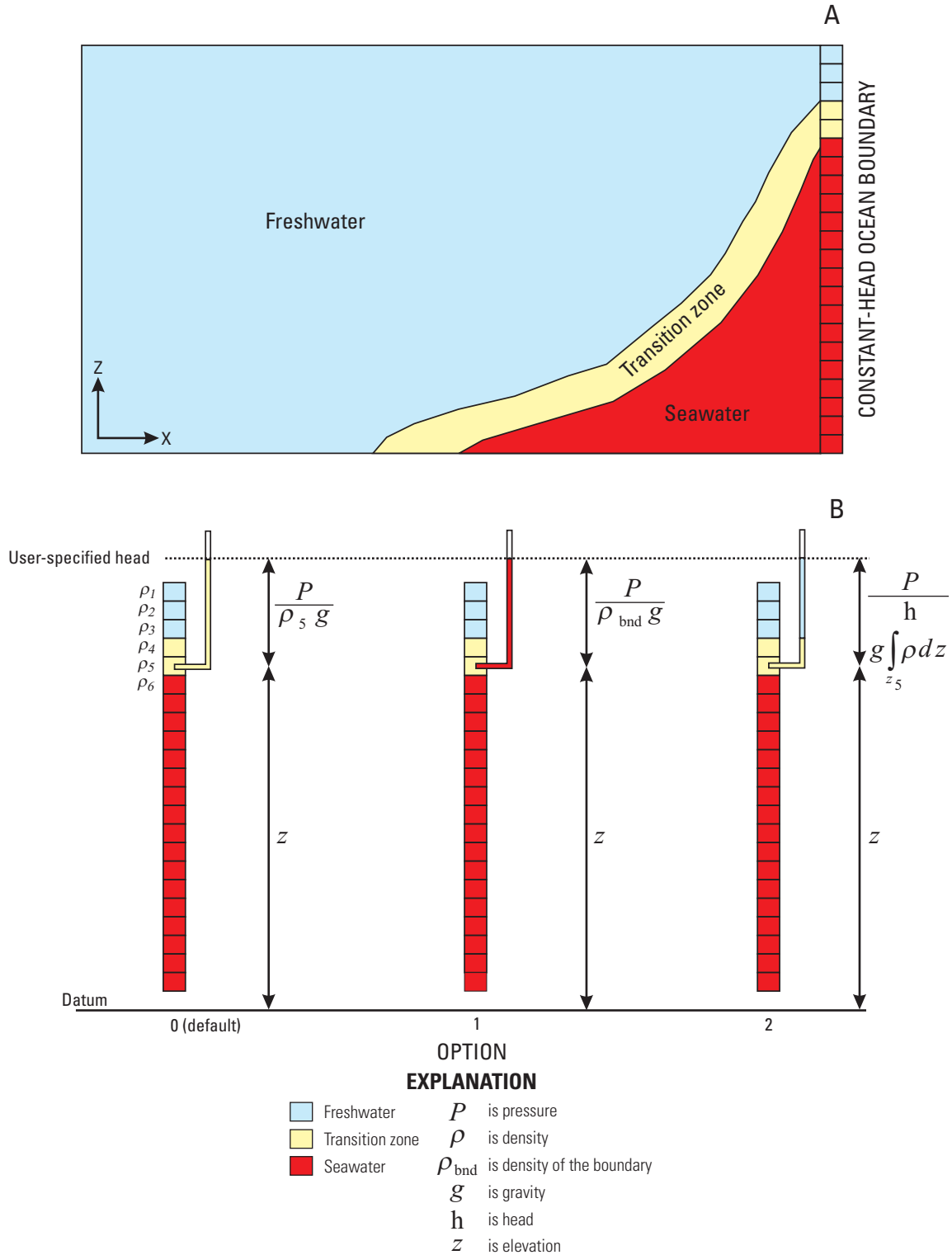
Figure 1. Density options used at constant-head boundaries to calculate boundary reference head: (A) a typical model section where the density at the boundary cells is calculated based on the flow system, and (B) different representations of the ocean boundary.

To increase flexibility in assigning boundary heads, three additional options were added for the CHD Package in SEAWAT_V4. As described later, the options are activated using auxiliary variables in the CHD Package. Figure 1B shows three of the four options available for representing boundary heads with the CHD Package. The options differ only in the assumed vertical density profile that is used to convert the assigned boundary head to the reference head (referenced to ρ_0) used in the solution to the flow equation. Option 0 is the default option, and was first implemented in SEAWAT-2000. With Option 0, the input head represents the point-water head in terms of the calculated density at the cell. With Option 1, the user also enters (within the CHD Package) the density (ρ_{bnd}) for which the input head is referenced. This option is appropriate for most types of ocean boundaries, where ρ_{bnd} would be assigned equal to the density of seawater. For Option 2, the density value used in the conversion of the input head to reference head is the average density of the overlying active cells. This option may be useful for inland settings with vertically stratified density distributions. With Option 2, the input head value can be conceptualized as environmental head (Lusczynski, 1961). Environmental heads are unique in that there is no vertical flow if the vertical gradient of the environmental head is zero. Thus, if the same input head value is assigned to all of the constant-head cells in a vertical column, this boundary type will result in hydrostatic conditions at that column. With Option 3, the final option, the user enters the reference head (freshwater head) directly and there is no adjustment in the program for density.

An important consequence of using either Option 1 or 2 is that the output heads written by SEAWAT_V4 may not equal the constant-head values that were entered as part of the CHD Package. This outcome is produced because SEAWAT writes point-water heads in terms of the calculated densities. Thus, extreme caution is necessary when using output heads from one model run as input to another when the CHD Package is used with either Option 1 or 2.

Input Instructions and Evaluation of Temperature Output

Multi-diffusive solute transport, whereby a unique diffusion coefficient can be entered for each MT3DMS species, is activated through the input file for the MT3DMS Dispersion (DSP) Package. The effect of multiple species on fluid density is invoked through the input file for the VDF Process. The effect of fluid viscosity on ground-water flow is activated through a new package in SEAWAT_V4, called the Viscosity (VSC) Package. The VSC Package works only with the LPF Package and is not compatible with the BCF or HUF2 Packages. Moreover, the VSC Package is compatible only with the VDF Process, and will not function for constant-density simulations (the VDF option is not included in the name file). Details on the input structure for the DSP, VDF, VSC, and CHD input files and an evaluation of simulated temperatures are presented herein.

MT3DMS Dispersion (DSP) Input File

In MT3DMS version 5.2, users can enter different diffusion coefficients for each species. With this option, the diffusion coefficient is entered as a three-dimensional array with one value for each model cell. In addition, users can enter molecular diffusion coefficients for solute species and a thermal conductivity parameter (eq. 25) for the temperature species. The new multi-diffusion option is described by Zheng (2006) and consists of entering the keyword "$MultiDiffusion" (case insensitive and without quotation marks) to the first non-commented line of the DSP input file. If this keyword is detected, MT3DMS (and SEAWAT_V4) uses the RARRAY utility (described in Zheng and Wang, 1999) to read a two-dimensional diffusion coefficient array for each layer. This process is repeated for each mobile solute component.

Variable-Density Flow (VDF) Process Input File

Input for the VDF Process is read from the file that is specified in the name file with "VDF" as the file type. All single-valued variables are free format if the option "FREE" is specified in the BAS6 Package input file; otherwise, the variables have 10-character fields. New input variables or variables that have new meaning in SEAWAT_V4 are underlined.

FOR EACH SIMULATION

0.   [#Text]

Item 0 is optional and the symbol # must be in column 1. Item 0 can be repeated multiple times, but it cannot be used in the file after the first data record.

1. MT3DRHOFLG MFNADVFD NSWTCPL IWTABLE

2. DENSEMIN DENSEMAX

Read Item 3 if NSWTCPL > 1 or NSWTCPL = -1

3. DNSCRIT

Read Item 4 if MT3DRHOFLG ≥ 0

4. DENSEREF DRHODC(1)

Read Item 4a through 4c if MT3DRHOFLG = -1

4a. DENSEREF DRHODPRHD PRHDREF

4b. NSRHOEOS

4c. MTRHOSPEC(NSRHOEOS) DRHODC(NSRHOEOS) CRHOREF(NSRHOEOS)

Item 4c is read as a table, with one row representing each MT3DMS species to be included in the equation of state for fluid density. There is no requirement that this table be sorted by MTRHOSPEC.

5. FIRSTDT

FOR EACH STRESS PERIOD

Read Items 6 and 7 only if MT3DRHOFLG = 0

6. INDENSE

Read Item 7 only if INDENSE is greater than zero

7. [DENSE(NCOL,NROW)] – U2DREL

Item 7 is read for each layer in the grid.

Explanation of Variables Read from the VDF Process Input File

Text—is a character variable (199 characters) that starts in column 2. Any characters can be included in Text. The "#" character must be in column 1. Except for the name file, lines beginning with # are restricted to these first lines of the file. Text is printed when the file is read.

MT3DRHOFLG—is the MT3DMS species number that will be used in the equation of state to compute fluid density. This input variable was formerly referred to as MTDNCONC (Langevin and others, 2003).

> If MT3DRHOFLG = 0, fluid density is specified using items 6 and 7, and flow will be uncoupled with transport if the IMT Process is active.

> If MT3DRHOFLG > 0, fluid density is calculated using the MT3DMS species number that corresponds with MT3DRHOFLG. A value for MT3DRHOFLG greater than zero indicates that flow will be coupled with transport.

> If MT3DRHOFLG = -1, fluid density is calculated using one or more MT3DMS species. Items 4a, 4b, and 4c will be read instead of item 4.

The dependence of fluid density on pressure head can only be activated when MT3DRHOFLG = -1. A value for MT3DRHOFLG of -1 indicates that flow will be coupled with transport.

MFNADVFD—is a flag that determines the method for calculating the internodal density values used to conserve fluid mass.

> If MFNADVFD = 2, internodal conductance values used to conserve fluid mass are calculated using a central-in-space algorithm.

> If MFNADVFD ≠ 2, internodal conductance values used to conserve fluid mass are calculated using an upstream-weighted algorithm.

NSWTCPL—is a flag used to determine the flow and transport coupling procedure.

> If NSWTCPL = 0 or 1, flow and transport will be explicitly coupled using a one-timestep lag. The explicit coupling option is normally much faster than the iterative option and is recommended for most applications.

> If NSWTCPL > 1, NSWTCPL is the maximum number of non-linear coupling iterations for the flow and transport solutions. SEAWAT-2000 will stop execution after NSWTCPL iterations if convergence between flow and transport has not occurred.

> If NSWTCPL = -1, the flow solution will be recalculated only for:

>> The first transport step of the simulation, or

>> The last transport step of the MODFLOW timestep, or

>> The maximum density change at a cell is greater than DNSCRIT.

IWTABLE—is a flag used to activate the variable-density water-table corrections (Guo and Langevin, 2002, eq. 82).

> If IWTABLE = 0, the water-table correction will not be applied.

> If IWTABLE > 0, the water-table correction will be applied.

DENSEMIN—is the minimum fluid density. If the resulting density value calculated with the equation of state is less than DENSEMIN, the density value is set to DENSEMIN.

If DENSEMIN = 0, the computed fluid density is not limited by DENSEMIN (this is the option to use for most simulations).

If DENSEMIN > 0, a computed fluid density less than DENSEMIN is automatically reset to DENSEMIN.

DENSEMAX—is the maximum fluid density. If the resulting density value calculated with the equation of state is greater than DENSEMAX, the density value is set to DENSEMAX.

If DENSEMAX = 0, the computed fluid density is not limited by DENSEMAX (this is the option to use for most simulations).

If DENSEMAX > 0, a computed fluid density larger than DENSEMAX is automatically reset to DENSEMAX.

DNSCRIT—is a user-specified density value. If NSWTCPL is greater than 1, DNSCRIT is the convergence criterion, in units of fluid density, for convergence between flow and transport. If the maximum fluid density difference between two consecutive implicit coupling iterations is not less than DNSCRIT, the program will continue to iterate on the flow and transport equations, or will terminate if NSWTCPL is reached. If NSWTCPL is -1, DNSCRIT is the maximum density threshold, in units of fluid density. If the fluid density change (between the present transport timestep and the last flow solution) at one or more cells is greater than DNSCRIT, then SEAWAT_V4 will update the flow field (by solving the flow equation with the updated density field).

DENSEREF—is the fluid density at the reference concentration, temperature, and pressure. For most simulations, DENSEREF is specified as the density of freshwater at 25 °C and at a reference pressure of zero.

DRHODC—formerly referred to as DENSESLP (Langevin and others, 2003), is the slope of the linear equation of state that relates fluid density to solute concentration. In SEAWAT_V4, separate values for DRHODC can be entered for as many MT3DMS species as desired. If DRHODC is not specified for a species, then that species does not affect fluid density. Any measurement unit can be used for solute concentration, provided DENSEREF and DRHODC are set properly. DRHODC can be approximated by the user by dividing the density difference over the range of end-member fluids by the difference in concentration between the end-member fluids.

For many applications, the end-member fluids are freshwater and seawater. Therefore, if the measurement units for both density and solute concentration are either kilograms per cubic meter or pounds per cubic feet, the value for DRHODC is about 0.7143. Users may also prefer to use relative concentrations, such that freshwater has a concentration of zero, and seawater has a concentration of 1.0. If relative concentrations are used with density values in units of kilograms per cubic meter, the appropriate DRHODC value is about 25.

SEAWAT_V4 offers the flexibility to use a variety of different solute concentrations to calculate fluid density, provided DRHODC is specified correctly. For example, users can utilize MT3DMS to simulate the concentration of total dissolved solids (TDS), chloride concentration, or the relative seawater concentration on a scale from 0 to 1. Use of TDS as the solute species for the fluid density calculation is straightforward, and is described in Guo and Langevin (2002, p. 18). If chloride is used for the fluid density calculation, a constant ratio between chloride concentration and TDS normally has to be assumed. For seawater and mixtures of seawater with freshwater, the ratio between chloride concentration and TDS is about 55 percent (19 g/L of chloride per 35 g/L of TDS). In some cases, particularly at relatively low TDS concentrations, this constant ratio may no longer hold. In these cases, caution is necessary in defining the relation between concentration and fluid density. If the linear relation implemented in SEAWAT_V4 is not appropriate, users may need to add a new equation of state and recompile the program. Regardless of the approach, simple hand calculations of fluid density are suggested as a way of ensuring that the correct input values are being used.

DRHODPRHD—is the slope of the linear equation of state that relates fluid density to the height of the pressure head (in terms of the reference density). Note that DRHODPRHD can be calculated from the volumetric expansion coefficient for pressure using equation 15. If the simulation is formulated in terms of kilograms and meters, DRHODPRHD has an approximate value of 4.46×10^{-3} kg/m^4. A value of zero, which is typically used for most problems, inactivates the dependence of fluid density on pressure.

PRHDREF—is the reference pressure head. This value should normally be set to zero.

NSRHOEOS—is the number of MT3DMS species to be used in the equation of state for fluid density. This value is read only if MT3DRHOFLG = -1.

MTRHOSPEC—is the MT3DMS species number corresponding to the adjacent DRHODC and CRHOREF.

CRHOREF—is the reference concentration (C_0) for species, MTRHOSPEC. For most simulations, CRHOREF should be specified as zero. If MT3DRHOFLG > 0, CRHOREF is assumed to equal zero (as was done in previous versions of SEAWAT).

FIRSTDT—is the length of the first transport timestep used to start the simulation if both of the following two conditions are met:

1. The IMT Process is active, and

2. Transport timesteps are calculated as a function of the user-specified Courant number (the MT3DMS input variable, PERCEL, is greater than zero)

INDENSE—is a flag. INDENSE is read only if MT3DRHOFLG is equal to zero.

If INDENSE < 0, values for the DENSE array will be reused from the previous stress period. If it is the first stress period, values for the DENSE array will be set to DENSEREF.

If INDENSE = 0, values for the DENSE array will be set to DENSEREF.

If INDENSE ≥ 1, values for the DENSE array will be read from item 7.

If INDENSE = 2, values read for the DENSE array are assumed to represent solute concentration, and will be converted to density values using the equation of state.

DENSE—is the fluid density array read for each layer using the MODFLOW-2000 U2DREL array reader. The DENSE array is read only if MT3DRHOFLG is equal to zero. The DENSE array may also be entered in terms of solute concentration, or any other units, if INDENSE is set to 2 and the constants used in the density equation of state are specified appropriately.

Viscosity (VSC) Package Input File

Input for the VSC Package is read from the file that is specified in the name file with "VSC" as the file type. The VDF Process must be active in order to use the VSC Package. In addition, the VSC Package works only with the LPF Package and is not compatible with the BCF or HUF2 Packages. All variables in the VSC input file are read using free format.

FOR EACH SIMULATION

0.   [#Text]

Item 0 is optional and the symbol # must be in column 1. Item 0 can be repeated multiple times.

1. MT3DMUFLG

2. VISCMIN VISCMAX

Read item 3 if MT3DMUFLG ≥ 0

3. VISCREF DMUDC(1) CMUREF(1)

Read item 3a through 3c if MT3DMUFLG = -1

3a. VISCREF

3b. NSMUEOS MUTEMPOPT

3c. MTMUSPEC(NSMUEOS) DMUDC(NSMUEOS) CMUREF(NSMUEOS)

Item 3c is read NSMUEOS times, once for each MT3DMS species to be included in the viscosity equation.

3d. MTMUTEMPSPEC AMUCOEFF(MUNCOEFF)

Item 3d is read if MUTEMPOPT > 0. The size of the AMUCOEFF coefficient array depends on the selected equation for viscosity.

FOR EACH STRESS PERIOD

Read items 4 and 5 only if MT3DMUFLG = 0

4. INVISC

Read item 5 only if INVISC is greater than zero

5. [VISC(NCOL,NROW)] – U2DREL

Item 5 is read for each layer in the grid.

Explanation of Variables Read from the VSC Package Input File

Text—is a character variable (199 characters) that starts in column 2. Any characters can be included in Text. The "#" character must be in column 1. Except for the name file, lines beginning with # are restricted to these first lines of the file. Text is printed when the file is read.

MT3DMUFLG—is the MT3DMS species number that will be used in the equation to compute fluid viscosity.

If MT3DMUFLG ≥ 0, fluid density is calculated using the MT3DMS species number that corresponds with MT3DMUFLG.

If MT3DMUFLG = -1, fluid viscosity is calculated using one or more MT3DMS species.

VISCMIN—is the minimum fluid viscosity. If the resulting viscosity value calculated with the equation is less than VISCMIN, the viscosity value is set to VISCMIN.

If VISCMIN = 0, the computed fluid viscosity is not limited by VISCMIN (this is the option to use for most simulations).

If VISCMIN > 0, a computed fluid viscosity less than VISCMIN is automatically reset to VISCMIN.

VISCMAX—is the maximum fluid viscosity. If the resulting viscosity value calculated with the equation is greater than VISCMAX, the viscosity value is set to VISCMAX.

If VISCMAX = 0, the computed fluid viscosity is not limited by VISCMAX (this is the option to use for most simulations).

If VISCMAX > 0, a computed fluid viscosity larger than VISCMAX is automatically reset to VISCMAX.

VISCREF—is the fluid viscosity at the reference concentration and reference temperature. For most simulations, VISCREF is specified as the viscosity of freshwater.

DMUDC—is the slope of the linear equation that relates fluid viscosity to solute concentration.

NSMUEOS—is the number of MT3DMS species to be used in the *linear* equation for fluid viscosity (this number does not include the temperature species if the nonlinear option is being used). This value is read only if MT3DMUFLG = -1. A value of zero indicates that none of the MT3DMS species have a linear effect on fluid viscosity (the nonlinear temperature dependence may still be activated); nothing should be entered for item 3c in this case.

MUTEMPOPT—is a flag that specifies the option for including the effect of temperature on fluid viscosity.

If MUTEMPOPT = 0, the effect of temperature on fluid viscosity is not included or is a simple linear relation that is specified in item 3c.

If MUTEMPOPT = 1, fluid viscosity is calculated using equation 18. The size of the AMUCOEFF array in item 3e is 4 (MUNCOEFF = 4).

If MUTEMPOPT = 2, fluid viscosity is calculated using equation 19. The size of the AMUCOEFF array in item 3e is 5 (MUNCOEFF = 5).

If MUTEMPOPT = 3, fluid viscosity is calculated using equation 20. The size of the AMUCOEFF array in item 3e is 2 (MUNCOEFF = 2).

If NSMUEOS and MUTEMPOPT are both set to zero, all fluid viscosities are set to VISCREF.

MTMUSPEC—is the MT3DMS species number corresponding to the adjacent DMUDC and CMUREF.

CMUREF—is the reference concentration for species, MTMUSPEC.

DMUDC—is the slope of the linear equation that relates fluid viscosity to solute concentration.

MTMUTEMPSPEC—is the MT3DMS species number that corresponds to temperature. This value must be between 1 and NCOMP and should not be listed in MTMUSPEC of item 3c.

AMUCOEFF—is the coefficient array of size MUNCOEFF. AMUCOEFF is "A" in equations 18, 19, and 20.

MUNCOEFF—is the size of the AMUCOEFF array.

INVISC—is a flag. INVISC is read only if MT3DMUFLG is equal to zero.

    If INVISC < 0, values for the VISC array will be reused from the previous stress period. If it is the first stress period, values for the VISC array will be set to VISCREF.

    If INVISC = 0, values for the VISC array will be set to VISCREF.

    If INVISC ≥ 1, values for the VISC array will be read from item 5.

    If INVISC = 2, values read for the VISC array are assumed to represent solute concentration, and will be converted to viscosity values.

VISC—is the fluid viscosity array read for each layer using the MODFLOW-2000 U2DREL array reader. The VISC array is read only if MT3DMUFLG is equal to zero. The VISC array may also be entered in terms of solute concentration (or any other units) if INVISC is set to 2, and the simple linear expression in item 3 can be used to represent the relation to viscosity.

Time-Variant Constant-Head (CHD) Package Input File

    The new options for specifying the density value assumed to correspond to the head values entered in the CHD Package are activated using auxiliary variables (Harbaugh and others, 2000). If the auxiliary variable "CHDDENSOPT" (in all uppercase) is detected in the CHD input file, then the program will read the CHD density option as an additional field. If all the values assigned to CHDDENSOPT are either 0 or 2, then no additional auxiliary variable is required. If, however, one or more CHD cells are assigned a value of 1 for CHDDENSOPT, then SEAWAT_V4 requires a user-specified density value for those cells. This density value must be entered through an additional auxiliary variable with the name "CHDDENS" (again in all uppercase). All three CHDDENSOPT options may be used within a single simulation. If option 1 is used for one or more CHD cells, the CHDDENS value will be required for all the CHD cells. The CHDDENS value will only be used, however, for those CHD cells with a CHDDENSOPT of 1. Table 4 provides a list of these options.

    An example of a simple CHD input file is shown below:

```
3 AUX CHDDENSOPT AUX CHDDEN
3           0
1           1           1 0.0000000 0.0000000  0 1025.000
2           1           1 0.0000000 0.0000000  1 1025.000
3           1           1 0.0000000 0.0000000  2 1025.000
```

This CHD input file will result in the assignment of CHD cells in layers 1, 2, and 3 of row 1 and column 1. CHD option 0 will be used for the CHD cell in layer 1. This option means that the assigned head value will be converted to reference head using the simulated density at that cell. CHD option 1 will be used for the CHD cell in layer 2. This option means that the assigned head value will be converted to a reference head using a density value of 1,025 kg/m^3 (entered in auxiliary variable "CHDDEN"). CHD option 2, used for the CHD cell in layer 3, indicates that the assigned head value is an environmental head that will be converted to a reference head using an average density value of the overlying CHD cells.

Table 4. Description of the options available for the Time-Variant Constant Head (CHD) Package.

CHDDENSOPT	CHDDEN	Description
0	Not used	Default option. Input head is converted to reference head (h_0) using calculated fluid density value at the cell.
1	Required	Input head is converted to reference head (h_0) using the density value specified in the CHDDEN auxiliary variable.
2	Not used	Input head is an environmental head and is converted to a reference head (h_0) using the average of the calculated fluid density values of the overlying active cells.
3	Not used	Input head is the reference head (h_0). No conversion is made.

Evaluating Temperature Output

Evaluating simulated temperatures is straightforward, and can be done using the same types of post-processing programs that are used to evaluate concentrations. Calculation of thermal energies, however, can be confusing because the "mass" values reported in the listing and mass budget files do not directly correspond with temperature or heat energy. The "mass" values reported by SEAWAT_V4 are calculated by multiplying temperature by a volumetric flux and the length of the transport timestep. Thus, for the temperature species, a reported mass value might have units of $m^3\,°C$ (or $\frac{m^3\,°C}{d}$ for a mass flux). These "mass" values (M_T) can be converted into thermal energy (E), using the following simple relation: $E = M_T \rho c_{Pfluid}$.

Example Problem

An example problem was developed to illustrate the new model features presented in this report. The problem consists of a two-dimensional cross section of a confined coastal aquifer initially saturated with relatively cold seawater at a temperature of 5 °C. Warmer freshwater with a temperature of 25 °C is injected into the coastal aquifer along the left boundary to represent flow from inland areas (fig. 1). The warmer freshwater flows to the right, where it discharges into a vertical ocean boundary. The ocean boundary is represented with hydrostatic conditions based on a fluid density calculated from seawater salinities at 5 °C. No-flow conditions are assigned to the top and bottom boundaries. A complete list of the input values used for the problem is given in table 5. This problem is a simplified representation of what might occur in a coastal carbonate platform.

Table 5. Input values for the example problem.

[m, meter; m/d, meter per day; J/(kg °C), joules per kilogram degrees Celsius; kg/m^3, kilogram per cubic meter; W/(m °C), watts per meter degrees Celsius; m^2/d, square meter per day; m^3/kg, cubic meter per kilogram; kg/(m^3 °C), kilogram per cubic meter degrees Celsius; kg/m^4, kilogram per meter to the 4th power]

	Input parameter	Value	Units	Comments
Grid properties	Number of columns (NCOL)	200	–	Assigned
	Number of rows (NROW)	1	–	Assigned
	Number of layers (NLAY)	100	–	Assigned
	Δx (DELR)	10	m	Assigned
	Δy (DELC)	1	m	Assigned
	Δz (DZ)	10	m	Assigned
Aquifer properties	Horizontal hydraulic conductivity (K_{h0})	10	m/d	
	Vertical hydraulic conductivity (K_{v0})	0.1	m/d	Assigned in terms of the reference fluid (at reference concentration and reference temperature)
	Specific storage (S_s)	1.00×10^{-5}	m	
	Porosity (θ)	0.35	–	Assigned
	Longitudinal dispersivity (α_L)	1	m	Assigned
	Transverse dispersivity (α_T)	0.1	m	Assigned
	Heat capacity of the solid (C_{Psolid})	835	J/(kg °C)	Approximate value for calcite
	Density of the solid (ρ_s)	2,710	kg/m^3	Approximate value for calcite
	Bulk density (ρ_b)	1,761.5	kg/m^3	Calculated from θ and ρ_s, $\rho_b = \rho_s(1-\theta)$
	Thermal conductivity of solid (k_{Tsolid})	3.59	W/(m °C)	Approximate value for calcite
	Bulk thermal conductivity (k_{Tbulk})	2.547	W/(m °C)	Volumetric weighted average (35% water, 65% calcite)
	Diffusion coefficient ($D_{m\_salinity}$)	1.00×10^{-10}	m^2/d	Assigned
	Bulk thermal diffusivity (D_{m_temp})	0.150309621	m^2/d	Calculated using eq. 25
Fluid properties	Heat capacity of the fluid (C_{Pfluid})	4,183	J/(kg °C)	Approximate value for water
	Thermal conductivity of water (k_{Tfluid})	0.61	W/(m °C)	Approximate value for water
	Distribution coefficient for salinity ($K_{d\_salinity}$)	0	m^3/kg	Assigned
	Distribution coefficient for temperature (K_{d_temp})	2.00×10^{-4}	m^3/kg	Calculated using eq. 24
	Reference density (ρ_0)	1,000	kg/m^3	Assigned
	$\delta\rho/\delta C$	0.7	–	Approximate change in density over change in salinity
	Reference concentration for density ($C_{\rho 0}$)	0	kg/m^3	Assigned
	$\delta\rho/\delta T$	-0.375	kg/(m^3 °C)	Approximate change in density over change in temperature
	Reference temperature (T_0)	25	°C	Assigned
	Reference viscosity	0.001	kg/(m s)	Assigned
	$\delta\mu/\delta C$	1.92×10^{-6}	m^2/d	Approximate change in viscosity over change in salinity
	Reference concentration for viscosity ($C_{\mu 0}$)	0	kg/m^3	Assigned
	Constants used for viscosity-temperature relation			Based on eq. 18
	A_1	2.394×10^{-5}	–	From Hughes and Sanford (2004)
	A_2	10	–	From Hughes and Sanford (2004)
	A_3	248.37	–	From Hughes and Sanford (2004)
	A_4	133.15	–	From Hughes and Sanford (2004)
	$\delta\rho/\delta\ell$	4.46×10^{-3}	kg/m^4	Calculated from water compressibility and eq. 15
Boundary conditions	Q_{inflow}	10	m^2/d	Assigned
	T_{inflow}	25	°C	Assigned
	C_{inflow}	0	kg/m^3	Assigned
	h_{ocean}	0	m	Head (or stage) of the ocean—not the freshwater head
	C_{ocean}	35	kg/m^3	Assigned
	T_{ocean}	5	°C	Assigned

To demonstrate the process of developing a numerical simulation of this problem, seven different cases are presented. For all of the cases, salinity is represented using species 1, and temperature is represented using species 2. For each case, a new process or feature is implemented in the model. A description of the seven cases is given in table 6.

Flow and transport were solved using identical solution procedures in all seven cases. Flow was solved using the Pre-Conditioned Conjugate Gradient (PCG2) Package. The head and flow convergence parameters were set at 1×10^{-5} m and 1 kg/d (mass per time), respectively. The advective term of the solute transport equation was solved using the Total-Variation Diminishing (TVD) option; the remaining terms (dispersion, source/sink mixing, reaction) were solved using the iterative Generalized Conjugate Gradient (GCG) solver with SSOR pre-conditioner. Each case was run in transient mode for 200,000 days (about 550 years). A Courant number of 1.0 was used to calculate the length of the transport timesteps. A length of 0.01 day was specified for the first transport timestep.

Table 6. Description of the cases simulated for the example problem.

Case	Salinity affects		Temperature affects		Heat conduction	Thermal equilibration with solid	Boundary heat conduction	Pressure affects density
	Density	Viscosity	Density	Viscosity				
1	x							
2	x		x					
3	x		x		x			
4	x		x		x	x		
5	x		x		x	x	x	
6	x	x	x	x	x	x	x	
7	x	x	x	x	x	x	x	x

Case 1

Case 1 is the simplest case and can be simulated with previous versions of SEAWAT. It is a variable-density simulation in which the fluid density is a function only of salinity. Although temperature is represented as species 2, it is represented as a conservative tracer in which thermal equilibration with the solid as well as heat conduction are not represented.

The name file for case 1 is as follows:

```
#SEAWAT LISTING FILE
LIST          7     coastal_flow.lst
#
#
#SEAWAT VDF INPUT FILE
VDF          80     coastal_flow.vdf
#
#
#MODFLOW INPUT FILES
BAS6          1     coastal_flow.bas
DIS          29     coastal_flow.dis
LPF          11     coastal_flow.lpf
WEL          12     coastal_flow.wel
OC           22     coastal_flow.oc
PCG          19     coastal_flow.pcg
#
#
```

```
#MT3DMS INPUT FILES
BTN           81      coastal_flow.btn
ADV           82      coastal_flow.adv
DSP           83      coastal_flow.dsp
SSM           84      coastal_flow.ssm
GCG           86      coastal_flow.gcg
#
#
#OUTPUT FILES
DATA(BINARY) 50 coastal_flow.cbb
DATA(BINARY) 30 coastal_flow.hds
```

All of the files listed in the name file are either output files created during the simulation, or standard MODFLOW or MT3DMS input files. The only exception to this is the VDF input file, which is specific to SEAWAT. The contents of the VDF input file (coastal_flow.vdf) are as follows:

```
        1           1      0      0     MT3DRHOFLG MFNADVFD NSWTCPL IWTABLE
    0.0000      0.0000                  DENSEMIN DENSEMAX
 1000.0000      0.7000                  DENSEREF DRHODC
1.0000e-02                              FIRSTDT
```

Three important values in this input file are MT3DRHOFLG = 1, DENSEREF = 1,000.0 kg/m^3, and DRHODC = 0.7. An MT3DRHOFLG value of 1 indicates that fluid density will be calculated using species 1 (salinity) in the equation of state. DENSEREF is the reference density (ρ_0), and DRHODC is the slope of the linear relation between density and salinity ($\delta\rho/\delta C$). With these values, density will vary linearly between 1,000.0 kg/m^3 for freshwater and 1,024.5 kg/m^3 for seawater.

The transient movement of the transition zone between freshwater and seawater is shown in figure 2 for five different simulation times. Temperature is not shown because the results are identical to the salinity results. Model results show that the transition zone, which is initially vertical, tilts toward the upper-right corner during the simulation due to the effects of fluid density. At the end of the 200,000-day simulation, the interface slopes gently upward toward the outflow boundary.
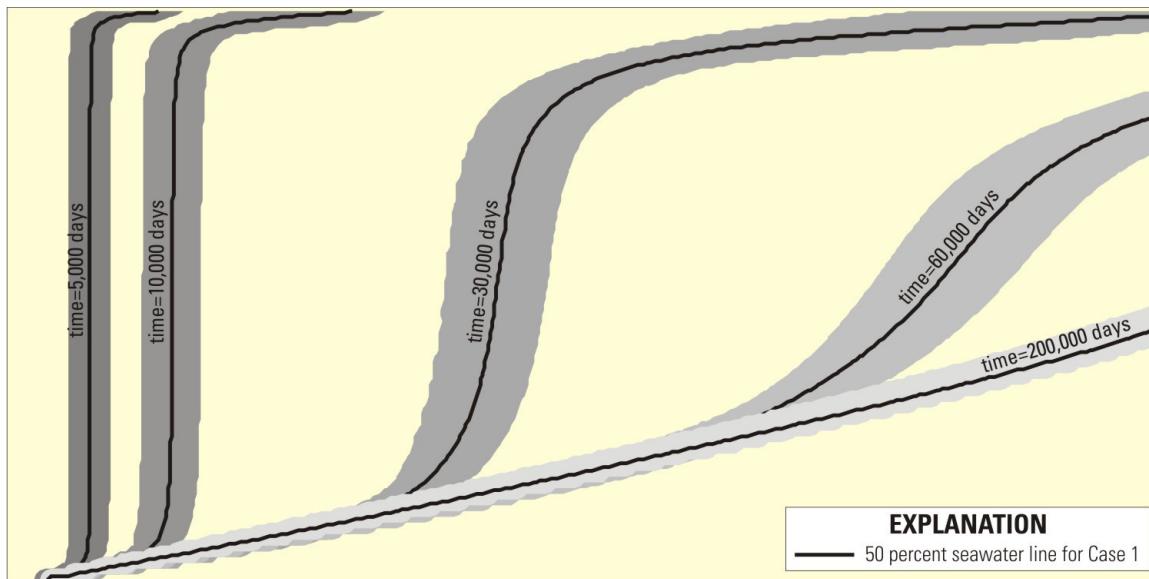

Figure 2. Transient movement of the freshwater-seawater transition zone for Case 1. Gray shading represents salinity values between 1 and 99 percent of seawater. The black lines represent a salinity value equal to 50-percent seawater.

Case 2

The effect of temperature on fluid density is activated for Case 2 (table 6). A linear expression is used to relate fluid density to temperature. The slope of that linear relation ($\frac{\partial \rho}{\partial T}$) is about -0.375 $\frac{\text{kg}}{\text{m}^3 \text{°C}}$. The negative sign indicates the fluid density increases as temperature decreases. As described earlier, more than one MT3DMS species can affect fluid density by entering -1 for MT3DRHOFLG in the VDF input file:

```
       -1          1         0         0      MT3DRHOFLG MFNADVFD NSWTCPL IWTABLE
   0.0000     0.0000                          DENSEMIN DENSEMAX
1000.0000     0.0000        0.                DENSEREF DRHODPRHD PRHDREF
        2                                     NSRHOEOS
        1     0.7000        0.                MTRHOSPEC(1) DRHODC(1) CRHOREF(1)
        2    -0.3750       25.                MTRHOSPEC(2) DRHODC(2) CRHOREF(2)
1.0000e-02                                    FIRSTDT
```

By entering a -1 for MT3DRHOFLG and a value of 2 for NSRHOEOS, the contributions of species 1 and 2 to the density equation of state are both included (as shown in lines 5 and 6 of the VDF input file).

Results from the Case 2 simulation are shown in figure 3. As before, temperature results are not shown because they correspond directly with salinities. The 50-percent seawater line for the five different times from Case 1 are also shown in figure 3 (as dashed lines) to illustrate the effect of including the temperature dependence on fluid density. By adding the temperature effect on fluid density, the transition zone moves more quickly at the top of the model than at the center or bottom of the model. The final shape of the transition zone is also sloped more steeply than for Case 1.

The Case 2 simulation could also have been performed using only a single species. Because no transport processes operate differently on salinity than on temperature, it is possible to reformulate the density equation of state to include the effects of both temperature and salinity. For example, temperature is a simple linear function of salinity for Case 2, where:

$$T = \left(\frac{T_{inflow} - T_{ocean}}{C_{inflow} - C_{ocean}} \right) C + \left(T_{inflow} - T_{ocean} \right) = -\frac{4}{7} C + 20 \ . \tag{29}$$

By substituting this equation into the equation of state for fluid density, the resulting DENSEREF and DRHODC values would be 1,000.0 kg/m³ and 0.914, respectively. If these values had been used for the Case 1 simulation, the results would be identical to the results shown for Case 2. This is true only because salinity and temperature are directly related. Heat conduction is included in the next case, and as a consequence, temperature is not directly related to salinity.
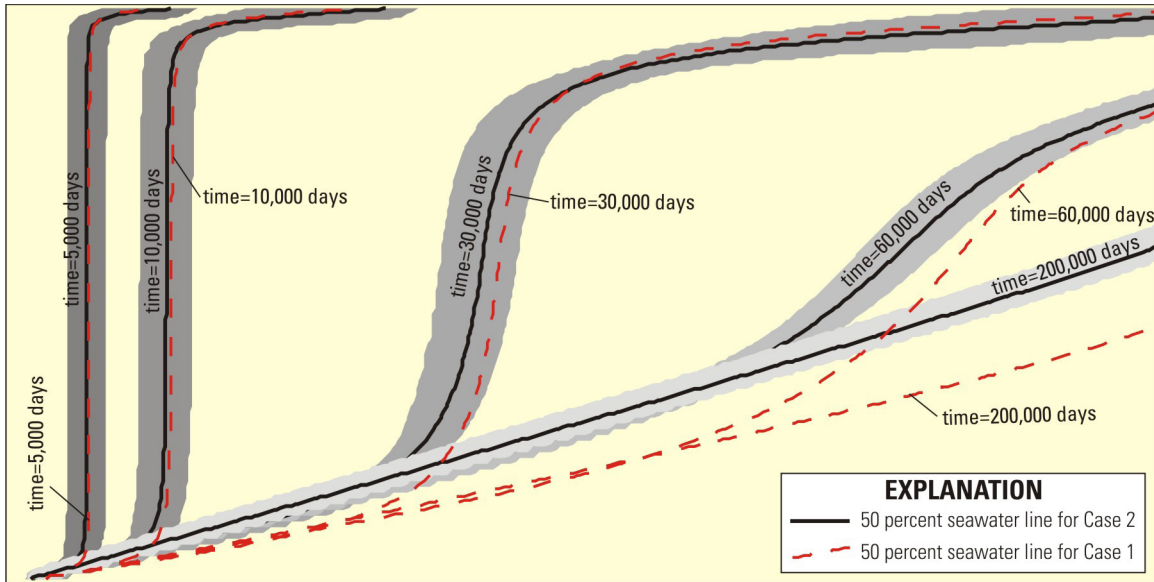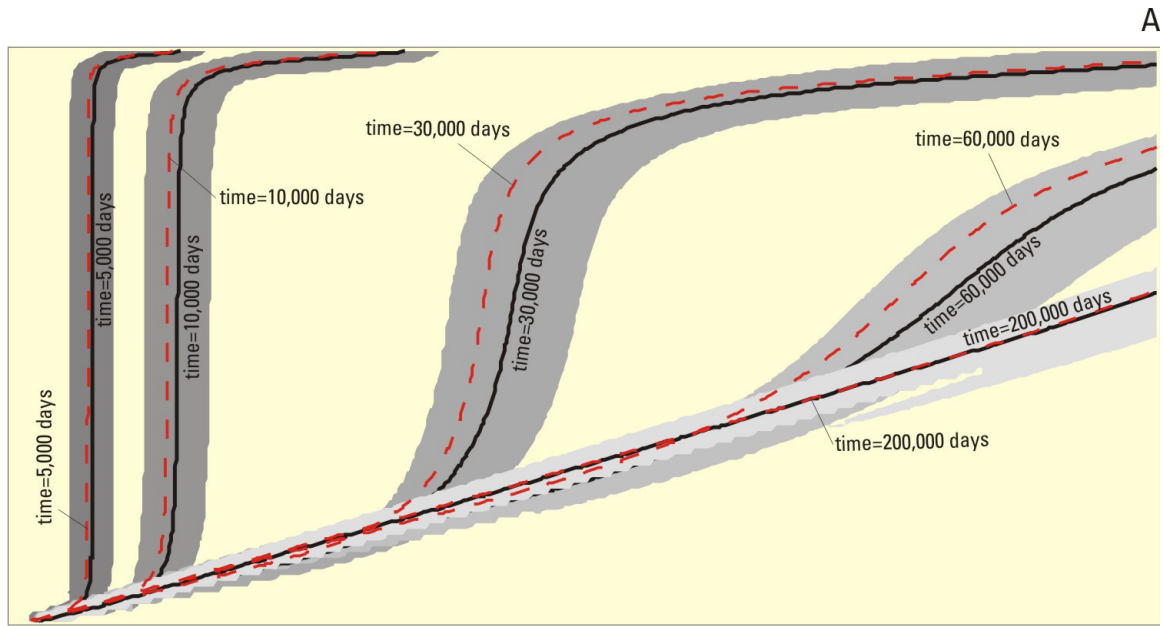
Figure 3. Transient movement of the freshwater-seawater transition zone for Case 2. Gray shading represents salinity values between 1 and 99 percent of seawater. The solid black lines represent a salinity value equal to 50-percent seawater for Case 2. Dashed lines represent the 50-percent seawater line for Case 1.

Case 3

In Case 3, heat conduction is included in the simulation by specifying a value for bulk thermal diffusivity (D_{m_temp}) within the DSP input file. A bulk thermal diffusivity value of 0.15 m^2/d (1.74 × 10^{-6} m^2/s) was calculated using equation 25; therefore, the following DSP input file is used for Case 3:

```
$MultiDiffusion
         0     1.000(10E12.4)        -1     DISPERSIVITY Layer    1
         0     1.000(10E12.4)        -1     DISPERSIVITY Layer    2
(layers 3 through 99 not shown)
         0     1.000(10E12.4)        -1     DISPERSIVITY Layer 100
         0     0.100(10E12.4)        -1     HZ DISPERSIVITY RATIO
         0     0.100(10E12.4)        -1     VT DISPERSIVITY RATIO
         0   1.0E-10                 -1     MOL DIFF SP 1 LAYER 001
         0   1.0E-10                 -1     MOL DIFF SP 1 LAYER 002
(layers 3 through 99 not shown)
         0   1.0E-10                 -1     MOL DIFF SP 1 LAYER 100
         0      0.15                 -1     MOL DIFF SP 2 LAYER 001
         0      0.15                 -1     MOL DIFF SP 2 LAYER 002
(layers 3 through 99 not shown)
         0      0.15                 -1     MOL DIFF SP 2 LAYER 100
```

For Case 3, the evolution of the salinity and temperature fields are no longer identical; the temperature transition zone is much more diffuse than the salinity transition zone (fig. 4).

A

EXPLANATION

— 50 percent seawater line for Case 3
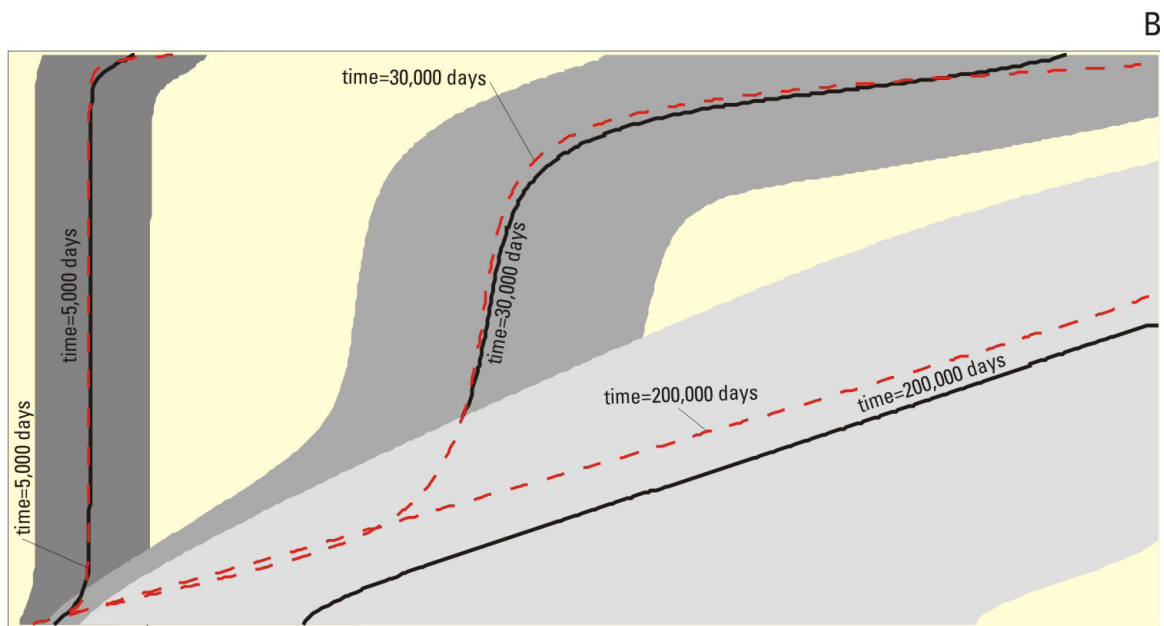
– – 50 percent seawater line for Case 2

B

Figure 4. Transient movement of the (a) salinity and (b) temperature transition zones for Case 3. Gray shading represents the 1 to 99 percent salinity or temperature values. The solid black lines represent the salinity or temperature value equal to 50 percent for Case 3. For comparison, dashed lines represent the 50-percent line for Case 2.
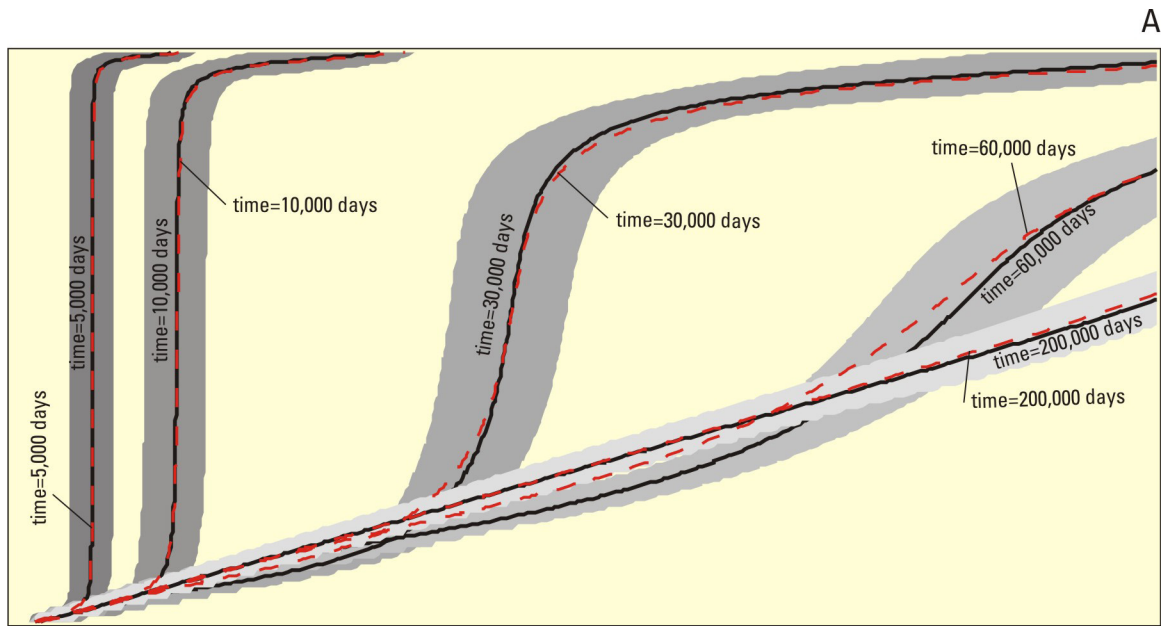
Case 4

In Case 4, thermal equilibration between the fluid and the solid matrix is included in the simulation. This feature is activated using the MT3DMS Reactions (RCT) Package, which has been added to the name file. This "reaction" process is activated only for the temperature species (species 2) by entering 2.0×10^{-4} m^3/kg for K$_{d\_temp}$. The following RCT input file is used for Case 4:

```
        1        0        2        0
        0 1760.000(10E12.4)           -1    Blk Dnsty         Lay   1
        0 1760.000(10E12.4)           -1    Blk Dnsty         Lay   2
(layers 3 through 99 not shown)
        0 1760.000(10E12.4)           -1    Blk Dnsty         Lay 100
        00.0000e+00(10E12.4)          -1    Kd Species 1      Lay   1
        00.0000e+00(10E12.4)          -1    Kd Species 1      Lay   2
(layers 3 through 99 not shown)
        00.0000e+00(10E12.4)          -1    Kd Species 1      Lay 100
        02.0000e-04(10E12.4)          -1    Kd Species 2      Lay   1
        02.0000e-04(10E12.4)          -1    Kd Species 2      Lay   2
(layers 3 through 99 not shown)
        02.0000e-04(10E12.4)          -1    Kd Species 2      Lay 100
        00.0000e+00(10E12.4)          -1    SP2 Sp 1 not used Lay   1
        00.0000e+00(10E12.4)          -1    SP2 Sp 1 not used Lay   2
(layers 3 through 99 not shown)
        00.0000e+00(10E12.4)          -1    SP2 Sp 1 not used Lay 100
        00.0000e+00(10E12.4)          -1    SP2 Sp 2 not used Lay   1
        00.0000e+00(10E12.4)          -1    SP2 Sp 2 not used Lay   2
(layers 3 through 99 not shown)
        00.0000e+00(10E12.4)          -1    SP2 Sp 2 not used Lay 100
```

Simulated salinities and temperatures for Case 4 are shown in figure 5. Simulated salinities are similar to the salinities from Case 3; however, the effect of including thermal equilibration with the solid substantially affects the transient response of the simulated temperatures. Inspection of figure 5 indicates that the temperature front in Case 4 is moving about half as fast as the temperature front in Case 3. This is consistent with a thermal retardation coefficient of about 2.0, which can be calculated directly from the thermal properties listed in table 5 and the pre-factor of the time derivative on the left-hand side of equation 23.

A

B

EXPLANATION

—————— 50 percent seawater line for Case 4

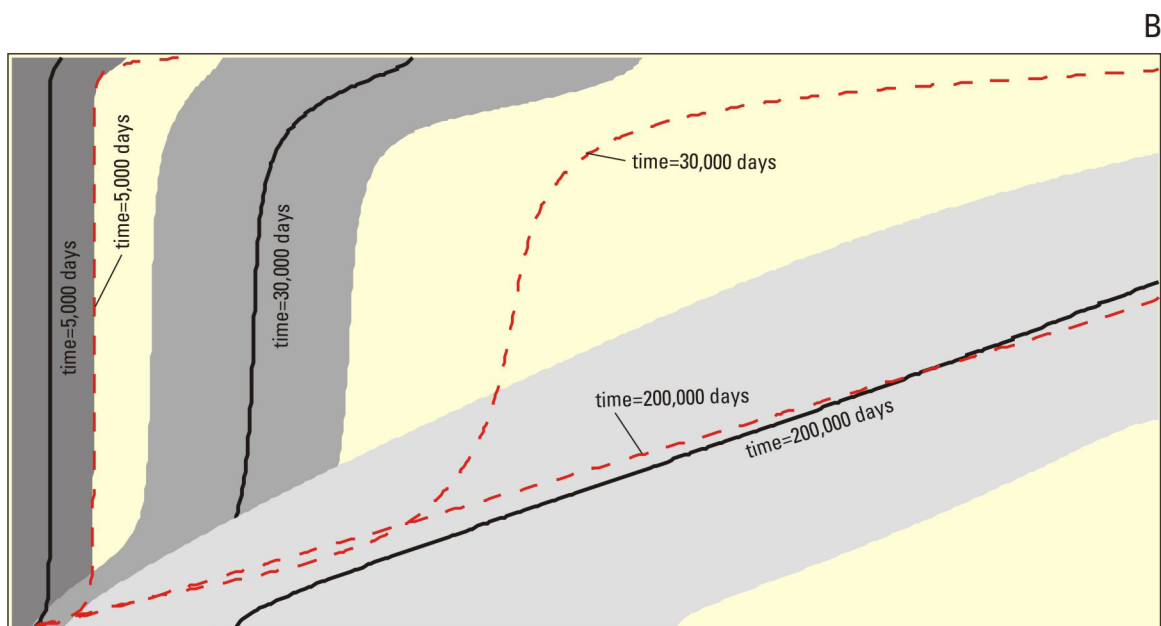– – – 50 percent seawater line for Case 3

Figure 5. Transient movement of the (a) salinity and (b) temperature transition zones for Case 4. Gray shading represents the 1 to 99 percent salinity or temperature values. The solid black lines represent the salinity or temperature value equal to 50 percent for Case 4. For comparison, dashed lines represent the 50-percent line for Case 3.
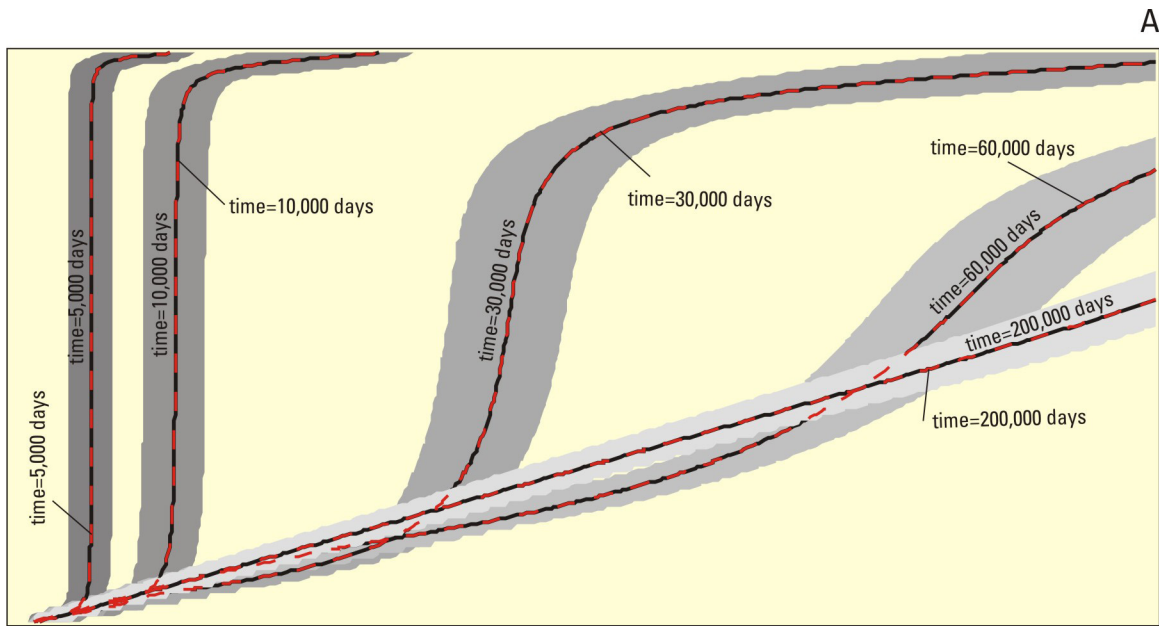
Case 5

Heat conduction at the seawater boundary is included in the Case 5 simulation by changing the MT3DMS boundary type for the temperature species to ITYPE = -1. By using the constant-head boundary type (ITYPE = 1 in the SSM input file), only advective transport (no dispersive transport) is allowed across the boundary. With this condition, the solute concentration (or temperature) value at the constant-head boundary can change from the value specified in the SSM input file. Without a dispersive flux across the boundary, there is no heat conduction. By setting ITYPE = -1 for temperature, the assigned temperature value will remain constant at the boundary, and heat conduction to or from the boundary will occur.

The SSM input file for Case 5 is as follows:

```
T F F F F F
      300
      300
        1          1      200 3.500e+01      1   3.500000e+001                    -1
        2          1      200 3.500e+01      1   3.500000e+001                    -1
(layers 3 through 99 not shown)
      100          1      200 3.500e+01      1   3.500000e+001                    -1
        1          1      200 3.500e+01     -1             -1  5.000000e+000
        2          1      200 3.500e+01     -1             -1  5.000000e+000
(layers 3 through 99 not shown)
      100          1      200 3.500e+01     -1             -1  5.000000e+000
        1          1        1 0.000e+00      2   0.000000e+000  2.500000e+001
        2          1        1 0.000e+00      2   0.000000e+000  2.500000e+001
(layers 3 through 99 not shown)
      100          1        1 0.000e+00      2   0.000000e+000  2.500000e+001
```

The first line indicates which flow packages are active. The "T" indicates that the well package is active. The second line specifies the maximum number of sources and sinks present in the simulation. The third line indicates the number of sources or sinks that are specified in the subsequent data record. The subsequent 300 lines contain layer, row, column, a dummy value, ITYPE, and the concentration value for each species. A negative concentration value indicates that this boundary type does not apply for this species. Thus, the first 100 lines indicate the right boundary has a zero dispersive flux (ITYPE = 1) for salinity (species 1) and that any solute entering from the boundary will have a concentration of 35 kg/m^3. The next 100 lines with an ITYPE = -1 indicate that temperature will be held constant at 5 ℃. The remaining 100 lines specify the salinity and temperature values for the inflow along the left boundary.

For this particular problem, the use of a constant temperature boundary does not have a substantial effect on the results (fig. 6). Simulated salinities for Case 5 are the same as those for Case 4. Including the boundary, heat conduction affects simulated temperatures slightly, but only near the vertical ocean boundary.
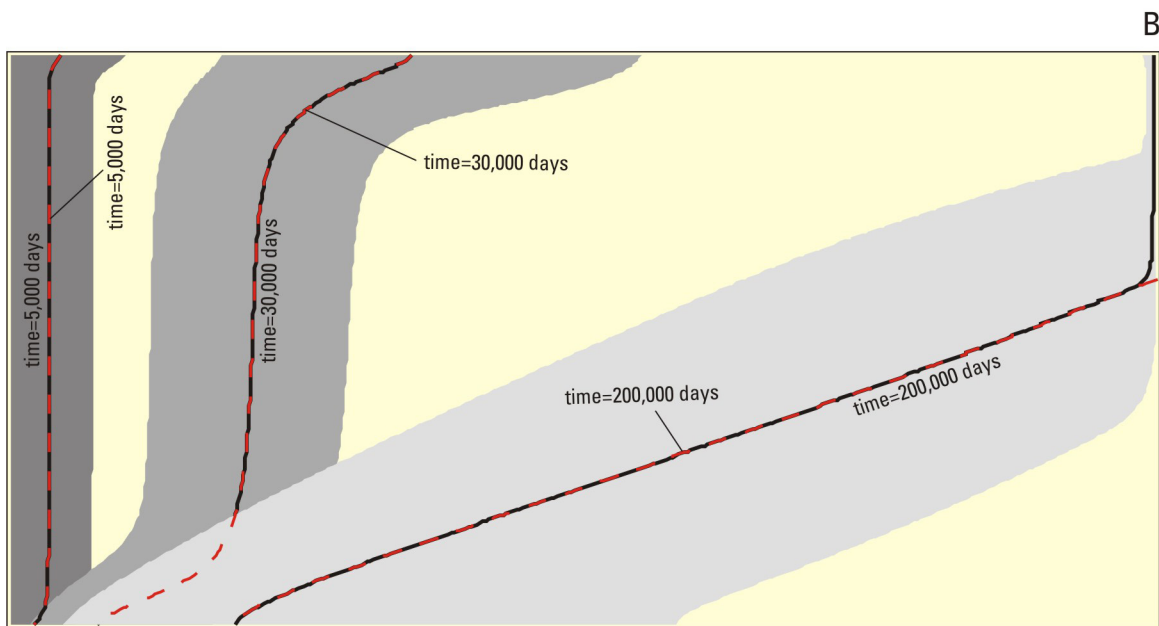
Figure 6. Transient movement of the (a) salinity and (b) temperature transition zones for Case 5. Gray shading represents the 1 to 99 percent salinity or temperature values. The solid black lines represent the salinity or temperature value equal to 50 percent for Case 5. For comparison, dashed lines represent the 50-percent line for Case 4.
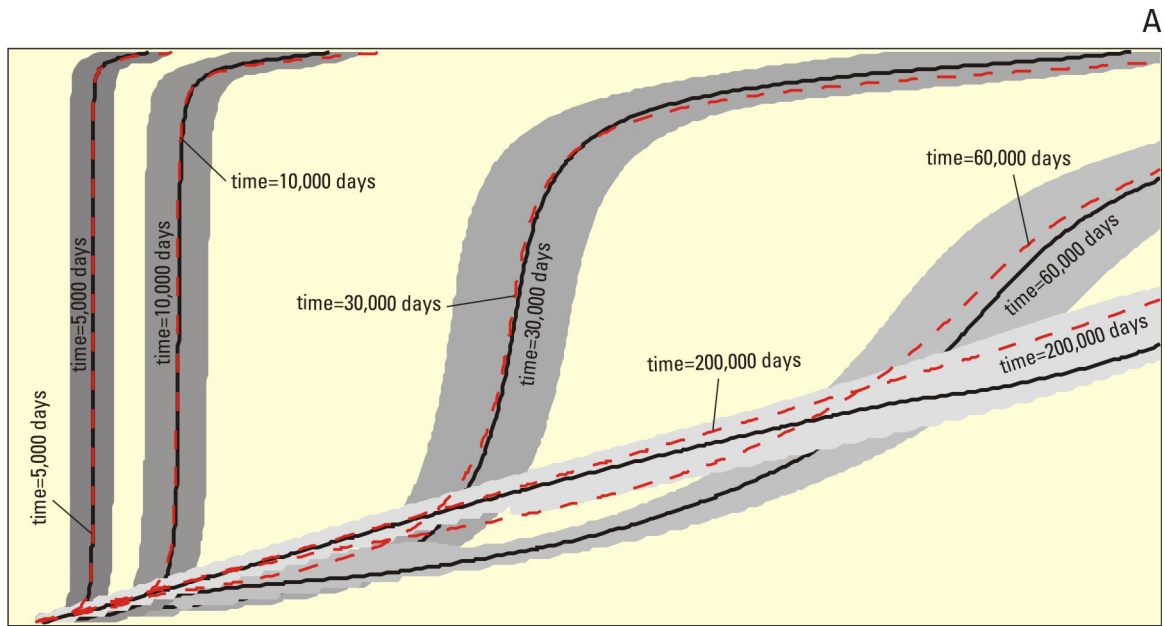
Case 6

For Case 6, the effects of fluid viscosity variation on salinity and temperature have been included in the simulation. Viscosity effects are included by activating the VSC Package in the name file. The input file for the VSC Package is as follows:

```
#Viscosity Package
-1                              MT3DMUFLG
0. 0.                           VISCMIN VISCMAX
8.904e-4                        VISCREF
1 1                             NSMUEOS MUTEMPOPT
1 1.923e-6 0.                   MTMUSPEC(1) DMUDC(1) CMUREF(1)
2 239.4e-7 10. 248.37 133.15    MTMUTEMPSPEC A1 A2 A3 A4
```

The first line is a comment. The second line indicates that viscosity is a function of one or more MT3DMS species. The third line contains the viscosity limiters, which are not active because of the zero value. The fourth line is the reference viscosity. The fifth line contains two important flags. The first indicates that one of the species has a linear effect on fluid density, and that information for the species will be read on the following line. The second flag contains information about the effects of temperature on fluid viscosity. A value of 1 indicates that fluid viscosity is calculated using equation 18, and that additional information regarding the temperature/viscosity relation will be read later. The sixth line contains the MT3DMS species number that has a linear effect on fluid density, the slope of this relation, and the reference concentration this relation is based upon. The last line indicates that species 2 is the temperature species and provides constants used in equation 18.

Results from the Case 6 simulation are shown in figure 7, and suggest that viscosity variations have a minimal effect on simulated salinities and temperatures for this particular problem. There are some minor differences between Cases 5 and 6, particularly at later times, but the overall results are similar.
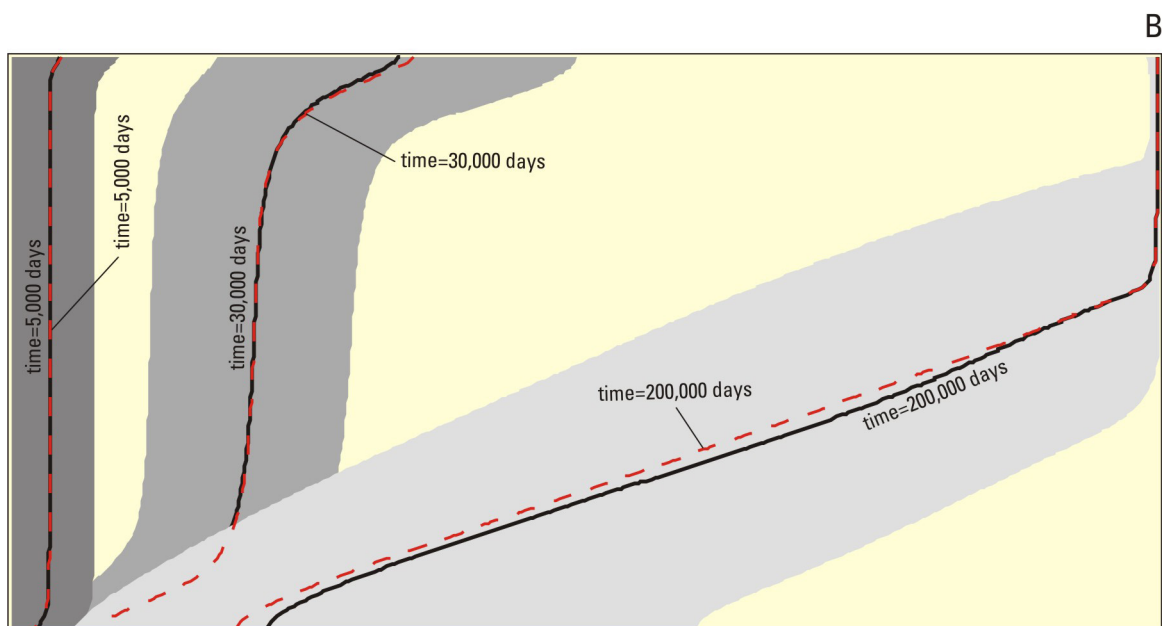
Figure 7. Transient movement of the (a) salinity and (b) temperature transition zones for Case 6. Gray shading represents the 1 to 99 percent salinity or temperature values. The solid black lines represent the salinity or temperature value equal to 50 percent for Case 6. For comparison, dashed lines represent the 50-percent line for Case 5.
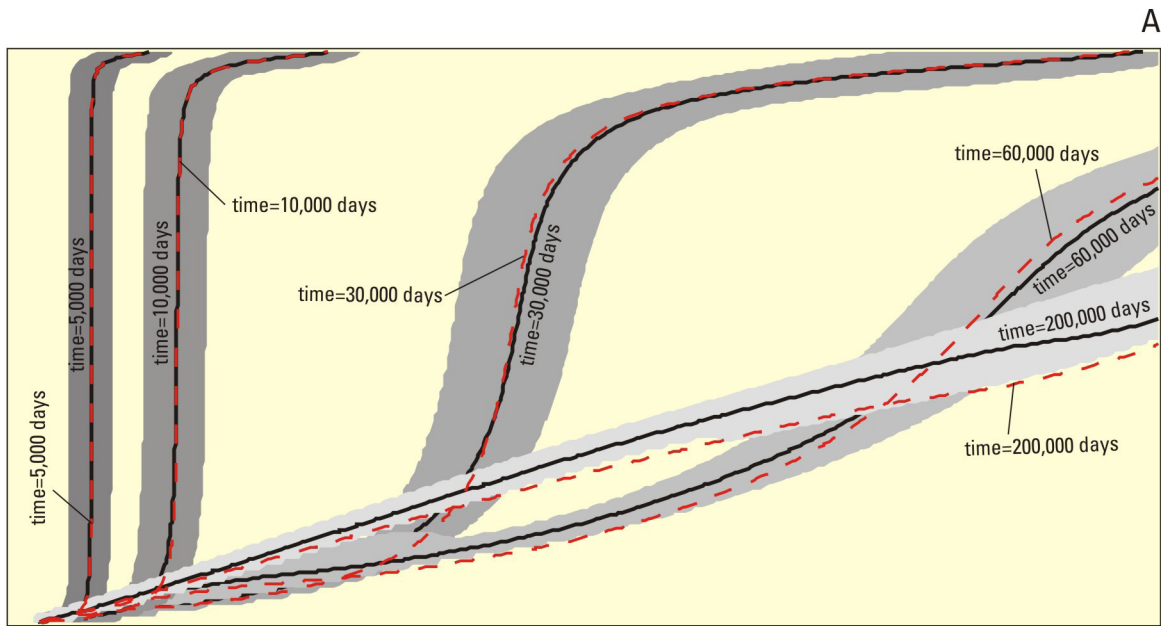
Case 7

For the last case, the effects of pressure (the weight of the overlying column of fluid) on fluid density are considered. The pressure effects are included through the VDF input file (shown below) by entering 4.46×10^{-3} kg m^{-4} for the change in density with the change in pressure head (DRHODPRHD), and a value of zero for the reference pressure head (PRHDREF).

```
      -1           1         -1         0    MT3DRHOFLG   MFNADVFD   NSWTCPL   IWTABLE
   0.0000     0.0000                         DENSEMIN DENSEMAX
   0.0000                                     DNSCRIT
 1000.0000   4.46E-03         0.             DENSEREF DRHODPRHD PRHDREF
      2                                       NSRHOEOS
      1       0.7000          0.             MTRHOSPEC(1) DRHODC(1) CRHOREF(1)
      2      -0.3750         25.             MTRHOSPEC(2) DRHODC(2) CRHOREF(2)
1.0000e-02                                   FIRSTDT
```

Results from the Case 7 simulation are shown in figure 8. The compressibility of water due to pressure appears to have a minor effect on the simulated salinities and temperatures, particularly at later times. This minor effect is largely due to the deep aquifer system (1 km) considered here. For shallow surficial aquifers, the effect of pressure on fluid density is expected to be negligible.
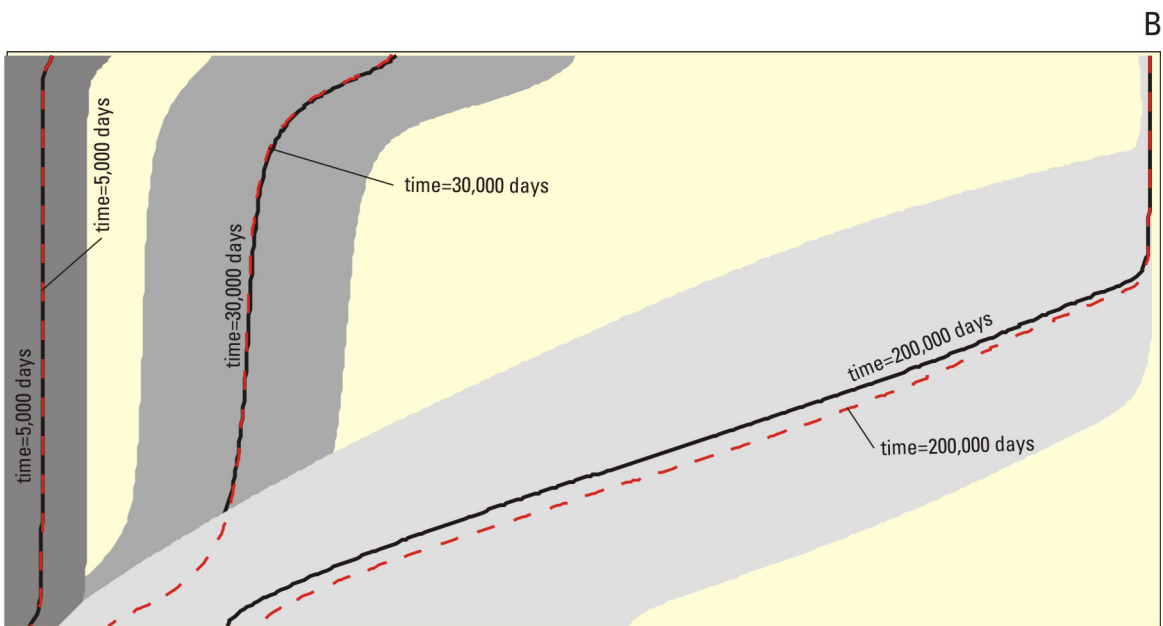
Figure 8. Transient movement of the (a) salinity and (b) temperature transition zones for Case 7. Gray shading represents the 1 to 99 percent salinity or temperature values. The solid black lines represent the salinity or temperature value equal to 50 percent for Case 7. For comparison, dashed lines represent the 50-percent line for Case 6.

References Cited

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