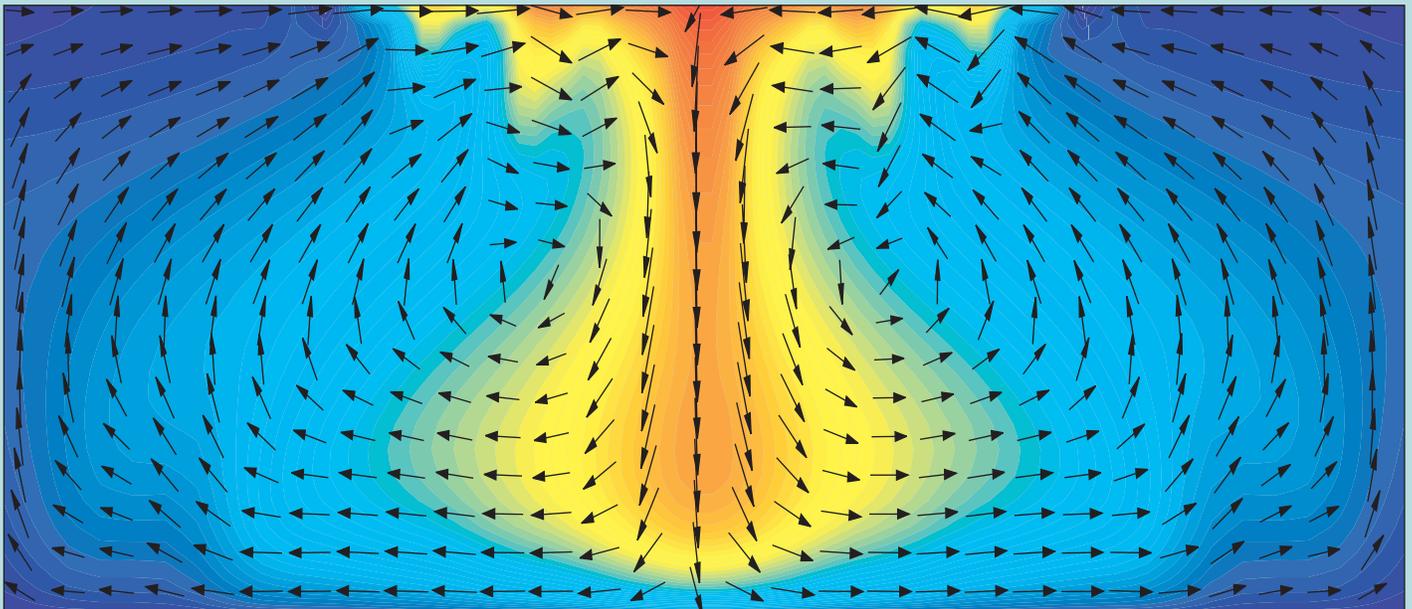# User's Guide to SEAWAT:

A Computer Program For Simulation of Three-Dimensional Variable-Density Ground-Water Flow

Techniques of Water-Resources Investigations of the U.S. Geological Survey

BOOK 6
Chapter A7

User's Guide to SEAWAT: A Computer Program for Simulation of Three-Dimensional Variable-Density Ground-Water Flow

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Techniques of Water-Resources Investigations 6-A7

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PREFACE

This report describes the SEAWAT program, which can be used to simulate three-dimensional, variable-density, ground-water flow. 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 encouraged to notify the U.S. Geological Survey of any errors found in this User Guide for the computer program by using the address on the back of the report title page. Updates might occasionally be made to both the User Guide and SEAWAT program. Users can check for updates on the Internet at URL **http://water.usgs.gov/software/ground_water.html/**.

CONTENTS

CONVERSION FACTORS AND VERTICAL DATUM

Multiply	By	To obtain
gram (g)	0.03527	ounce
liter (L)	0.2642	gallon
meter (m)	3.281	foot
meter per day (m/d)	3.281	foot per day
kilogram (kg)	2.205	pound
kilogram per day (kg/d)	2.205	pound per day
kilogram per cubic meter (kg/m^3)	0.06243	pound per cubic foot
square meter per day (m^2/d)	10.76	square foot per day
cubic meter per day (m^3/d)	35.31	cubic foot per day

Sea level: In this report, "sea level" refers to the National Geodetic Vertical Datum of 1929 (NGVD of 1929)–a geodetic datum derived from a general adjustment of the first-order levels nets of the United States and Canada, formerly called Sea Level Datum of 1929.

User's Guide to SEAWAT: A Computer Program for Simulation of Three-Dimensional Variable-Density Ground-Water Flow

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Abstract

The SEAWAT program was developed to simulate three-dimensional, variable-density, transient ground-water flow in porous media. The source code for SEAWAT was developed by combining MODFLOW and MT3DMS into a single program that solves the coupled flow and solute-transport equations. The SEAWAT code follows a modular structure, and thus, new capabilities can be added with only minor modifications to the main program. SEAWAT reads and writes standard MODFLOW and MT3DMS data sets, although some extra input may be required for some SEAWAT simulations. This means that many of the existing pre- and post-processors can be used to create input data sets and analyze simulation results. Users familiar with MODFLOW and MT3DMS should have little difficulty applying SEAWAT to problems of variable-density ground-water flow.

MODFLOW was modified to solve the variable-density flow equation by reformulating the matrix equations in terms of fluid mass rather than fluid volume and by including the appropriate density terms. Fluid density is assumed to be solely a function of the concentration of dissolved constituents; the effects of temperature on fluid density are not considered. Temporally and spatially varying salt concentrations are simulated in SEAWAT using routines from the MT3DMS program. SEAWAT uses either an explicit or implicit procedure to couple the ground-water flow equation with the solute-transport equation. With the explicit procedure, the flow equation is solved first for each timestep, and the resulting advective velocity field is then

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used in the solution to the solute-transport equation. This procedure for alternately solving the flow and transport equations is repeated until the stress periods and simulation are complete. With the implicit procedure for coupling, the flow and transport equations are solved multiple times for the same timestep until the maximum difference in fluid density between consecutive iterations is less than a user-specified tolerance.

The SEAWAT code was tested by simulating five benchmark problems involving variable-density ground-water flow. These problems include two box problems, the Henry problem, Elder problem, and HYDROCOIN problem. The purpose of the box problems is to verify that fluid velocities are properly calculated by SEAWAT. For each of the box problems, SEAWAT calculates the appropriate velocity distribution. SEAWAT also accurately simulates the Henry problem, and SEAWAT results compare well with those of SUTRA. The Elder problem is a complex flow system in which fluid flow is driven solely by density variations. Results from SEAWAT, for six different times, compare well with results from Elder's original solution and results from SUTRA. The HYDROCOIN problem consists of fresh ground water flowing over a salt dome. Simulated contours of salinity compare well for SEAWAT and MOCDENSE.

CHAPTER 1

INTRODUCTION

Ground water contains dissolved constituents, such as the salts commonly found in seawater. At relatively low concentrations, dissolved constituents do not substantially affect fluid density. As solute concentrations increase, however, the mass of the dissolved constituents can substantially affect the fluid density. If the spatial variations in fluid density are minimal, regardless of the actual density value, field and mathematical methods for quantifying rates and patterns of ground-water flow are relatively straightforward. Where spatial variations in fluid density are present, such as in coastal aquifers, investigations of ground-water flow are more complicated because the density variations can substantially affect rates and patterns of fluid flow. In many of these hydrogeologic settings, an accurate representation of variable-density ground-water flow is necessary to characterize and predict ground-water flow rates, travel paths, and residence times.

Spatial variations in fluid density that affect ground-water flow have been observed in a wide range of hydrogeologic settings. For example, in coastal aquifers, an interface exists between fresh ground water flowing toward the ocean and saline ground water. Across the interface, the fluid density may increase from that of freshwater (about 1,000 kg/m^3) to that of seawater (about 1,025 kg/m^3), an increase of about 2.5 percent. Field observations and mathematical analyses have shown that this relatively minor variation in ground-water density has a substantial effect on ground-water flow rates and patterns. An understanding of variable-density ground-water flow, therefore, can be important in many types of studies of coastal aquifers, such as studies of saltwater intrusion, contaminated site remediation, and fresh ground-water discharge into oceanic water bodies.

Characterization of variable-density ground-water flow also can be important for studies of aquifer storage and recovery (ASR). ASR projects typically involve the injection of surface water into an aquifer during times of surplus and retrieval of this same water during times of demand. If the native water quality of the aquifer selected for ASR is brackish or saline, the storage times and recovery efficiencies can be affected by the density differences between the injected water and the native aquifer water. In some situations, the freshwater "bubble" can migrate upward in response to the differences in fluid density.

The theory of variable-density ground-water flow has been studied for many years, beginning with the early work of Ghyben (1888) and Herzberg (1901). Later, Hubbert (1940) presented a simple equation relating the elevation of a sharp interface to freshwater heads measured on the interface and to the densities of saltwater and freshwater. Henry (1964) used a semianalytical solution to define the location and shape of the interface under the condition of a constant seaward flux of freshwater toward an oceanic boundary. Several other analytical and numerical solutions since then have been developed for the original Henry problem, including Pinder and Cooper (1970), Lee and Cheng (1974), Huyakorn and others (1987), Voss and Souza (1987), and Croucher and O'Sullivan (1995).

There is a wide range of private and public domain computer codes that can be used to simulate variable-density ground-water flow. For example, the U.S. Geological Survey (USGS) offers the finite-element SUTRA code (Voss, 1984) and the finite-difference HST3D (Kipp, 1997) and MOCDENSE (Sanford and Konikow, 1985) codes. These codes contain powerful options for simulating a wide range of complex problems. Although many hydrogeologists are familiar with the constant-density MODFLOW (McDonald and Harbaugh, 1988) code, there are fewer hydrogeologists familiar with the complex variable-density codes.This manual describes the SEAWAT code, which is based on the 1988 version of the MODFLOW code, and demonstrates how those familiar with MODFLOW and the solute-transport code, MT3DMS (Zheng and Wang, 1998), should have little difficulty developing variable-density models of ground-water flow.

Purpose and Scope

The purpose of this report is to document a computer program (SEAWAT) that simulates variable-density, transient, ground-water flow in three dimensions. Two popular computer programs, MODFLOW and MT3DMS, were used in the development of SEAWAT. This report is divided into seven chapters. Chapter 1 is an introduction to the development of SEAWAT. Chapter 2 contains a mathematical development of variable-density ground-water flow in terms of freshwater head and includes a discussion of Darcy's law for variable-density flow. The finite-difference equation for flow of variable-density water, using a block-centered scheme, is presented in Chapter 3. The design and structure of the SEAWAT program are presented in Chapter 4. Additionally, this chapter discusses the solution procedures implemented in MODFLOW and MT3DMS and describes how the timestep calculated by MT3DMS (based on stability criteria) is used as the timestep in SEAWAT. The major modifications made to the block-centered flow (BCF) package and the stress packages (RIV, DRN, WEL, RCH, EVT, CHD, and GHB) of MODFLOW are discussed in Chapter 5. Instructions for preparing input files for individual MODFLOW and MT3DMS packages for use in SEAWAT are explained in Chapter 6. Several benchmark problems solved using SEAWAT are presented in Chapter 7.

This report should be used to supplement the documentations of MODFLOW and MT3DMS, which are available in the public domain. The documentation for MODFLOW and MT3DMS can be obtained from the USGS and the Hydrogeology Group at the University of Alabama, respectively.

Development of SEAWAT

The original SEAWAT concept of combining MODFLOW and MT3D into a single program to simulate three-dimensional variable-density ground-water flow was first documented by Guo and Bennett (1998). Later, as part of a U.S. Geological Survey project to quantify submarine ground-water discharge to Biscayne Bay, Fla. (Langevin, 2001), the SEAWAT program was improved, updated, and verified against a number of benchmark test problems (Langevin and Guo, 1999; Guo and others, 2001). This user's manual presents the concept behind the original SEAWAT code (Guo and Bennett, 1998) and documents the recent changes and improvements that extend the applicability of the SEAWAT code to a wide range of variable-density ground-water flow problems.

The source code for SEAWAT was developed by combining MODFLOW and MT3DMS into a single program that solves the coupled flow and solute-transport equations. The SEAWAT code follows a modular structure, so new capabilities can be added with only minor modifications to the source code. MODFLOW was modified to conserve fluid mass rather than fluid volume and uses equivalent freshwater head as the principal dependent variable. In the revised form of MODFLOW, the cell-by-cell flow is calculated from freshwater head gradients and relative density-difference terms. The resulting flow field is passed to MT3DMS for transport of solute; an updated density field is then calculated from the new solute concentrations and incorporated back into MODFLOW as relative density-difference terms.

For the convenience of hydrologists and modelers familiar with MODFLOW and MT3DMS, the changes in input files for MODFLOW and MT3DMS were kept to a minimum. Thus, existing input files for the standard versions of MODFLOW and MT3DMS can be revised for SEAWAT with minor modifications. Because no additional data files are needed to run SEAWAT, individuals familiar with MODFLOW and MT3DMS should be able to use SEAWAT with few difficulties. SEAWAT reads and writes standard MODFLOW and MT3DMS data sets, which are easily manipulated with the commercially available pre- and post-processors. These processors substantially reduce the length of time it takes to create input data sets and evaluate model results.

Acknowledgments

CHAPTER 2
MATHEMATICAL DESCRIPTION OF VARIABLE-DENSITY GROUND-WATER FLOW

This chapter develops the governing equations that describe variable-density ground-water flow and solute transport in porous media. The theory of variable-density ground-water flow is usually developed and presented in terms of fluid pressure and fluid density. In this chapter, however, the variable-density ground-water flow equation is developed in terms of equivalent freshwater head and fluid density. The purpose for developing the flow equation in terms of equivalent freshwater head, rather than pressure, is discussed in this chapter and later in Chapter 5 where modifications to the MODFLOW computer program are presented.

Basic Assumptions

The development presented here is based on the usual assumptions that Darcy's law is valid (laminar flow); the standard expression for specific storage in a confined aquifer is applicable; the diffusive approach to dispersive transport based on Fick's law can be applied; and isothermal conditions prevail. The porous medium is assumed to be fully saturated with water. A single, fully miscible liquid phase of very small compressibility also is assumed.

Concept of Equivalent Freshwater Head

SEAWAT is based on the concept of freshwater head, or equivalent freshwater head, in a saline ground-water environment. A thorough understanding of this concept is required in developing the equations of variable-density ground-water flow as used in the SEAWAT program and in interpreting calculated results. The subsequent discussion is intended to provide readers with an understanding of equivalent freshwater head and its relation to head.

Two piezometers open to a given point, N, in an aquifer containing saline water are shown in figure 1. Piezometer A contains freshwater and is equipped with a mechanism that prevents saline water in the aquifer from mixing with freshwater in the piezometer, while still allowing the piezometer to respond accurately to the pressure at point N. Piezometer B contains water identical to that present in the saline aquifer at point N. The height of the water level in piezometer A above point N is $P_N/\rho_f g$. The freshwater head at point N is the elevation of the water level in piezometer A above datum, and thus is given by:

$$h_f = \frac{P_N}{\rho_f g} + Z_N, \qquad (1)$$

where:

   h_f is equivalent freshwater head [L],
   P_N is pressure at point N [ML^{-1}T^{-2}],
   ρ_f is density of freshwater [ML^{-3}]
   g is acceleration due to gravity [LT^{-2}], and
   Z_N is elevation of point N above datum [L].

Piezometers filled with freshwater would seldom if ever be used in field studies of a saline aquifer (although pressure transducers calibrated to read values of freshwater head could certainly be implemented without difficulty). However, the point here is not that field measurements would ever be made in terms of freshwater head, but rather that because pressure and elevation are defined at all points in any aquifer,

Figure 1. Two piezometers, one filled with freshwater and the other with saline aquifer water, open to the same point in the aquifer.
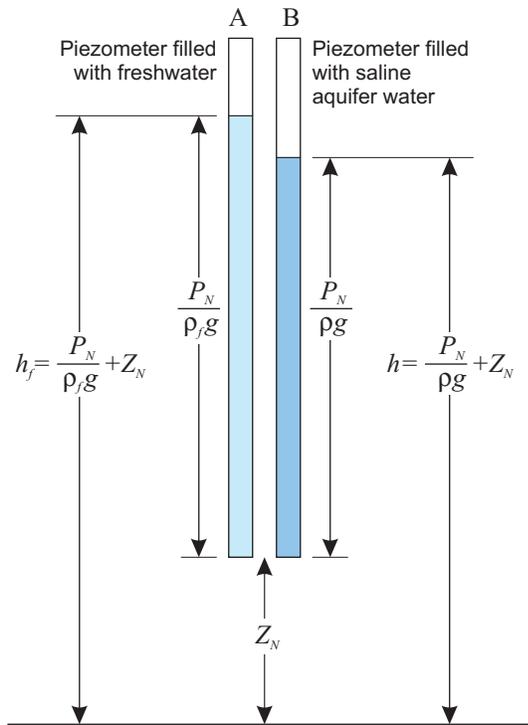
EXPLANATION

h_f Equivalent freshwater head [L]

h Head [L]

P_N Pressure [ML^{-1}T^{-2}]

ρ_f Density of freshwater [ML^{-3}]

ρ Density of saline aquifer water [ML^{-3}]

g Acceleration due to gravity [LT^{-2}]

Z_N Elevation [L]

NOTE: L = length, M = mass, T = time

freshwater head also can be defined as a function at all points in any aquifer; in certain cases, this leads to convenience in calculation or software application.

The elevation of the water level in piezometer B above point N is $P_N/\rho g$. The head expressed in terms of the saline aquifer is the level in piezometer B above datum and is given by:

$$h = \frac{P_N}{\rho g} + Z_N,\qquad(2)$$

where:

h is head [L], and
ρ is density of saline ground water at point N [ML^{-3}].

Head in terms of the aquifer water, h, varies not only as do pressure and elevation, but also as the water density, ρ, varies. Thus, at two points having equal pressures and the same elevation but different water densities, different values of h will be recorded. The equation of ground-water flow can be formulated in terms of h, but the result includes cumbersome expressions involving density and its derivatives, and no computational advantage is gained. On the other hand, formulation of the flow equation in terms of freshwater head causes no increase in complexity and allows the use of software, such as MODFLOW, with relatively little modification.

The values calculated by the SEAWAT program in a variable-density simulation are freshwater head values corresponding to the level in piezometer A (fig. 1). They can be used in a variable-density form of Darcy's law to calculate volumetric ground-water flows. However, the calculated value of freshwater head at a given point in the aquifer does not represent the level to which ambient saline ground water will rise in a piezometer open to that point. As discussed above and shown in figure 1, native ground water will rise to the level h in a tightly cased piezometer. Conversion between head as measured by the native aquifer water and equivalent freshwater head is, therefore, necessary in converting model results or field data, and in model calibration or in the interpretation of calculated results. These conversions can be made using the following relations:

$$h_f = \frac{\rho}{\rho_f}h - \frac{\rho - \rho_f}{\rho_f}Z\qquad(3)$$

and:

$$h = \frac{\rho_f}{\rho}h_f + \frac{\rho - \rho_f}{\rho}Z\qquad(4)$$

where Z is elevation [L]. Equations 3 and 4 are obtained by eliminating pressure between equations 1 and 2, and solving for the respective head value.

Governing Equation for Ground-Water Flow

A representative elementary volume (REV) in a porous medium is shown in figure 2. Based on the principle of mass conservation for fluid and solute, the rate of accumulation of mass stored in the REV is equal to the algebraic sum of the mass fluxes across the faces of the element and the mass exchange due to sinks or sources. The mathematical expression for the conservation of mass is:

$$-\nabla \cdot (\rho \vec{q}) + \bar{\rho} q_s = \frac{\partial(\rho\theta)}{\partial t}, \quad (5)$$

where:

∇ is the gradient operator $\dfrac{\partial}{\partial x} + \dfrac{\partial}{\partial y} + \dfrac{\partial}{\partial x}$,

ρ is the fluid density [ML^{-3}],

$\vec{q}$ is the specific discharge vector [LT^{-1}],

$\bar{\rho}$ is the density of water entering from a source or leaving through a sink [ML^{-3}],

q_s is the volumetric flow rate per unit volume of aquifer representing sources and sinks [T^{-1}],

θ is porosity [dimensionless], and

t is time [T].
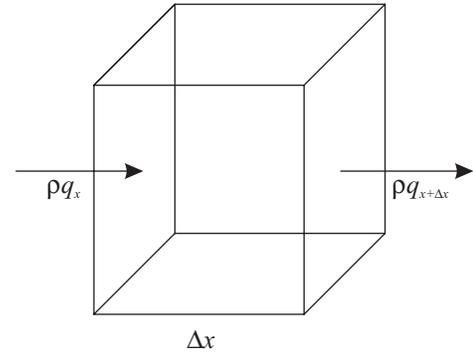
EXPLANATION

ρ Fluid density [ML^{-3}]

q_x Specific discharge at x [LT^{-1}]

$q_{x+\Delta x}$ Specific discharge at $x+\Delta x$ [LT^{-1}]

Δx Distance along the x axis [L]

NOTE: L = length, M = mass, T = time

Figure 2. Representative elementary volume in a porous medium.

The left-hand side of equation 5 is the net flux of mass through the faces of the REV, $\nabla \cdot (\rho \vec{q})$ plus the rate $(\bar{\rho} q_s)$ at which mass enters from sources or leaves through sinks located in the REV. The right-hand side of equation 5 is the time rate of change in the mass stored in the REV over a given period and can be expanded with the chain rule as:

$$\frac{\partial(\rho\theta)}{\partial t} = \rho\frac{\partial\theta}{\partial t} + \theta\frac{\partial\rho}{\partial t}. \quad (6)$$

The changes of porosity considered here are restricted to those associated with the change of fluid pressure; therefore, the change of porosity with time is mathematically represented as:

$$\frac{\partial\theta}{\partial t} = \frac{\partial\theta}{\partial P}\frac{\partial P}{\partial t}. \quad (7)$$

Under isothermal conditions, fluid density is a function of fluid pore pressure and solute concentration; therefore, the equation of the state for fluid density is:

$$\rho = f(P, C), \quad (8)$$

where:

P is fluid pore pressure [ML^{-1}T^{-2}], and

C is solute concentration [ML^{-3}].

Differentiating equation 8 with respect to time gives:

$$\frac{\partial \rho}{\partial t} = \frac{\partial \rho}{\partial P}\frac{\partial P}{\partial t} + \frac{\partial \rho}{\partial C}\frac{\partial C}{\partial t} . \qquad (9)$$

Substituting equations 7 and 9 into equation 6 gives:

$$\frac{\partial(\rho\theta)}{\partial t} = \rho\frac{\partial \theta}{\partial t} + \theta\frac{\partial \rho}{\partial t} = \rho\frac{\partial \theta}{\partial P}\frac{\partial P}{\partial t} + \theta\frac{\partial \rho}{\partial P}\frac{\partial P}{\partial t} + \theta\frac{\partial \rho}{\partial C}\frac{\partial C}{\partial t} . \qquad (10)$$

The first two terms in the right-hand side of equation 10 represent the rate of fluid mass accumulation due to ground-water storage effects (for example, due to the compressibility of the bulk porous material and fluid compressibility). The third term on the right-hand side of equation 10 represents the rate of fluid mass accumulation due to the change of solute concentration.

The relation between porosity, pressure, and the compressibility of a bulk porous material is given by Bear (1979) as:

$$\xi = \frac{1}{(1-\theta)}\frac{\partial \theta}{\partial P} , \qquad (11)$$

where ξ is the compressibility of the bulk porous material [M^{-1}LT^2]. The coefficient of water compressibility is defined as (Bear, 1979):

$$\zeta = \frac{1}{\rho}\frac{\partial \rho}{\partial P} , \qquad (12)$$

where ζ is the coefficient of water compressibility [M^{-1}LT^2]. Using equations 11 and 12, equation 10 can be rewritten as:

$$\frac{\partial(\rho\theta)}{\partial t} = \rho(\xi[1-\theta] + \zeta\theta)\frac{\partial P}{\partial t} + \theta\frac{\partial \rho}{\partial C}\frac{\partial C}{\partial t} . \qquad (13)$$

The term, $\rho(\xi[1-\theta] + \zeta\theta)$, represents the volume of water released from storage in a unit volume of a confined elastic aquifer per unit change in pressure:

$$S_p = (\xi[1-\theta] + \zeta\theta) , \qquad (14)$$

where S_p is the specific storage in terms of pressure [M^{-1}LT^2]. Substitution of equation 14 into 13 gives:

$$\frac{\partial(\rho\theta)}{\partial t} = \rho S_p\frac{\partial P}{\partial t} + \theta\frac{\partial \rho}{\partial C}\frac{\partial C}{\partial t} . \qquad (15)$$

A more thorough discussion of storativity is presented by Bear (1979).

The first term in the right-hand side of equation 15 is the rate of fluid mass accumulation due to fluid pore pressure change, and the second term is the rate of fluid mass accumulation due to the change of solute concentration. Further discussion of the second term in the right-hand side of equation 15 is presented later.

Substituting equation 15 into equation 5, the flow equation becomes:

$$-\nabla \cdot (\rho \vec{q}) + \bar{\rho} q_s = \rho S_p \frac{\partial P}{\partial t} + \theta \frac{\partial \rho}{\partial C} \frac{\partial C}{\partial t} . \tag{16}$$

Equation 16 is the general form of the partial differential equation for variable-density ground-water flow in porous media.

If density is constant, the term $\partial \rho / \partial C$ in equation 16 is zero, and the remaining density terms cancel. The resulting equation would conserve fluid mass and fluid volume for a constant density system, but would conserve only fluid volume for a variable-density system. The flow equation based on fluid volume conservation is often cited for the case of uniform density (for example, de Marsily, 1986). As Bear (1972) points out, however, the use of an equation based on volume balance is inappropriate when substantial density or temperature gradients are present. Evans and Raffensperger (1992) compared the mass- and volume-based stream functions for variable-density ground-water flow and found that the differences between the stream functions, calculated using the mass-based stream function and volume-based stream function, could reach 9.55 percent for their particular test problem after a calculation period of 600 years. They concluded that mass fluxes rather than volumetric fluxes must be used to describe the flow of ground water if the variation in fluid density is substantial.

Darcy's Law for Variable-Density Ground-Water Flow

The governing equation for variable-density ground-water flow includes a term for specific discharge, which is calculated with Darcy's law. In this section, the variable-density form of Darcy's law is presented.

General Form of Darcy's Law

Mass fluxes are defined as the product of fluid density and the specific discharge, or volumetric flow per unit cross-sectional area of bulk porous medium. Darcy's law for a fluid of variable density can be expressed by the equations:

$$q_x = -\frac{k_x}{\mu} \frac{\partial P}{\partial x} , \tag{17}$$

$$q_y = -\frac{k_y}{\mu} \frac{\partial P}{\partial y} , \tag{18}$$

and:

$$q_z = -\frac{k_z}{\mu} \left[\frac{\partial P}{\partial z} + \rho g \right] , \tag{19}$$

where:
q_x, q_y, q_z are the individual components of specific discharge,
μ is the dynamic viscosity [ML^{-1}T^{-1}],
k_x, k_y, k_z represent intrinsic permeabilities [L^2] in the three coordinate directions, and
g is the gravitational constant [LT^{-2}] and treated here as a positive scalar quantity.

In this formulation, it is assumed that the three principal directions of permeability are aligned with the orthogonal *x*-, *y*-, and *z*-coordinate system. The *z*-coordinate axis, representing the vertical, is positive upward.

Note that in equation 19, the density, ρ, is that of the fluid at the calculation point (and time) for which specific discharge is to be determined. The density term reflects the direct action of gravity on a fluid element at the calculation point and only affects the component of specific discharge in the vertical direction. It should be kept in mind, however, that the overall pressure distribution in a porous medium is controlled, in part, by the overall fluid density distribution, and thus, horizontal components of specific discharge also are affected by density variations in the system.

Assumption of Axes Alignment with Principal Permeability Directions

The assumption that the principal axes of permeability are horizontal and vertical is usually acceptable for an aquifer with horizontal bedding. A more general form of Darcy's law is required when the principal directions of permeability do not coincide with the horizontal and vertical *x*-, *y*-, and *z*-coordinate system. The simplest approach is to abandon the *x*-, *y*-, and *z*-coordinate system, and instead use a coordinate system aligned with the principal directions of permeability as shown in figure 3. If γ represents the direction normal to the bedding and α and β represent the principal directions of permeability parallel to the bedding, the pressure gradients acting in the α, β, and γ directions can be formulated independently. Because none of the coordinate directions are horizontal, although they are orthogonal to one another, a component of the gravitational force applies in each coordinate direction. This leads to the following expression of Darcy's law:

$$q_\alpha = -\frac{k_\alpha}{\mu}\left(\frac{\partial P}{\partial \alpha} + \rho g \cos \delta_\alpha\right), \qquad (20)$$

$$q_\beta = -\frac{k_\beta}{\mu}\left(\frac{\partial P}{\partial \beta} + \rho g \cos \delta_\beta\right), \qquad (21)$$

and:

$$q_\gamma = -\frac{k_\gamma}{\mu}\left(\frac{\partial P}{\partial \gamma} + \rho g \cos \delta_\gamma\right), \qquad (22)$$

where:

$q_\alpha, q_\beta, q_\gamma$ represent the specific discharge components in the coordinate axes aligned with permeability directions [LT^{-1}],

$k_\alpha, k_\beta, k_\gamma$ are the permeabilities in these directions [L^2], and

$\delta_\alpha, \delta_\beta, \delta_\gamma$ are the angles between the respective coordinate axes and the upward vertical direction.

Darcy's Law in Terms of Equivalent Freshwater Head

Darcy's law can also be expressed in terms of the freshwater head or elevation above an arbitrary datum of the water surface in a piezometer filled with freshwater. Note that it is not assumed that the aquifer itself contains freshwater of uniform density, but rather that piezometers open to the aquifer have been filled with freshwater, and a mechanism prevents the dissolved salts in the aquifer water from mixing with the water in the piezometers. As shown in figure 1, the elevation of the

Figure 3. Relation between a coordinate system aligned with the principal axes of permeability and the upward z-axis.

water surface in a piezometer has two components: the elevation of the point of measurement above some datum, z, and the height of the fluid column in the piezometer itself. Because the piezometer is assumed to contain freshwater having a fixed density, ρ_f, the height of the water column within the piezometer is $P/\rho_f g$, where P is the pressure at the piezometer opening. Thus, the freshwater head, h_f, at this point is equal to $(P/\rho_f g) + z$ and the pressure is given by:

$$P = \rho_f g(h_f - z).$$

(23)

For the dipping-aquifer problem (fig. 3), equation 23 is first differentiated with respect to the coordinate direction α, which yields:

$$\frac{\partial P}{\partial \alpha} = \rho_f g \frac{\partial h_f}{\partial \alpha} - \rho_f g \frac{\partial z}{\partial \alpha}.$$

(24)

Substituting this expression into equation 20 and noting that $\cos \delta_\alpha = \dfrac{\partial z}{\partial \alpha}$, the following relation is obtained:

$$q_\alpha = \frac{-k_\alpha}{\mu}\left[\rho_f g \frac{\partial h_f}{\partial \alpha} - \rho_f g \frac{\partial z}{\partial \alpha} + \rho g \frac{\partial z}{\partial \alpha}\right].$$

(25)

It is important to note that both ρ_f, the density of freshwater in the piezometers and ρ, the density of water in the formation at the point of velocity calculation, appear in equation 25. These two density terms should not be confused.

The freshwater hydraulic conductivity, K_f, in the α direction is defined as:

$$K_{f\alpha} = \frac{k_\alpha \rho_f g}{\mu_f},$$

(26)

where $\mu_f [ML^{-1}T^{-1}]$ represents the viscosity of freshwater under standard conditions (for example, 20 degrees Celsius and 1 atmospheric pressure). Using this term for freshwater hydraulic conductivity, equation 20 can be written as:

$$q_\alpha = -K_{f\alpha}\frac{\mu_f}{\mu}\left[\frac{\partial h_f}{\partial \alpha} + \left(\frac{\rho - \rho_f}{\rho_f}\right)\frac{\partial z}{\partial \alpha}\right].$$

(27)

Similarly, equation 21 can be written as:

$$q_\beta = -K_{f\beta}\frac{\mu_f}{\mu}\left[\frac{\partial h_f}{\partial \beta} + \left(\frac{\rho - \rho_f}{\rho_f}\right)\frac{\partial z}{\partial \beta}\right],$$

(28)

and equation 22 as:

$$q_\gamma = -K_{f\gamma}\frac{\mu_f}{\mu}\left[\frac{\partial h_f}{\partial \gamma} + \left(\frac{\rho - \rho_f}{\rho_f}\right)\frac{\partial z}{\partial \gamma}\right].$$

(29)

Note that for a horizontally stratified aquifer, equations 27 to 29 would reduce to:

$$q_x = -K_{fx}\frac{\mu_f}{\mu}\left[\frac{\partial h_f}{\partial x}\right],$$

(30)

$$q_y = -K_{fy}\frac{\mu_f}{\mu}\left[\frac{\partial h_f}{\partial y}\right], \tag{31}$$

and:

$$q_z = -K_{fz}\frac{\mu_f}{\mu}\left[\frac{\partial h_f}{\partial z} + \left(\frac{\rho - \rho_f}{\rho_f}\right)\right]. \tag{32}$$

For many practical applications, the term μ_f/μ in equations 27 to 32 can be considered equal to one; it can be assumed that the viscosity of water in the formation is essentially the same as that of freshwater, even though differences in density are present. Variations in fluid viscosity arise primarily because of variations in water temperature. Where substantial temperature variations are absent and where hydraulic conductivity has been measured at the same water temperature for which velocity is to be calculated, the viscosity correction usually can be neglected.

Governing Equation for Flow in Terms of Freshwater Head

With the definition of freshwater head and Darcy's law in terms of freshwater head, the governing equation for ground-water flow (eq. 16) can be written in terms of equivalent freshwater head. Expanding the left-hand side of equation 16 and rearranging yield:

$$-\frac{\partial}{\partial\alpha}(\rho\dot{q}_\alpha) - \frac{\partial}{\partial\beta}(\rho\dot{q}_\beta) - \frac{\partial}{\partial\gamma}(\rho\dot{q}_\gamma) = \rho S_P\frac{\partial P}{\partial t} + \theta\frac{\partial\rho}{\partial C}\frac{\partial C}{\partial t} - \bar{\rho}q_s. \tag{33}$$

Differentiation of equation 23 with respect to time shows that $\partial P/\partial t$ can be expanded as $\rho_f g\ \partial h_f/\partial t$. Using this form and substituting Darcy's law as given in equations 27 to 29 for the components of specific discharge yield:

$$\begin{aligned}
&\frac{\partial}{\partial\alpha}\left(\rho K_{f\alpha}\left[\frac{\partial h_f}{\partial\alpha} + \frac{\rho - \rho_f}{\rho_f}\frac{\partial Z}{\partial\alpha}\right]\right) + \frac{\partial}{\partial\beta}\left(\rho K_{f\beta}\left[\frac{\partial h_f}{\partial\beta} + \frac{\rho - \rho_f}{\rho_f}\frac{\partial Z}{\partial\beta}\right]\right)\\
&+ \frac{\partial}{\partial\gamma}\left(\rho K_{f\gamma}\left[\frac{\partial h_f}{\partial\gamma} + \frac{\rho - \rho_f}{\rho_f}\frac{\partial Z}{\partial\gamma}\right]\right) = \rho S_p g\rho_f\frac{\partial h_f}{\partial t} + \theta\frac{\partial\rho}{\partial C}\frac{\partial C}{\partial t} - \bar{\rho}q_s.
\end{aligned} \tag{34}$$

The specific storage in terms of pressure, S_p (eq. 14), includes the compressibility of the water, which in turn, depends on the water density, ρ, at the point of calculation (eq. 12). The assumption is made here that the difference between the compressibility coefficients of saltwater and freshwater can be neglected in that:

$$\zeta = \frac{1}{\rho}\frac{\partial\rho}{\partial P} \approx \zeta_f = \frac{1}{\rho_f}\frac{\partial\rho}{\partial P}, \tag{35}$$

where ζ_f is the compressibility coefficient for freshwater. The specific storage, in terms of freshwater head, $S_f[\text{L}^{-1}]$, or the volume of water released from storage in a unit volume of aquifer per unit decline in freshwater head is given by Bear (1979) as:

$$S_f = g\rho_f[\xi(1 - \theta) + \zeta_f\theta] . \tag{36}$$

By using equations 14 and 35, the term $S_p g \rho_f$ in equation 34 can be replaced by the term S_f, which yields:

$$\frac{\partial}{\partial \alpha}\left(\rho K_{f\alpha}\left[\frac{\partial h_f}{\partial \alpha} + \frac{\rho - \rho_f}{\rho_f}\frac{\partial Z}{\partial \alpha}\right]\right) + \frac{\partial}{\partial \beta}\left(\rho K_{f\beta}\left[\frac{\partial h_f}{\partial \beta} + \frac{\rho - \rho_f}{\rho_f}\frac{\partial Z}{\partial \beta}\right]\right)$$
$$+ \frac{\partial}{\partial \gamma}\left(\rho K_{f\gamma}\left[\frac{\partial h_f}{\partial \gamma} + \frac{\rho - \rho_f}{\rho_f}\frac{\partial Z}{\partial \gamma}\right]\right) = \rho S_f \frac{\partial h_f}{\partial t} + \theta \frac{\partial \rho}{\partial C}\frac{\partial C}{\partial t} - \bar{\rho} q_s. \quad (37)$$

Equation 37 is the governing equation for variable-density flow in terms of freshwater head as used in SEAWAT.

Governing Equation for Solute Transport

In addition to the flow equation that was developed (eq. 37), a second partial differential equation is required to describe solute transport in the aquifer. Ground-water flow causes the redistribution of solute concentration, and the redistribution of solute concentration alters the density field, thus, affecting ground-water movement. Therefore, the movement of ground water and the transport of solutes in the aquifer are coupled processes, and the two equations must be solved jointly.

Solute mass is transported in porous media by the flow of ground water (advection), molecular diffusion, and mechanical dispersion. The transport of solute mass in ground water can be described by the following partial differential equation (Zheng and Bennett, 1995):

$$\frac{\partial C}{\partial t} = \nabla \cdot (D \cdot \nabla C) - \nabla \cdot (\grave{v}C) - \frac{q_s}{\theta}C_s + \sum_{k=1}^{N} R_k, \quad (38)$$

where:
  D is the hydrodynamic dispersion coefficient [$L^2 T^{-1}$],
  $\grave{v}$ is the fluid velocity [LT^{-1}],
  C_s is the solute concentration of water entering from sources or sinks [ML^{-3}], and
  R_k ($k=1, ..., N$) is the rate of solute production or decay in reaction k of N different reactions [$ML^{-3}T^{-1}$].

When fluid density varies, the concentration gradient, ∇C, should actually be formulated as $\rho \nabla(C/\rho)$ (de Marsily, 1986, p. 239). This is only necessary for brines of high density; however for fluid densities in the seawater range, the change introduced by this expression is negligible, and the transport equation as formulated in equation 38 may be used.

Boundary and Initial Conditions

Boundary and initial conditions must be specified to solve the differential equations for flow (eq. 37) and transport (eq. 38) in a particular problem. Mathematical boundaries are commonly defined in three categories: Dirichlet (constant head or concentration), Neumann (specific flux), and Cauchy (head-dependent flux or mixed boundary condition). The physical features and processes, which impose boundary conditions on ground-water regimes, normally include streams and other surface-water bodies, drains, low-permeability boundaries, seepage faces, evapotranspiration, discharging wells, injection wells and recharge. In simulation theory, many of the boundary conditions are commonly implemented through the sink/source term in equations 37 and 38; that approach is followed in this model. There is a separate section that further describes sink and source terms.

Dirichlet Boundary

A Dirichlet boundary (also referred to as Type I) is one in which the value of head or concentration is specified at all points along the boundary. The head or concentration value may vary from point to point or as a function of time and is treated as a known quantity in the solution of the equation. In terms of flow simulation, a specified head implies that flow toward or away from the boundary occurs in proportion to the difference between the specified head at the boundary and the calculated head at points directly adjacent to the boundary. This is simulated by not solving a flow equation at the specified-head cell. In terms of solute transport, a specified concentration implies that the dispersive flux toward or away from the boundary occurs in response to the difference between the specified boundary concentration and the calculated concentration at points directly adjacent to the boundary. Advective solute flux into the modeled area from a specified concentration boundary depends on the flow from the boundary and the specified concentration value. Advective solute flux toward any type of boundary depends on the calculated concentration of the water at points adjacent to the boundary and on the flow toward the boundary.

A physical example of an external Dirichlet boundary might be a fully penetrating stream or other surface-water body on the boundary of the model domain along which head or concentration is specified. An example of an internal Dirichlet boundary might be a drain operating at a specified water level in the interior of the model domain.

Neumann Boundary

The Neumann boundary (also referred to as Type II) represents the condition in which the gradient of the dependent variable is specified normal to the boundary. For ground-water flow, this boundary condition results in a specified flux of water into or out of the modeled area. For solute transport, the concentration gradient is specified normal to the boundary. This results in a specified dispersive flux of solute across the Neumann boundary. Although the Neumann boundary for solute transport ensures a specified dispersive flux, the advective solute flux depends on the ground-water flow velocity normal to the boundary and the calculated concentration on the boundary. Thus, the total solute flux across a Neumann boundary cannot be specified prior to simulation.

An impermeable boundary represents a special case of the Neumann condition for flow and transport, where the gradients of head and concentration are zero such that neither flow nor dispersive solute flux may occur, and advective solute flux is precluded by the absence of flow. An impermeable boundary (commonly called a no-flow boundary) is simulated by specifying cells for which a flow equation is not solved. Additionally, the flow between a no-flow cell and an adjacent cell is zero. A nonzero Neumann boundary is simulated using sink/source terms. An example of a nonzero Neumann boundary in flow simulation might be a surface-water body from which seepage occurs at a prescribed rate.

Cauchy Boundary

A head-dependent flow condition represents a Cauchy boundary (also referred to as Type III) for the simulation of flow (Anderson and Woessner, 1992). The Cauchy boundary for solute transport, however, is not analogous because boundary conditions for solute transport may contain both advective and dispersive components, whereas boundary conditions for flow contain only the flow component. With the Cauchy boundary for flow, a control head is specified, but this control head prevails at some hydraulic separation from the boundary. The head on the boundary itself is calculated in the simulation, but is linked to the control head through a conductance term, which may represent, for example, the semipermeable material on the bed of a stream or the local head loss through convergent flow into a drain. The flow, Q_b, into or from a head-dependent flow boundary is calculated as:

$$Q_b = COND(h_c - h_{i,j,k}),\qquad\qquad(39)$$

where:

$COND$ is the conductance term,

h_c is the specified control head, and

$h_{i,j,k}$ is the calculated head at the boundary cell, which is linked through the conductance term.

Examples of the head-dependent condition are provided by the River (RIV), Drain (DRN), Evapotranspiration (EVT), and General-Head Boundary (GHB) packages of MODFLOW; the first three of these nonlinear variations involve limiting values of head beyond which the flow value, Q_b, takes on a fixed value, making these nonlinear variations of the head-dependent flux boundary condition.

The Cauchy boundary for solute transport represents a boundary on which both concentration and concentration gradient are specified (Zheng and Bennett, 1995). This implies that the dispersive flux across the boundary is specified and that the advective flux across the boundary will vary only to the extent that the flow across the boundary in the transport simulation varies. A Cauchy boundary condition in the transport model, which coincides with a Neumann boundary condition in the flow regime, will result in a specified total flux of solute mass across the boundary.

Initial Conditions

Initial conditions represent starting values for the dependent variable, such as freshwater head for ground-water flow and concentration for solute transport, at some starting time. Initial conditions for both flow and transport must be specified for transient simulations.

Sink and Source Terms

The third term on the right-hand side of equation 37 and the third term on the left-hand side of equation 38 are the sink/source terms for water and solute, respectively. These terms quantify the exchange of water and solute mass between the aquifer and such features as discharging wells, injection wells, and recharge. Sinks and sources may be areally distributed or localized. Areally distributed sinks or sources include recharge and evapotranspiration; localized sinks and sources may include wells, drains, and rivers. In the case of sources, which provide a mechanism for bringing solute mass into the flow systems, solute concentration of the source water must be specified. The concentration of water removed at a sink generally is the simulated value for the cell containing the sink and may represent information useful in model calibration. Evapotranspiration, which is typically thought to remove only freshwater from the flow system, is an exception.

The strength (that is, the mass of solute per unit time) of a source or sink component in the transport equation depends on the volumetric flow rate and solute concentration of the water entering the sink or leaving through the source. For a transport source, the concentration is specified; for a sink, the calculated concentration of the water in the aquifer as it enters the sink is used. The flow terms are identical to those used for the corresponding source or sink in the flow equation. Solutes entering the flow field by dissolution of minerals from the aquifer generally would not be treated as part of the source term, but rather as part of the chemical reaction term, R_k, in equation 38.

Concentration and Density

The second term on the right-hand side of equation 37 represents the change of fluid mass in the REV due to the change in solute concentration. To evaluate this term, the relation between solute concentration and fluid density is required. For isothermal conditions, fluid density is predominantly affected by the solute concentration and fluid pore pressure. The effects of pore pressure on fluid density are included in the storage term (eq. 9). An empirical relation between the density of saltwater and concentration was developed by Baxter and Wallace (1916):

$$\rho = \rho_f + EC, \tag{40}$$

where:

E is a dimensionless constant having an approximate value of 0.7143 for salt concentrations ranging from zero to that of seawater, and

C is the salt concentration [ML^{-3}].

The derivative of equation 40 with respect to salt concentration is:

$$\frac{\partial \rho}{\partial C} = E. \tag{41}$$

Substituting this relation into equation 37, the governing equation is rewritten as:

$$\frac{\partial}{\partial \alpha}\left(\rho K_{f\alpha}\left[\frac{\partial h_f}{\partial \alpha} + \frac{\rho - \rho_f}{\rho_f}\frac{\partial Z}{\partial \alpha}\right]\right) + \frac{\partial}{\partial \beta}\left(\rho K_{f\beta}\left[\frac{\partial h_f}{\partial \beta} + \frac{\rho - \rho_f}{\rho_f}\frac{\partial Z}{\partial \beta}\right]\right)$$
$$+ \frac{\partial}{\partial \gamma}\left(\rho K_{f\gamma}\left[\frac{\partial h_f}{\partial \gamma} + \frac{\rho - \rho_f}{\rho_f}\frac{\partial Z}{\partial \gamma}\right]\right) = \rho S_f \frac{\partial h_f}{\partial t} + \theta E \frac{\partial C}{\partial t} - \bar{\rho} q_s. \tag{42}$$

Sometimes salt concentration is measured as salinity and expressed as mass/mass (for example, grams per kilogram or parts per thousand). Salinity is defined as the total amount of solid material in grams contained in 1 kg of seawater when all the carbonate is converted to oxide, the bromine and iodine are replaced by chloride, and all organic matter is completely oxidized (Chow, 1964). The value of salinity is often close to the dissolved-solids concentration; however, the salinity cannot be used directly in equation 40, but must rather be converted to concentration in units of mass/volume. The conversion for a dilute solution is relatively simple; for example, parts per million can approximately be treated as milligrams per liter (Freeze and Cherry, 1979). For a solution with higher concentrations of solute, such as seawater, the conversion is more complicated because of the change in volume of the solution, which accompanies a change in salt concentration. For example, the solution volume increases about 1 percent when 35 g of salt are added to 1 L of water. The volume change of a solution with high concentration depends on many factors, and the conversion from units of mass/mass to units of mass/volume must, therefore, generally be based on empirical relations.

Equations 40 to 42 are applied only for typical seawaters for which the relation between fluid density and solute concentration can be expressed as a linear function as in equation 40. If the fluid has a different composition from typical seawater or the salt concentration in the fluid is much higher than normal seawater concentration, then these equations may not be valid. In that case, a different empirical relation between salt concentration and fluid density (similar to eq. 40) should be developed for that particular application.

CHAPTER 3

FINITE-DIFFERENCE APPROXIMATION FOR THE VARIABLE-DENSITY GROUND-WATER FLOW EQUATION

For variable-density ground-water conditions, flow and solute transport are linked processes. This means that a fully coupled solution to the flow and transport equations is required to properly represent dynamic ground-water flow. For most problems, it is difficult, if not impossible, to develop analytical solutions for these coupled governing equations; therefore, numerical methods generally are required.

This chapter contains the development of the finite-difference approximation for the variable-density flow equation that is used in SEAWAT. The finite-difference equation for variable-density ground-water flow is developed using sign conventions and nomenclature similar to those used by McDonald and Harbaugh (1988) in the documentation of MODFLOW. As a result, the similarities and differences between the flow equation in MODFLOW and the flow equation in SEAWAT are readily apparent.

The numerical methods used by the MT3DMS program to simulate solute transport in a constant-density flow field are directly used in SEAWAT to simulate solute transport in a variable-density flow field. Because the solute-transport equation is applicable for both constant and variable-density flow conditions, it was not necessary to make substantial changes to the MT3DMS program prior to the incorporation into SEAWAT. For this reason, the finite-difference and other methods used to solve the solute-transport equation are not presented. Instead, interested users are referred to the MT3DMS documentation (Zheng and Wang, 1998) for a detailed description of the equations and methods used to solve the solute-transport equation.

Finite-Difference Approximation for the Flow Equation

The finite-difference method is commonly used to solve partial differential equations, wherein a grid is overlain on the area of interest, dividing the domain into individual model cells. The finite-difference approximation to the partial differential equation is then applied to the discretized model domain. The assumption is then made that the concept of an REV can be applied to each model cell. Both MODFLOW and MT3DMS use cell-centered grids. In this formulation, the dependent variables obtained in the finite-difference solution represent average values (assumed to exist at the cell center) for the respective cells. SEAWAT also uses a block-centered grid because it is used for both MODFLOW and MT3DMS. The subsequent discussion of the finite-difference approximation of the variable-density ground-water flow equation, therefore, is based on the concept of a cell-centered grid, although the general approach could easily be applied to other grid designs.

The terms on the left-hand side of the governing equation for variable-density ground-water flow (eq. 42) account for the difference between inflow and outflow of mass per unit volume of aquifer across the faces of a differential element of aquifer (for example, a model cell). The first term on the right-hand side of equation 42 represents the time rate of change of liquid mass (which includes both water and solute) per unit volume of aquifer due to pressure changes in the system. The second term on the right-hand side of equation 42 represents the time rate of change of fluid mass per unit volume of aquifer due to the change in solute concentration. This second term is calculated from the concentrations obtained in the solution of the solute-transport equation. As the concentrations reach dynamic equilibrium, this term becomes negligible. Thus, the flow field does not reach steady state until the solute concentrations remain constant in time. The third term on the right-hand side represents the mass flux due to sources and sinks.

With a central finite-difference scheme in space and a backward finite-difference scheme in time, the finite-difference approximation for the partial differential equation of ground-water flow is:

$$
\hat{\rho}_{i+1/2,j,k}\frac{K_{\alpha,i+1/2,j,k}}{\Delta\alpha_{i+1/2,j,k}}A_{j,k}\left[h_{f,i+1,j,k}-h_{f,i,j,k}+\frac{\rho_{i+1/2,j,k}-\rho_f}{\rho_f}(Z_{i+1,j,k}-Z_{i,j,k})\right]
$$

$$
-\hat{\rho}_{i-1/2,j,k}\frac{K_{\alpha,i-1/2,j,k}}{\Delta\alpha_{i-1/2,j,k}}A_{j,k}\left[h_{f,i,j,k}-h_{f,i-1,j,k}+\frac{\rho_{i-1/2,j,k}-\rho_f}{\rho_f}(Z_{i,j,k}-Z_{i-1,j,k})\right]
$$

$$
+\hat{\rho}_{i,j+1/2,k}\frac{K_{\beta,i,j+1/2,k}}{\Delta\beta_{i,j+1/2,k}}A_{i,k}\left[h_{f,i,j+1,k}-h_{f,i,j,k}+\frac{\rho_{i,j+1/2,k}-\rho_f}{\rho_f}(Z_{i,j+1,k}-Z_{i,j,k})\right]
$$

$$
-\hat{\rho}_{i,j-1/2,k}\frac{K_{\beta,i,j-1/2,k}}{\Delta\beta_{i,j-1/2,k}}A_{i,k}\left[h_{f,i,j,k}-h_{f,i,j-1,k}+\frac{\rho_{i,j-1/2,k}-\rho_f}{\rho_f}(Z_{i,j,k}-Z_{i,j-1,k})\right] \tag{43}
$$

$$
+\hat{\rho}_{i,j,k+1/2}\frac{K_{\gamma,i,j,k+1/2}}{\Delta\gamma_{i,j,k+1/2}}A_{i,j}\left[h_{f,i,j,k+1}-h_{f,i,j,k}+\frac{\rho_{i,j,k+1/2}-\rho_f}{\rho_f}(Z_{i,j,k+1}-Z_{i,j,k})\right]
$$

$$
-\hat{\rho}_{i,j,k-1/2}\frac{K_{\gamma,i,j,k-1/2}}{\Delta\gamma_{i,j,k-1/2}}A_{i,j}\left[h_{f,i,j,k}-h_{f,i,j,k-1}+\frac{\rho_{i,j,k-1/2}-\rho_f}{\rho_f}(Z_{i,j,k}-Z_{i,j,k-1})\right]
$$

$$
=\left(\rho_{i,j,k}S_{f,i,j,k}\frac{h_{f,i,j,k}^{n+1}-h_{f,i,j,k}^{n}}{t_{n+1}-t_n}+\theta E\frac{\partial C}{\partial t}\right)V_{i,j,k}-(\bar{\rho}Q_s)_{i,j,k},
$$

where:

i,j,k are row, column, and layer indices, respectively.

$A_{j,k}$ is the area of the finite-difference cell normal to the α axis [L^2] such that $A_{j,k} = \Delta\beta_j \cdot \Delta\gamma_k$, and similarly for other coordinate directions,

$Z_{i,j,k}$ is the cell center elevation [L],

n is the timestep number,

$V_{i,j,k}$ is the volume of the cell [L^3] such that $V_{i,j,k} = \Delta\alpha_i \Delta\beta_j \Delta\gamma_k$, and

Q_s is the volumetric flow rate of the sink/source term [L^{3}T^{-1}].

The subscripts $i+1/2, i-1/2, j+1/2, j-1/2, k+1/2$ and $k-1/2$ refer to the value of a property or variable between two neighboring cells (for example, the harmonic mean for hydraulic conductivity). In equation 43, the f subscript is dropped for convenience from the freshwater-equivalent hydraulic conductivity terms, and this simplified notation is used throughout the rest of this section. The equivalent freshwater head values on the left-hand side of equation 43 refer to the $n+1$ timestep. If the timestep superscript is not listed with the variable, as is the case with the freshwater head values on the left-hand side of equation 43, the variable is evaluated at the $n+1$ timestep.

In equation 43, there are two types of density terms calculated at boundaries between model cells. The density term, $\hat{\rho}$, converts the volumetric flow rate to a mass flux. In SEAWAT, this density term is calculated before each iteration of the flow equation using an upstream weighting algorithm. For example, if flow is from cell i,j,k to cell $i,j,k+1$, then the term $\hat{\rho}_{i,j,k+1/2}$ would be assigned a density value equal to $\rho_{i,j,k}$. If, however, the flow direction were reversed (from $i,j,k+1$ to i,j,k), then $\hat{\rho}_{i,j,k+1/2}$ would be assigned a value equal to $\rho_{i,j,k+1}$. The other density term calculated at cell boundaries in equation 43 is denoted by ρ and is simply the arithmetic average of fluid density between neighboring cells. These density values are used in

the density-difference terms within the brackets on the left side of equation 43; as discussed previously, the density-difference terms are required in Darcy's Law when gradients of freshwater head are used in a saline environment.

Following the concepts of McDonald and Harbaugh (1988), several of the coefficients in equation 43 can be grouped together to form the conductance term, $COND$ $[L^2T^{-1}]$:

$$COND = \frac{AK}{L},$$

(44)

where:
A represents the area normal to flow $[L^2]$, and
L represents the distance along the flow path $[L]$.

Following this convention, equation 43 can be rewritten as:

$$\hat{\rho}_{i+1/2, j, k} CC_{i+1/2, j, k}\left[h_{f, i+1, j, k} - h_{f, i, j, k} + \frac{\rho_{i+1/2, j, k} - \rho_f}{\rho_f}(Z_{i+1, j, k} - Z_{i, j, k})\right]$$

$$-\hat{\rho}_{i-1/2, j, k} CC_{i-1/2, j, k}\left[h_{f, i, j, k} - h_{f, i-1, j, k} + \frac{\rho_{i-1/2, j, k} - \rho_f}{\rho_f}(Z_{i, j, k} - Z_{i-1, j, k})\right]$$

$$+\hat{\rho}_{i, j+1/2, k} CR_{i, j+1/2, k}\left[h_{f, i, j+1, k} - h_{f, i, j, k} + \frac{\rho_{i, j+1/2, k} - \rho_f}{\rho_f}(Z_{i, j+1, k} - Z_{i, j, k})\right]$$

$$-\hat{\rho}_{i, j-1/2, k} CR_{i, j-1/2, k}\left[h_{f, i, j, k} - h_{f, i, j-1, k} + \frac{\rho_{i, j-1/2, k} - \rho_f}{\rho_f}(Z_{i, j, k} - Z_{i, j-1, k})\right]$$

(45)

$$+\hat{\rho}_{i, j, k+1/2} CV_{i, j, k+1/2}\left[h_{f, i, j, k+1} - h_{f, i, j, k} + \frac{\rho_{i, j, k+1/2} - \rho_f}{\rho_f}(Z_{i, j, k+1} - Z_{i, j, k})\right]$$

$$-\hat{\rho}_{i, j, k-1/2} CV_{i, j, k-1/2}\left[h_{f, i, j, k} - h_{f, i, j, k-1} + \frac{\rho_{i, j, k-1/2} - \rho_f}{\rho_f}(Z_{i, j, k} - Z_{i, j, k-1})\right]$$

$$= \left(\rho_{i, j, k} S_{f, i, j, k} \frac{h_{f, i, j, k}^{n+1} - h_{f, i, j, k}^{n}}{t_{n+1} - t_n} + \theta E \frac{\partial C}{\partial t}\right) V_{i, j, k} - (\bar{\rho} Q_s)_{i, j, k},$$

where *CC*, *CR*, and *CV* refer to the conductance factors along columns, rows, and normal to layers, respectively [L^2T^{-1}]. Equation 45 can be rewritten as:

$$\hat{\rho}_{i+1/2,j,k}CC_{i+1/2,j,k}[h_{f,i+1,j,k}-h_{f,i,j,k}]$$

$$+\hat{\rho}_{i+1/2,j,k}CC_{i+1/2,j,k}\left[\frac{\rho_{i+1/2,j,k}-\rho_f}{\rho_f}(Z_{i+1,j,k}-Z_{i,j,k})\right]$$

$$-\hat{\rho}_{i-1/2,j,k}CC_{i-1/2,j,k}[h_{f,i,j,k}-h_{f,i-1,j,k}]$$

$$-\hat{\rho}_{i-1/2,j,k}CC_{i-1/2,j,k}\left[\frac{\rho_{i-1/2,j,k}-\rho_f}{\rho_f}(Z_{i,j,k}-Z_{i-1,j,k})\right]$$

$$+\hat{\rho}_{i,j+1/2,k}CR_{i,j+1/2,k}[h_{f,i,j+1,k}-h_{f,i,j,k}]$$

$$+\hat{\rho}_{i,j+1/2,k}CR_{i,j+1/2,k}\left[\frac{\rho_{i,j+1/2,k}-\rho_f}{\rho_f}(Z_{i,j+1,k}-Z_{i,j,k})\right]$$

$$-\hat{\rho}_{i,j-1/2,k}CR_{i,j-1/2,k}[h_{f,i,j,k}-h_{f,i,j-1,k}] \qquad (46)$$

$$-\hat{\rho}_{i,j-1/2,k}CR_{i,j-1/2,k}\left[\frac{\rho_{i,j-1/2,k}-\rho_f}{\rho_f}(Z_{i,j,k}-Z_{i,j-1,k})\right]$$

$$+\hat{\rho}_{i,j,k+1/2}CV_{i,j,k+1/2}[h_{f,i,j,k+1}-h_{f,i,j,k}]$$

$$+\hat{\rho}_{i,j,k+1/2}CV_{i,j,k+1/2}\left[\frac{\rho_{i,j,k+1/2}-\rho_f}{\rho_f}(Z_{i,j,k+1}-Z_{i,j,k})\right]$$

$$-\hat{\rho}_{i,j,k-1/2}CV_{i,j,k-1/2}[h_{f,i,j,k}-h_{f,i,j,k-1}]$$

$$-\hat{\rho}_{i,j,k-1/2}CV_{i,j,k-1/2}\left[\frac{\rho_{i,j,k-1/2}-\rho_f}{\rho_f}(Z_{i,j,k}-Z_{i,j,k-1})\right]$$

$$=\left(\rho_{i,j,k}S_{f,i,j,k}\frac{h_{f,i,j,k}^{n+1}-h_{f,i,j,k}^{n}}{t_{n+1}-t_n}+\theta E\frac{\partial C}{\partial t}\right)V_{i,j,k}-(\bar{\rho}Q_s)_{i,j,k}.$$

The signs in equation 46 can be rearranged to give:

$$
\begin{aligned}
&\hat{\rho}_{i+1/2,j,k} CC_{i+1/2,j,k} [h_{f,i+1,j,k} - h_{f,i,j,k}] \\
&+ \hat{\rho}_{i+1/2,j,k} CC_{i+1/2,j,k} \left[\frac{\rho_{i+1/2,j,k} - \rho_f}{\rho_f} (Z_{i+1,j,k} - Z_{i,j,k}) \right] \\
&+ \hat{\rho}_{i-1/2,j,k} CC_{i-1/2,j,k} [h_{f,i-1,j,k} - h_{f,i,j,k}] \\
&+ \hat{\rho}_{i-1/2,j,k} CC_{i-1/2,j,k} \left[\frac{\rho_{i-1/2,j,k} - \rho_f}{\rho_f} (Z_{i-1,j,k} - Z_{i,j,k}) \right] \\
&+ \hat{\rho}_{i,j+1/2,k} CR_{i,j+1/2,k} [h_{f,i,j+1,k} - h_{f,i,j,k}] \\
&+ \hat{\rho}_{i,j+1/2,k} CR_{i,j+1/2,k} \left[\frac{\rho_{i,j+1/2,k} - \rho_f}{\rho_f} (Z_{i,j+1,k} - Z_{i,j,k}) \right] \\
&+ \hat{\rho}_{i,j-1/2,k} CR_{i,j-1/2,k} [h_{f,i,j-1,k} - h_{f,i,j,k}] \\
&+ \hat{\rho}_{i,j-1/2,j,k} CR_{i,j-1/2,k} \left[\frac{\rho_{i,j-1/2,k} - \rho_f}{\rho_f} (Z_{i,j-1,k} - Z_{i,j,k}) \right] \\
&+ \hat{\rho}_{i,j,k+1/2} CV_{i,j,k+1/2} [h_{f,i,j,k+1} - h_{f,i,j,k}] \\
&+ \hat{\rho}_{i,j,k+1/2} CV_{i,j,k+1/2} \left[\frac{\rho_{i,j,k+1/2} - \rho_f}{\rho_f} (Z_{i,j,k+1} - Z_{i,j,k}) \right] \\
&+ \hat{\rho}_{i,j,k-1/2} CV_{i,j,k-1/2} [h_{f,i,j,k-1} - h_{f,i,j,k}] \\
&+ \hat{\rho}_{i,j,k-1/2} CV_{i,j,k-1/2} \left[\frac{\rho_{i,j,k-1/2} - \rho_f}{\rho_f} (Z_{i,j,k-1} - Z_{i,j,k}) \right] \\
&= \left(\rho_{i,j,k} S_{f,i,j,k} \frac{h_{f,i,j,k}^{n+1} - h_{f,i,j,k}^{n}}{t_{n+1} - t_n} + \theta E \frac{\partial C}{\partial t} \right) V_{i,j,k} - (\bar{\rho} Q_s)_{i,j,k}.
\end{aligned}
\tag{47}
$$

Equation 47 is the finite-difference equation for three-dimensional flow of variable-density ground water as implemented in SEAWAT. Using the following expression for the relative density-difference terms:

$$
D_{i,j,k} = D_{i+1/2,j,k} + D_{i-1/2,j,k} + D_{i,j+1/2,k} + D_{i,j-1/2,k} + D_{i,j,k+1/2} + D_{i,j,k-1/2},
\tag{48}
$$

where:

$$
D_{i+1/2,j,k} = \hat{\rho}_{i+1/2,j,k} CC_{i+1/2,j,k} \left[\frac{\rho_{i+1/2,j,k} - \rho_f}{\rho_f} (Z_{i+1,j,k} - Z_{i,j,k}) \right],
\tag{49a}
$$

$$
D_{i-1/2,j,k} = \hat{\rho}_{i-1/2,j,k} CC_{i-1/2,j,k} \left[\frac{\rho_{i-1/2,j,k} - \rho_f}{\rho_f} (Z_{i-1,j,k} - Z_{i,j,k}) \right],
\tag{49b}
$$

$$
D_{i,j+1/2,k} = \hat{\rho}_{i,j+1/2,k} CR_{i,j+1/2,k} \left[\frac{\rho_{i,j+1/2,k} - \rho_f}{\rho_f} (Z_{i,j+1,k} - Z_{i,j,k}) \right],
\tag{49c}
$$

$$D_{i,j-1/2,k} = \hat{\rho}_{i,j-1/2,k} CR_{i,j-1/2,k} \left[\frac{\rho_{i,j-1/2,k} - \rho_f}{\rho_f} (Z_{i,j-1,k} - Z_{i,j,k}) \right], \tag{49d}$$

$$D_{i,j,k+1/2} = \hat{\rho}_{i,j,k+1/2} CV_{i,j,k+1/2} \left[\frac{\rho_{i,j,k+1/2} - \rho_f}{\rho_f} (Z_{i,j,k+1} - Z_{i,j,k}) \right], \tag{49e}$$

and:

$$D_{i,j,k-1/2} = \hat{\rho}_{i,j,k-1/2} CV_{i,j,k-1/2} \left[\frac{\rho_{i,j,k-1/2} - \rho_f}{\rho_f} (Z_{i,j,k-1} - Z_{i,j,k}) \right]. \tag{49f}$$

Equation 47 becomes:

$$
\begin{aligned}
&\hat{\rho}_{i+1/2,j,k} CC_{i+1/2,j,k} [h_{f,i+1,j,k} - h_{f,i,j,k}] + \hat{\rho}_{i-1/2,j,k} CC_{i-1/2,j,k} [h_{f,i-1,j,k} - h_{f,i,j,k}] \\
&+ \hat{\rho}_{i,j+1/2,k} CR_{i,j+1/2,k} [h_{f,i,j+1,k} - h_{f,i,j,k}] + \hat{\rho}_{i,j-1/2,k} CR_{i,j-1/2,k} [h_{f,i,j-1,k} - h_{f,i,j,k}] \\
&+ \hat{\rho}_{i,j,k+1/2} CV_{i,j,k+1/2} [h_{f,i,j,k+1} - h_{f,i,j,k}] + \hat{\rho}_{i,j,k-1/2} CV_{i,j,k-1/2} [h_{f,i,j,k-1} - h_{f,i,j,k}] + D_{i,j,k} \\
&= \left(\rho_{f,i,j,k} S_{f,i,j,k} \frac{h_{f,i,j,k}^{n+1} - h_{f,i,j,k}^{n}}{t_{n+1} - t_n} + \theta E \frac{\partial C}{\partial t} \right) V_{i,j,k} - (\bar{\rho} Q_s)_{i,j,k}.
\end{aligned}
\tag{50}
$$

Equation 50 implies that model layers can be either horizontal or tilted. When model layers are tilted, $D_{i+1/2,j,k}$, $D_{i-1/2,j,k}$, $D_{i,j+1/2,k}$, $D_{i,j-1/2,k}$ contribute to the mass flux across the four faces normal to model layers. When the model layers are horizontal, $D_{i+1/2,j,k}$, $D_{i-1/2,j,k}$, $D_{i,j+1/2,k}$, $D_{i,j-1/2,k}$ become zero. For this case, equation 50 reduces to:

$$
\begin{aligned}
&\hat{\rho}_{i+1/2,j,k} CC_{i+1/2,j,k} [h_{f,i+1,j,k} - h_{f,i,j,k}] + \hat{\rho}_{i-1/2,j,k} CC_{i-1/2,j,k} [h_{f,i-1,j,k} - h_{f,i,j,k}] \\
&+ \hat{\rho}_{i,j+1/2,k} CR_{i,j+1/2,k} [h_{f,i,j+1,k} - h_{f,i,j,k}] + \hat{\rho}_{i,j-1/2,k} CR_{i,j-1/2,k} [h_{f,i,j-1,k} - h_{f,i,j,k}] \\
&+ \hat{\rho}_{i,j,k+1/2} CV_{i,j,k+1/2} \left[h_{f,i,j,k+1} - h_{f,i,j,k} + \frac{\rho_{i,j,k+1/2} - \rho_f}{\rho_f} (Z_{i,j,k+1} - Z_{i,j,k}) \right] \\
&+ \hat{\rho}_{i,j,k-1/2} CV_{i,j,k-1/2} \left[h_{f,i,j,k-1} - h_{f,i,j,k} + \frac{\rho_{i,j,k-1/2} - \rho_f}{\rho_f} (Z_{i,j,k-1} - Z_{i,j,k}) \right] \\
&= \left(\rho_{f,i,j,k} S_{f,i,j,k} \frac{h_{f,i,j,k}^{n+1} - h_{f,i,j,k}^{n}}{t_{n+1} - t_n} + \theta E \frac{\partial C}{\partial t} \right) V_{i,j,k} - (\bar{\rho} Q_s)_{i,j,k}.
\end{aligned}
\tag{51}
$$

If variations in fluid density are not considered, equation 51 reduces to:

$$CC_{i+1/2,j,k}[h_{f,i+1,j,k}-h_{i,j,k}] + CC_{i-1/2,j,k}[h_{i-1,j,k}-h_{i,j,k}]$$
$$+ CR_{i,j+1/2,k}[h_{i,j+1,k} - h_{i,j,k}] + CR_{i,j-1/2,k}[h_{i,j-1,k} - h_{i,j,k}]$$
$$+ CV_{i,j,k+1/2}[h_{i,j,k+1} - h_{i,j,k}] + CV_{i,j,k-1/2}[h_{i,j,k-1} - h_{i,j,k}]$$
$$= S_{f,i,j,k}\frac{h_{i,j,k}^{n+1} - h_{i,j,k}^{n}}{t_{n+1} - t_{n}}V_{i,j,k} - Q_{s,i,j,k}. \tag{52}$$

Equation 52 is the finite-difference equation solved in a conventional MODFLOW application (McDonald and Harbaugh, 1988).

Construction of System Equations

At timestep $n+1$, equation 50 can be rearranged so that all terms containing the dependent variable, h_f at time $n+1$, are on the left-hand side and all terms that do not contain the unknown are on the right-hand-side. The equation becomes:

$$\hat{\rho}_{i+1/2,j,k}CC_{i+1/2,j,k}h_{f,i+1,j,k}^{n+1} - \hat{\rho}_{i+1/2,j,k}CC_{i+1/2,j,k}h_{f,i,j,k}^{n+1}$$
$$+ \hat{\rho}_{i-1/2,j,k}CC_{i-1/2,j,k}h_{f,i-1,j,k}^{n+1} - \hat{\rho}_{i-1/2,j,k}CC_{i-1/2,j,k}h_{f,i,j,k}^{n+1}$$
$$+ \hat{\rho}_{i,j+1/2,k}CR_{i,j+1/2,k}h_{f,i,j+1,k}^{n+1} - \hat{\rho}_{i,j+1/2,k}CR_{i,j+1/2,k}h_{f,i,j,k}^{n+1}$$
$$+ \hat{\rho}_{i,j-1/2,k}CR_{i,j-1/2,k}h_{f,i,j-1,k}^{n+1} - \hat{\rho}_{i,j-1/2,k}CR_{i,j-1/2,k}h_{f,i,j,k}^{n+1} \tag{53}$$
$$+ \hat{\rho}_{i,j,k+1/2}CV_{i,j,k+1/2}h_{f,i,j,k+1}^{n+1} - \hat{\rho}_{i,j,k+1/2}CV_{i,j,k+1/2}h_{f,i,j,k}^{n+1}$$
$$+ \hat{\rho}_{i,j,k-1/2}CV_{i,j,k-1/2}h_{f,i,j,k-1}^{n+1} - \hat{\rho}_{i,j,k-1/2}CV_{i,j,k-1/2}h_{f,i,j,k}^{n+1}$$
$$+ D_{i,j,k} - \rho_{i,j,k}S_{f,i,j,k}\frac{V_{i,j,k}}{t_{n+1}-t_n}h_{f,i,j,k}^{n+1} = \left(\rho_{i,j,k}S_{f,i,j,k}\frac{-h_{f,i,j,k}^{n}}{t_{n+1}-t_n} + \theta E\frac{\partial C}{\partial t}\right)V_{i,j,k} - (\bar{\rho}Q_s)_{i,j,k}.$$

As noted in Chapter 2, the strength of the source/sink terms may be head dependent. Thus, the flux between a sink/source and an aquifer can be proportional to the head difference between the aquifer and sink/source feature, such as drains and rivers. For other cases, the flux between a sink/source and an aquifer may not depend on the head in the aquifer (for example, wells and recharge). Formulation of sink/source terms will be presented in Chapter 5, which discusses the modification of individual packages required in SEAWAT.

All the terms, except for the relative density-difference term $D_{i,j,k}$ in the left-hand side of equation 53, explicitly contain the dependent variable, h_f, at time level $n+1$. The terms in the right-hand side of equation 53 do not contain the dependent variable at time level $n+1$.

All density values, except for the freshwater density, should correspond to the same time level as the freshwater heads. In SEAWAT, the density terms are treated as "constants" when the flow equation is formulated and solved for freshwater head. This simplification is acceptable for most cases as long as the timestep is sufficiently short or the change of fluid density is relatively slow compared to the change of freshwater head. Because the relative density-difference term, $D_{i,j,k}$ is evaluated using the solute concentration from

the previous timestep (or previous iteration of the same timestep if the flow and transport equations are implicitly coupled), $D_{i,j,k}$ in equation 53 represents a "constant" value for each cell, in the sense that it is not affected by the heads at the new time level $n+1$. It follows that the relative density-difference term can be treated as a constant when the flow equation is solved iteratively. Thus, the relative density-difference term, $D_{i,j,k}$, can be moved to the right-hand side of equation 53. Then equation 53 becomes:

$$
\begin{aligned}
&\hat{\rho}_{i+1/2,j,k} CC_{i+1/2,j,k} h^{n+1}_{f,i+1,j,k} - \hat{\rho}_{i+1/2,j,k} CC_{i+1/2,j,k} h^{n+1}_{f,i,j,k} \\
&+ \hat{\rho}_{i-1/2,j,k} CC_{i-1/2,j,k} h^{n+1}_{f,i-1,j,k} - \hat{\rho}_{i-1/2,j,k} CC_{i-1/2,j,k} h^{n+1}_{f,i,j,k} \\
&+ \hat{\rho}_{i,j+1/2,k} CR_{i,j+1/2,k} h^{n+1}_{f,i,j+1,k} - \hat{\rho}_{i,j+1/2,k} CR_{i,j+1/2,k} h^{n+1}_{f,i,j,k} \\
&+ \hat{\rho}_{i,j-1/2,k} CR_{i,j-1/2,k} h^{n+1}_{f,i,j-1,k} - \hat{\rho}_{i,j-1/2,k} CR_{i,j-1/2,k} h^{n+1}_{f,i,j,k} \\
&+ \hat{\rho}_{i,j,k+1/2} CV_{i,j,k+1/2} h^{n+1}_{f,i,j,k+1} - \hat{\rho}_{i,j,k+1/2} CV_{i,j,k+1/2} h^{n+1}_{f,i,j,k} \\
&+ \hat{\rho}_{i,j,k-1/2} CV_{i,j,k-1/2} h^{n+1}_{f,i,j,k-1} - \hat{\rho}_{i,j,k-1/2} CV_{i,j,k-1/2} h^{n+1}_{f,i,j,k} \\
&- \rho_{i,j,k} S_{f,i,j,k} \frac{V_{i,j,k}}{t_{n+1} - t_n} h^{n+1}_{f,i,j,k} \\
&= \left(\rho_{i,j,k} S_{f,i,j,k} \frac{-h^n_{f,i,j,k}}{t_{n+1} - t_n} + \theta E \frac{\partial C}{\partial t} \right) V_{i,j,k} - (\bar{\rho} Q_s)_{i,j,k} - D_{i,j,k}.
\end{aligned}
\tag{54}
$$

Because none of the terms in the right-hand side of equation 54 explicitly contain the dependent variable, h_f at time level $n+1$, they can be lumped together and treated as one constant in the solution procedure.

Equation 54 is the finite-difference approximation of flow for cell (i,j,k). As previously mentioned, a similar equation can be written for each cell inside the model domain. If N active cells are inside the model domain, there are N equations similar to equation 54 for the N active cells. Following the general matrix notation:

$$
[A]\{h_f\} = \{B\},
\tag{55}
$$

where:

   $[A]$ is the coefficient matrix with size N by N (a sparse matrix where most entries are zero except for those falling on the seven diagonals for a three-dimensional model),

   $\{h_f\}$ is the unknown vector of size N (the freshwater head at each cell) at the new time level, and

   $\{B\}$ is a vector of size N, which accumulates all known or constant terms appearing on the right-hand side of equation 55.

For this reason, the vector B is sometimes referred to as the *RHS* (right-hand side) accumulator in MODFLOW. In SEAWAT, the *RHS* accumulator is different compared with MODFLOW because each term is multiplied by fluid density. Thus, the *RHS* accumulator in SEAWAT has dimensions of $[MT^{-1}]$ compared with the *RHS* accumulator in MODFLOW, which has dimensions of $[L^3 T^{-1}]$.

Equation 55 can be solved using standard methods applicable to a system of linear equations and is identical to the system of equations solved by MODFLOW. Readers should refer to the MODFLOW documentation (McDonald and Harbaugh, 1988) for further information.

CHAPTER 4
DESIGN AND STRUCTURE OF THE SEAWAT PROGRAM

The SEAWAT code is MODFLOW and MT3DMS combined into a single program that solves the coupled flow and solute-transport equations. Parts of the original MODFLOW code were modified to include the relative density-difference terms and the term that quantifies the rate of mass accumulation due to changes in solute concentration, and the entire flow equation was reformulated to conserve mass rather than fluid volume. The coupling between flow and transport is performed through a synchronous timestepping approach that cycles between MODFLOW solutions of the flow equation and MT3DMS solutions of the transport equation (fig. 4).

SEAWAT includes both explicit and implicit methods for coupling the flow and solute-transport equations. With the explicit method, a lagged approach is used for assigning fluid densities in the flow equation. This means that fluid densities are calculated with solute concentrations from the previous timestep. Advective fluxes from the flow solution for the current timestep are then used in the current solution to the transport equation. This cycling mechanism results in an explicit coupling of the flow and transport equations.

With the implicit coupling method, solutions to the flow and transport equations are repeated, and concentrations and densities are updated within each timestep until the maximum difference in fluid density at a single cell for consecutive iterations is less than a user-specified value.

The present version of SEAWAT is written with MODFLOW-88 and MT3DMS. In linking these two codes, the SEAWAT program was coded and designed to meet the following three objectives in order of importance:

1. Simulations provide an accurate solution to the variable-density ground-water flow equation;

2. The program maintains a modular structure, which makes it easy to modify and improve; and

3. Modifications to the original MODFLOW and MT3DMS subroutines and input files are kept to a minimum to allow users of these programs to gain rapid familiarity with SEAWAT and to allow newer versions of MODFLOW and MT3DMS to be easily incorporated into SEAWAT.

The third objective was only partially achieved because many of the MODFLOW procedures required modification to accommodate the variable-density form of the ground-water flow equation.

This chapter presents the overall design and structure of the SEAWAT program and provides the framework for Chapter 5, which provides details of the modifications of MODFLOW and MT3DMS. MODFLOW and MT3DMS are lengthy programs that do much more than simply solve equations. Both programs perform read and write operations, track volumetric and mass budgets, and so forth. For
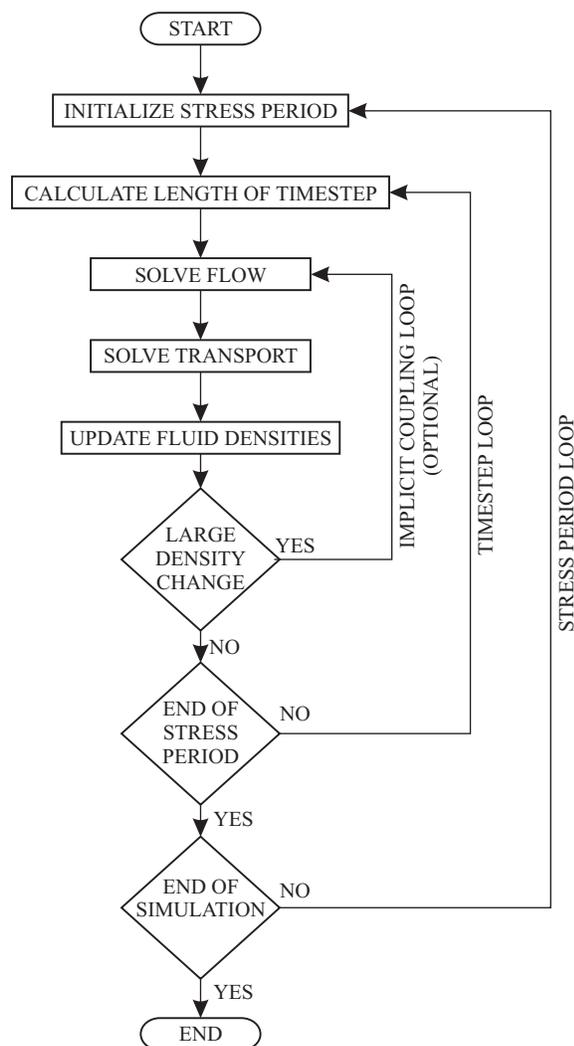
Figure 4. Generalized flow chart of the SEAWAT program.

this reason, the phrases "solve the flow equation" or "solve the transport equation" are used herein to refer to only those parts of MODFLOW or MT3DMS, respectively, which are actually required to solve the particular equation.

Temporal Discretization

The temporal discretization scheme implemented in the SEAWAT code is a combination of the schemes used by MODFLOW and MT3DMS. This section reviews the temporal discretization schemes implemented in the conventional versions of MODFLOW and MT3DMS and presents the approach implemented in SEAWAT.

For a conventional MODFLOW application, the total simulation period is divided into one or more stress periods. During a single stress period, flow rates and boundary heads—with the exception of the Time-Varying Constant Head (CHD) package—remain constant. Each stress period is further divided into one or more timesteps to produce results that are more accurate or to allow output from the model to be saved for selected times. During each timestep, MODFLOW solves the flow equation for the period from t_n to t_{n+1}.

MT3DMS was originally designed to work with MODFLOW. In a conventional MODFLOW-MT3DMS application, spatial and temporal variations in fluid density are assumed to be so small as to have no measurable effect on the flow field. Thus, a practical procedure was developed in which the flow simulation is first performed with MODFLOW, and during the simulation, flow information (saturated thickness, cell-by-cell discharge rates, and boundary flows) required by MT3DMS to solve the solute-transport equation is stored in a MODFLOW-MT3DMS link file. This link file is then used in a subsequent MT3DMS run in which only solute transport is simulated.

MT3DMS further divides each MODFLOW timestep into transport steps. The term, transport step, was introduced to avoid confusion with a MODFLOW timestep. A transport step, however, is the timestep or time increment used by MT3DMS to solve the transport equation (eq. 38), and thus, is conceptually analogous to a MODFLOW timestep. MODFLOW timesteps are further divided into transport steps in MT3DMS because of stability requirements with the explicit solution schemes implemented in MT3DMS. For example, Zheng and Wang (1998) list the stability constraints and accuracy requirements for the transport of conservative species with the explicit finite-difference scheme as:

$$\text{advection, } \Delta t \leq \frac{1}{\dfrac{v_x}{\Delta x} + \dfrac{v_y}{\Delta y} + \dfrac{v_z}{\Delta z}}, \tag{56a}$$

$$\text{dispersion, } \Delta t \leq \frac{0.5}{\dfrac{D_{xx}}{\Delta x^2} + \dfrac{D_{yy}}{\Delta y^2} + \dfrac{D_{zz}}{\Delta z^2}}, \tag{56b}$$

and:

$$\text{sink/source, } \Delta t \leq \frac{\theta}{|q_s|}, \tag{56c}$$

where:

Δt is the length of the timestep, and

$\Delta x, \Delta y, \Delta z$ are the dimensions of the model cell.

MT3DMS uses the stability constraints and accuracy requirements in equation 56a-c to calculate the maximum permissible length of transport steps; therefore, the lengths of transport steps are not specified by the user, but rather calculated by the program. The stability constraint for advection requires flow velocities

to calculate transport step lengths. For a given MODFLOW timestep, extending from t_n to t_{n+1}, MT3DMS uses the velocities calculated for the end of the timestep, t_{n+1}, in equation 56a-c to calculate the length and number of transport steps required over the interval t_n to t_{n+1}.

In addition to the explicit solvers for the transport equation, MT3DMS also has an implicit iterative procedure called the generalized conjugate gradient (GCG) solver (Zheng and Wang, 1998). With the implicit solver, the user is allowed to specify the lengths of transport steps. In many cases, the implicit solver may reduce the number of transport steps required for a simulation. The lengths of transport steps, however, may be limited by accuracy requirements, and convergence issues may arise if the specified transport lengths are too long.

The above procedure involves the calculation of the full sequence of head and flow values prior to the start of transport calculation and cannot be used in a variable-density program because of the interdependence of the flow and transport equations. In SEAWAT, stress periods are divided into timesteps. If an explicit solver is used for transport, the timestep lengths are calculated during the simulation by SEAWAT to satisfy the stability constraints and accuracy requirements (eq. 56a-c), and thus, the number of timesteps is not known prior to execution. Both the flow and transport equations are solved during a SEAWAT timestep. For the coupling of the flow and the transport equations, the SEAWAT program contains two approaches, explicit and implicit. The explicit approach requires less computer time but may not be as accurate as the implicit approach. Additionally, smaller timesteps may be required for the explicit approach compared to those needed for the implicit approach. Descriptions of these coupling options are presented in the subsequent sections.

Explicit Coupling of Flow and Transport

The following sequence is used in SEAWAT to advance the simulation through time if the user specifies an explicit coupling between flow and transport (fig. 5).

ρ_n Distribution of fluid density at end of timestep n [ML^{-3}]

C_n Distribution of solute concentration at end of timestep n [ML^{-3}]

q_n Field of specific discharge at end of timestep n [LT^{-1}]
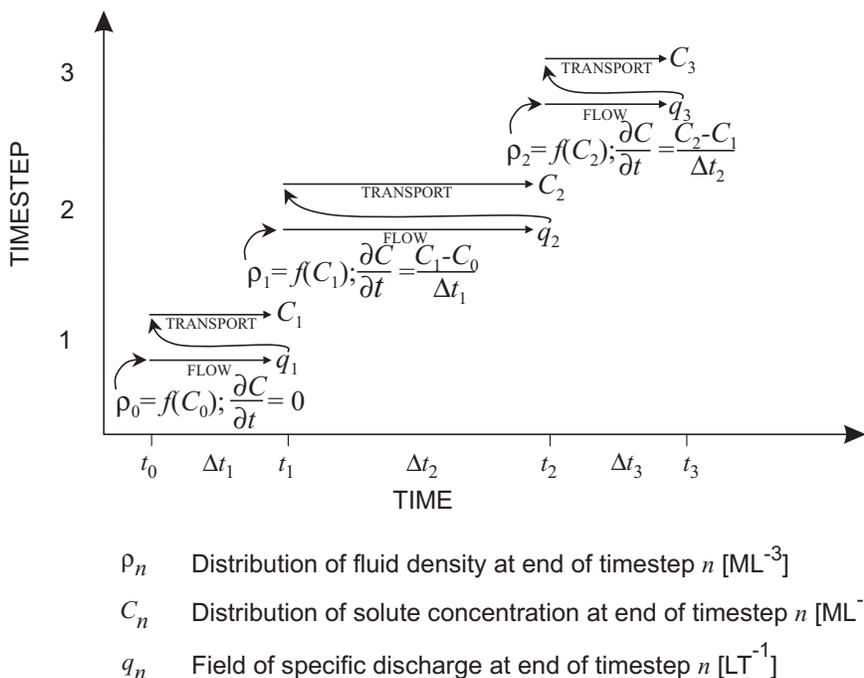
Figure 5. Example of the explicit scheme used to couple the flow and transport equations.

1. The flow equation is solved iteratively using the modified MODFLOW routines to calculate heads at a time t_1, representing the end of the initial timestep. This iterative solution procedure is performed with fluid densities from the previous stress period, or with densities calculated from the initial solute concentrations if it is the first stress period. The length of the initial timestep, Δt_1, is specified by the user through the input variable INITIALDT or is assigned a default value if no input is specified. The default value currently used in SEAWAT is 0.01 time units; the default value would be 0.01 day, for example, if the units selected for time are days.

2. Values of specific discharge for time t_1 at model boundaries and within the model domain are calculated from the results of the flow simulation and passed to the transport routines to represent flow over the time interval Δt_1.

3. Solute concentrations for time t_1 are determined by solving the transport equation over the time interval Δt_1.

4. Fluid densities for t_1, which are used in solving the flow equation for the second timestep, are calculated from the t_1 solute concentrations.

5. The length of Δt_2 is calculated according to the stability constraints and accuracy requirements, using velocities calculated for the beginning of that time period. This calculated timestep length for Δt_2 should always be greater than the length of the initial timestep length, Δt_1. A calculated value for Δt_2 less than Δt_1 indicates rapidly changing concentration and density fields at the beginning of the stress period. If Δt_1, which has a default value of 0.01 time units unless otherwise specified by the user, is greater than Δt_2, SEAWAT displays a warning message. At this point, the user needs to go back to step 1 and shorten the value of INITIALDT, and rerun SEAWAT.

6. The flow equation is solved to calculate heads and flows for the end of the second step, t_2, using the fluid densities that were calculated in the first timestep.

7. Solute concentrations for time t_2 are determined by solving the transport equation over the time interval Δt_2. These concentrations are then used to calculate fluid densities for t_2.

8. The stability constraints and accuracy requirements are used to calculate the maximum timestep length for Δt_3, and the sequence is repeated.

When the explicit coupling approach is used in SEAWAT, three criteria should be considered: (1) instability problems may occur during solution of the flow equation because densities are calculated using the previous timestep concentrations; (2) the lengths of timesteps, which are calculated to satisfy the stability constraints and accuracy requirements of the transport equation, are based on velocities calculated for the end of the preceding timestep; and thus (3) there is a lag of one timestep in the application of the stability constraints and accuracy requirements. The constraints that should be applied to timestep n are actually applied to timestep $n+1$. Because this coupling approach is explicit, additional simulations with reduced timestep lengths should be performed to verify that consistent results are obtained.

Implicit Coupling of Flow and Transport

The implicit approach involves the solution of the flow and transport equations in an iterative sequence for each timestep until the consecutive differences in the calculated fluid densities are less than a user-specified value (fig. 6). Referring to the explicit approach outlined previously, the implicit coupling approach will repeat steps 2, 3, and 4 within each timestep until the consecutive change in fluid density is less than a user-specified convergence value. The implicit coupling approach results in heads, concentrations, densities, and flows that pertain to the end of the timestep.

The implicit coupling approach in the current version of SEAWAT only works when a MT3DMS finite-difference method (as opposed to a particle-tracking-based method) is used to solve the solute-transport equation. The implicit coupling approach was not programmed for the particle-based solution methods because of the computer memory that would be required to store particle information. As the implicit coupling approach may solve the transport equation more than one time for each timestep, the same starting particle distribution would have to be used for each solution.
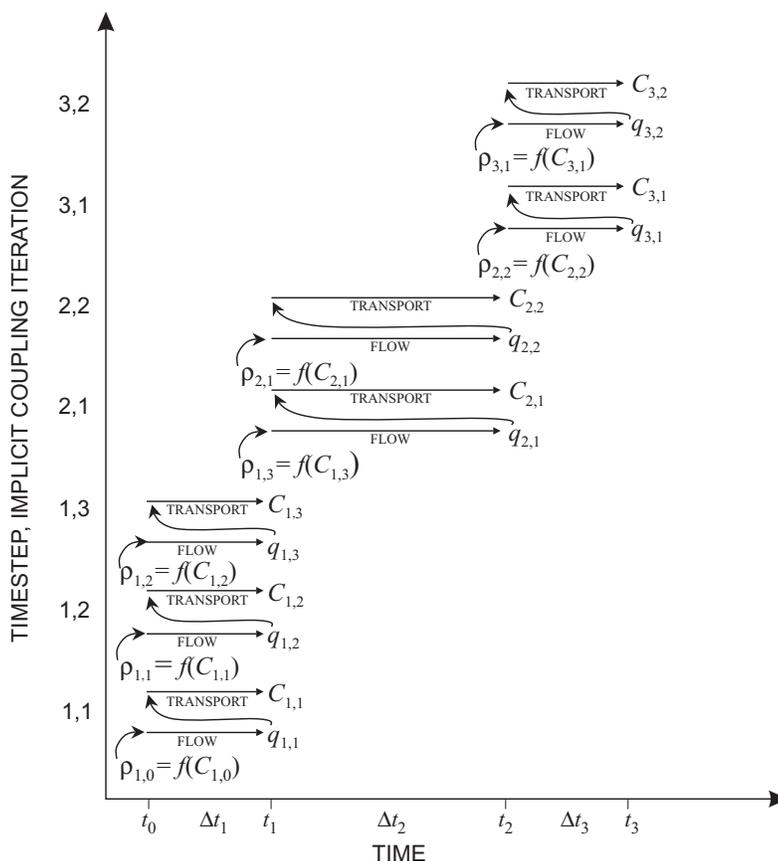
$\rho_{n,ncpl}$ Distribution of fluid density at end of timestep n and end of coupling iteration $ncpl$ [ML^{-3}]

$C_{n,ncpl}$ Distribution of solute concentration at end of timestep n and end of coupling iteration $ncpl$ [ML^{-3}]

$q_{n,ncpl}$ Field of specific discharge at end of timestep n and end of coupling iteration $ncpl$ [LT^{-1}]

Figure 6. Example of the implicit scheme used to couple the flow and transport equations.

With the implicit coupling approach, the user may specify the lengths of the timesteps. In a conventional application of MT3DMS, the implicit GCG solver can increase the lengths of transport steps, reduce the number of transport steps, and substantially reduce the amount of time required for a computer to perform the simulation. While the GCG solver may be used in SEAWAT to increase the lengths of timesteps, the advantages may not be as large as with conventional applications of MT3DMS because of the interdependence between flow and transport. As with the explicit coupling approach, repeated simulations with shorter timesteps can help verify the numerical accuracy of results.

Structure of the SEAWAT Program

The structure of the original MODFLOW and MT3DMS programs is a main program that performs calls to subroutines. This is the general approach used by SEAWAT, whereby the main SEAWAT program makes calls to MODFLOW, MT3DMS, and SEAWAT subroutines. The main SEAWAT program was written by adding appropriate MT3DMS and SEAWAT subroutine calls to the main MODFLOW program and synchronizing the timesteps.

The original MODFLOW and MT3DMS main programs are divided into "procedures," which are categories of tasks that fall under the same general purpose. Because SEAWAT primarily consists of MODFLOW and MT3DMS, the main SEAWAT program also is divided into procedures. The flow chart for SEAWAT procedures is presented in figure 7.
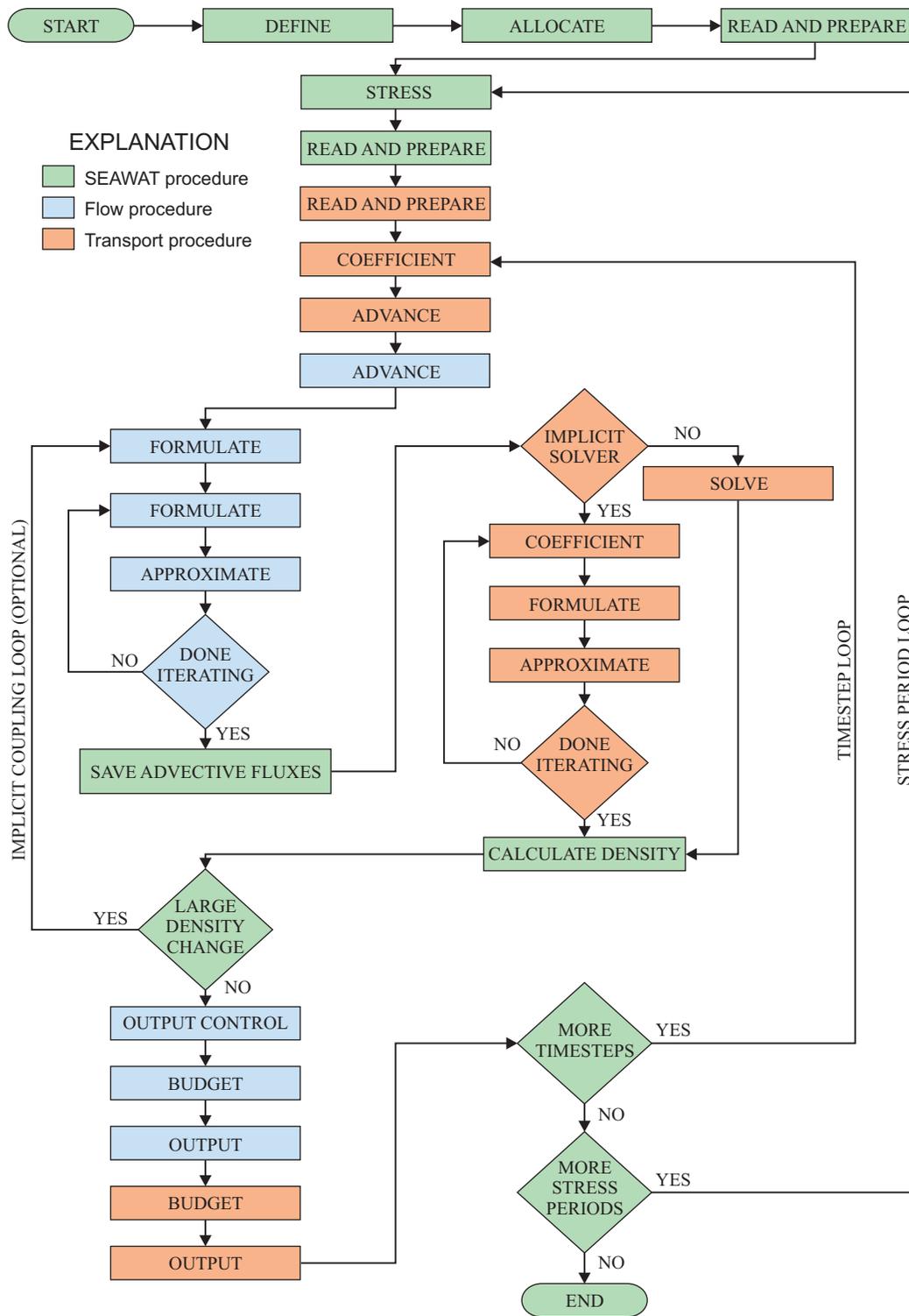
Figure 7. Step-by-step procedures of the SEAWAT program.

Packages

The 1988 version of MODFLOW and the MT3DMS version of MT3D are used in SEAWAT. Both of these codes utilize the "package" approach in which features and options may be turned on or off by users depending on the requirements of the specific problem. Table 1 lists the packages that are available in the current version of SEAWAT. Several additional MODFLOW packages, introduced after the 1988 version of MODFLOW was released, also are included in SEAWAT to extend the applicability of the program to a wide range of problems. These additional or updated packages include the BCF2 package (McDonald and others, 1992), EVT package that allows evapotranspiration to be withdrawn from the highest active cell (Swain and others, 1996), CHD package (Leake and Prudic, 1988), PCG2 package (Hill, 1990), and LKMT3D package (Zheng and Wang, 1998).

Array Structure and Memory Allocation

Both MODFLOW and MT3DMS utilize the same general approach for allocating computer memory. In the original versions of MODFLOW and MT3DMS, a single array, called the X array, is used to store most of the information for a simulation. In the SEAWAT code, four main arrays are used: X array (for MODFLOW information), Y array (for real MT3DMS information), IY array (for integer MT3DMS information), and Z array (for SEAWAT-specific information). Computer memory for each of these arrays is allocated during run time using the FORTRAN 90 statements—ALLOCATABLE and ALLOCATE.

Table 1. MODFLOW and MT3DMS packages used in SEAWAT

Package	Acronym	Program	Reference
Basic	BAS	MODFLOW	McDonald and Harbaugh (1988)
Block-Centered Flow	BCF2	MODFLOW	McDonald and others (1992)
Well	WEL	MODFLOW	McDonald and Harbaugh (1988)
Drain	DRN	MODFLOW	McDonald and Harbaugh (1988)
River	RIV	MODFLOW	McDonald and Harbaugh (1988)
Evapotranspiration	EVT	MODFLOW	Swain and others (1996)
General-Head Boundary	GHB	MODFLOW	McDonald and Harbaugh (1988)
Recharge	RCH	MODFLOW	McDonald and Harbaugh (1988)
Strongly Implicit Procedure	SIP	MODFLOW	McDonald and Harbaugh (1988)
Successive Over-Relaxation	SOR	MODFLOW	McDonald and Harbaugh (1988)
Preconditioned Conjugate Gradient Solver	PCG2	MODFLOW	Hill (1990)
Output Control	OC	MODFLOW	McDonald and Harbaugh (1988)
Time-Variant Constant Head	CHD	MODFLOW	Leake and Prudic (1988)
LinkMT3D	LKMT3D	MODFLOW	Zheng and Wang (1998)
Basic Transport	BTN	MT3DMS	Zheng and Wang (1998)
Advection	ADV	MT3DMS	Zheng and Wang (1998)
Dispersion	DSP	MT3DMS	Zheng and Wang (1998)
Source/Sink Mixing	SSM	MT3DMS	Zheng and Wang (1998)
Reaction	RCT	MT3DMS	Zheng and Wang (1998)
Generalized Conjugate Gradient Solver	GCG	MT3DMS	Zheng and Wang (1998)

CHAPTER 5

MODIFICATIONS OF MODFLOW AND MT3DMS

Under the SEAWAT approach, two separate computer programs, MODFLOW and MT3DMS, were modified and combined into one program. Among these modifications are the conversion of volumetric fluxes to mass fluxes and the addition of relative density-difference terms and solute-mass accumulation terms to the basic finite-difference equation solved by MODFLOW. Additionally, modifications were made to each of the stress packages of MODFLOW because mass fluxes and freshwater heads are used in SEAWAT. Modifications of MT3DMS are relatively minor and mainly affect internal data transfer and manipulation. This chapter focuses on the modifications made to the block-centered flow (BCF) package and the following stress packages implemented in MODFLOW:

- Well (WEL) package

- River (RIV) package

- Drain (DRN) package

- Recharge (RCH) package

- Evapotranspiration (EVT) package

- General-Head Boundary (GHB) package

- Time-Varying Constant Head (CHD) package

This chapter shows how the equations, as originally formulated in MODFLOW, were modified to represent variable-density ground-water flow. To simplify this documentation, presentation of the FORTRAN source code is excluded because much of the SEAWAT program is unmodified MODFLOW and MT3DMS code. Modifications to the original MODFLOW and MT3DMS programs are marked in the source code where the changes were made.

Matrix and Vector Accumulators

SEAWAT uses the same approach as MODFLOW for constructing the matrix equations that describe ground-water flow. Equation 55 shows the general form of the matrix equation solved by SEAWAT and is identical in form to the one solved by MODFLOW. The [A] matrix represents coefficients of equivalent freshwater head, of which a portion is stored in a three-dimensional array called the *HCOF* accumulator. The {B} vector represents constant terms on the right-hand side of equation 55 and is stored in a three-dimensional array called the *RHS* accumulator. MODFLOW and SEAWAT pass these accumulators and other terms into subroutines that solve for head or equivalent freshwater head, respectively.

As part of the solution procedure, a series of subroutines assemble the *RHS* and *HCOF* accumulators. Prior to assembly, the *RHS* and *HCOF* accumulators are initialized with values of zero. During the assembly, consecutive calls to various subroutines add to or subtract from the accumulators in order to include storage effects, sources, sinks, and other components. In the following sections, the *RHS* accumulator is referred to in mathematical expressions as $RHS_{i,j,k}^{old}$ and $RHS_{i,j,k}^{new}$. $RHS_{i,j,k}^{old}$ represents the value of *RHS* for cell (i,j,k) up to that point in the series of assembly subroutines. The term $RHS_{i,j,k}^{new}$ represents the new value of *RHS* at cell (i,j,k) after the mathematical expression from that subroutine has been applied. Note, however, that the final value of $RHS_{i,j,k}^{new}$ passed into the solver cannot be determined until the entire sequence of assembly routines has been called.

Modifications of the Basic Flow Equation

In Chapter 3, the finite-difference equation for freshwater head in cell (*i,j,k*) was developed with the simplification that relative density-difference terms are kept constant within each timestep (or within each solution of the flow equation if the implicit coupling approach is utilized). Inspection of the flow equation solved by SEAWAT (eq. 50) suggests that it is similar in mathematical form to the equation solved by MODFLOW (eq. 52). Thus, the solution techniques implemented in the original version of MODFLOW also can be used to solve the variable-density flow equation if the code is appropriately modified to include the density terms.

Addition of Relative Density-Difference Term

The relative density-difference term for a model cell, as defined in equation 48 (and in more detail in eq. 49a-f), is treated as constant during solution of the flow equation. With the explicit approach for coupling flow and transport, the density values are calculated from solute concentrations from the previous timestep (or initial concentrations for the first timestep). With the implicit approach for coupling flow and transport, the density values are calculated from solute concentrations from the previous iteration of that timestep.

SEAWAT adds the relative density-difference term to the *RHS* accumulator using the following expression:

$$RHS_{i,j,k}^{new} = RHS_{i,j,k}^{old} - D_{i,j,k}. \tag{57}$$

Note that one or more of the six components of the relative density-difference term (eq. 49a-f) may equal zero if the fluid density is the same as the density of freshwater, or if the elevations of two adjacent cell centers are the same.

Weiss (1982) developed a similar approach for the steady-state situation when fluid density does not change with time. With that approach, "pseudo sources" are calculated for each model cell prior to simulation. The "pseudo sources," which represent the relative density-difference terms, are then treated as constants during a simulation with a constant density ground-water flow model.

Addition of Solute Mass Accumulation Term

A similar approach to that used for the density-difference terms also can be used to include the term for solute mass accumulation. The term for solute mass accumulation can be added to the *RHS* accumulator because the term does not contain the principal variable, freshwater head. With the explicit coupling approach, the partial derivative for solute concentration, $\partial C / \partial t$, is evaluated using concentrations from the previous timestep. With the implicit coupling approach, $\partial C / \partial t$ is evaluated using concentrations from the previous coupling iteration. With either approach, $\partial C / \partial t$ is zero for the first timestep of a simulation.

For the explicit coupling approach, SEAWAT uses the following expression to include the term for solute mass accumulation in the *RHS* accumulator:

$$RHS_{i,j,k}^{new} = RHS_{i,j,k}^{old} + \theta E \frac{C_{i,j,k}^{n-1} - C_{i,j,k}^{n-2}}{\Delta t_{n-1}} V_{i,j,k}. \tag{58}$$

For the implicit coupling approach, a similar equation is used to update the *RHS* accumulator except that the concentrations from a previous coupling iteration are used rather than concentrations from a previous timestep.

Conversion from Volume Conservation to Mass Conservation

Volumetric fluxes are converted to mass fluxes by multiplying by fluid density. This is accomplished by multiplying the conductance terms by fluid density. In MODFLOW, three-dimensional arrays called *CC*, *CR* and *CV* contain values of conductance in each direction. The conductance values stored in these three arrays are calculated as the harmonic mean of the transmissivity between two adjacent nodes. For example, the conductance along a column is calculated with the following equation:

$$CC_{i+1/2,j,k} = 2DELR \frac{TC_{i,j,k}TC_{i+1,j,k}}{TC_{i,j,k}DELC_{i+1} + TC_{i+1,j,k}DELC_i}, \tag{59}$$

where:

$DELR$ is the grid width along the row [L],

TC is the transmissivity for each cell in the column direction [L^2T^{-1}], and

$DELC$ is the grid width along the column [L].

These conductance arrays may or may not be updated during simulations depending on the aquifer type (LAYCON) specified by the user.

In SEAWAT, three new arrays (*RHOCR, RHOCC,* and *RHOCV*) are used to hold the mass conductances, which are the conductance values multiplied by fluid density. The original conductance arrays (*CR, CC*, and *CV*) are still used to hold the values of conductance in each direction. The new arrays are calculated as the product of the conductance terms and the fluid density in the upstream direction. An example of the expression is:

$$RHOCC_{i+1/2,j,k} = \hat{\rho}_{i+1/2,j,k}CC_{i+1/2,j,k}. \tag{60}$$

Whether or not the conductance terms are updated, these three new arrays are recalculated within each iteration of the flow equation. The three mass conductance arrays are passed into the solver, rather than the original conductance arrays, because the system of equations is conserving fluid mass, not fluid volume.

Conversion from Fluid Volume Storage to Fluid Mass Storage

For a layer in which the storage coefficient remains constant during the simulation, the storage formulation is based on a direct application of the storage expression that applies to an individual cell, (i,j,k). In MODFLOW, the storage expression has the form:

$$\frac{\Delta V}{\Delta t} = SS_{i,j,k}(\Delta r_j \Delta c_i \Delta v_k)\frac{h^n_{i,j,k} - h^{n-1}_{i,j,k}}{t_n - t_{n-1}}, \tag{61}$$

where:

$\Delta V/\Delta t$ is the volumetric rate of accumulation of water in the cell;

$SS_{i,j,k}$ is the specific storage of the material in cell i,j,k; and

$\Delta r_j, \Delta c_i, \Delta v_k$ are the cell dimensions.

In SEAWAT, the storage formulation has the form:

$$\frac{\Delta m}{\Delta t} = \rho_{i,j,k}SS_{i,j,k}(\Delta r_j \Delta c_i \Delta v_k)\frac{h^n_{f,i,j,k} - h^{n-1}_{f,i,j,k}}{t_n - t_{n-1}}, \tag{62}$$

where $\Delta m / \Delta t$ is the rate of mass accumulation of water in the cell. Using the storage concept defined in MODFLOW, mass storage capacity, $SC1_{i,j,k}$, can be defined as:

$$SC1_{i,j,k} = \rho_{i,j,k} SS_{i,j,k} (\Delta r_j \Delta c_i \Delta v_k).$$ (63)

Equation 62 then can be rewritten as:

$$\frac{\Delta m}{\Delta t} = SC1_{i,j,k} \frac{h^n_{f,i,j,k} - h^{n-1}_{f,i,j,k}}{t_n - t_{n-1}}.$$ (64)

Conversion Between Confined and Unconfined Conditions

The primary value for specific storage is only adequate if the water level in each individual cell remains above the top of the cell during an entire simulation or below the top of the cell during an entire simulation. If the water level in a cell crosses the top of the cell during a simulation, the aquifer "converts" from confined to water-table (unconfined) conditions, or vice versa. When these conditions are likely, the user may invoke a storage term conversion by specifying the appropriate layer-type flag (LAYCON).

In SEAWAT, a check is made after each iteration of the flow equation to determine if the head in a cell is above the top of the cell. This check is only performed if the layer is specified as "convertible" (for example, LAYCON = 2 or 3). Because the check depends on the elevation of the water table, the head is used rather than the freshwater head. The expression for calculating head at cell (i,j,k) is:

$$h_{i,j,k} = \frac{\rho_f}{\rho_{i,j,k}} h_{f,i,j,k} + \frac{\rho_{i,j,k} - \rho_f}{\rho_{i,j,k}} Z_{i,j,k},$$ (65)

where $h_{i,j,k}$ is the head value [L]. The head value (as opposed to the value of freshwater head) is used to determine if the water table is above the top of the cell. The storage conversion mechanism is invoked only when the head crosses the top of the cell during the simulation. When the storage conversion is necessary, the rate of fluid mass accumulation in storage in cell (i,j,k) is formulated as follows:

$$\frac{\Delta m}{\Delta t} = \frac{SCB(h^n_{f,i,j,k} - TOP_{i,j,k}) + SCA(TOP_{i,j,k} - h^{n-1}_{f,i,j,k})}{t_n - t_{n-1}},$$ (66)

where:

SCB is the "current" storage capacity during the iteration in progress,
TOP is the elevation of the top of the model cell, and
SCA is the storage capacity in effect in cell (i,j,k) at the start of the timestep.

Note that the freshwater head value is used in the storage calculation, but the actual head is used to check for the onset of storage conversion. This is because the change in freshwater head serves as an indicator of pressure change, which is ultimately responsible for storage accumulation, whereas the actual head is required to measure water-level movement.

Vertical Flow Calculation for Dewatered Conditions

MODFLOW accounts for the special case of downward vertical flow into a dewatering cell by adding correction terms to the RHS accumulator (fig. 8). Similar conditions might be encountered in a SEAWAT simulation; therefore, correction terms based on the variable-density form of Darcy's law are used to account for downward flow into a dewatering cell.
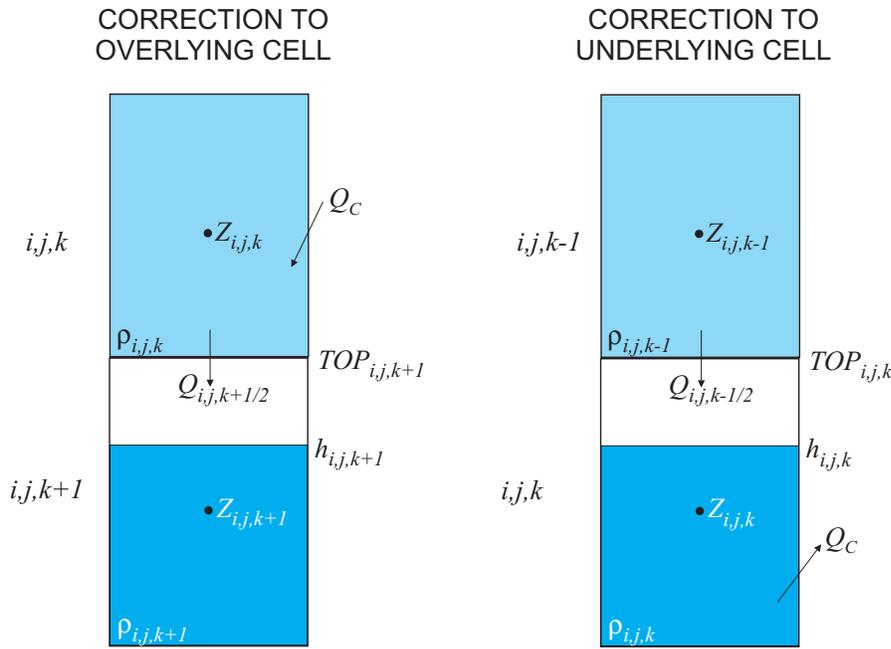
Figure 8. Cell indices and variable definitions for the case of a partially dewatered cell underlying an active model cell. A correction term is added to the overlying cell and subtracted from the underlying cell to account for the inaccurate flow rate that would be calculated with the uncorrected finite-difference equation. Note that in each case, cell indices are rewritten so that the correction is applied to cell i,j,k.

EXPLANATION

i,j,k	Indices that refer to row, column, and layer, respectively, of a finite-difference model grid
h_f	Equivalent freshwater head [L]
h	Head [L]
Q	Flow rate [L³T⁻¹]
Q_c	Flow correction [L³T⁻¹]
ρ	Fluid density [ML⁻³]
Z	Elevation of cell center [L]
TOP	Top elevation of model cell [L]

NOTE: L = length, M = mass, T = time

Noting that MODFLOW layers are numbered from top downward, the downward vertical flow from upper cell (i,j,k) to lower cell ($i,j,k+1$) is normally computed with the following equation:

$$Q^m_{i,j,k+1/2} = \hat{\rho}_{i,j,k+1/2} CV_{i,j,k+1/2} \left[h_{f,i,j,k+1} - h_{f,i,j,k} + \frac{\rho_{i,j,k+1/2} - \rho_f}{\rho_f}(Z_{i,j,k+1} - Z_{i,j,k}) \right], \quad (67)$$

where $Q^m_{i,j,k+1/2}$ is the mass flux of fluid between the two cells [MT⁻¹].

Equation 67 is based on the assumption that cell ($i,j,k+1$) is fully saturated, which means that the water level in cell ($i,j,k+1$) is higher than the top of the cell. There are, however, situations in which cell ($i,j,k+1$) could become partially unsaturated while the overlying cell remains saturated. In this case, flow between cell (i,j,k) and cell ($i,j,k+1$) does not depend on the head in cell ($i,j,k+1$). In this case, the "actual" mass flux, Q^m_a, between cell (i,j,k) and cell ($i,j,k+1$), which is partially dewatered, is:

$$Q_a^m = \hat{\rho}_{i,j,k+1/2} CV_{i,j,k+1/2} \left[Z_{i,j,k} - h_{f,i,j,k} + \frac{\rho_{i,j,k+1/2}}{\rho_f}(TOP_{i,j,k+1} - Z_{i,j,k}) \right].$$ (68)

Although equation 68 may not seem intuitive, it was derived from the variable-density form of Darcy's law. The correction term, Q_c^m, is calculated by subtracting equation 68 from equation 67 to give:

$$Q_c^m = \hat{\rho}_{i,j,k+1/2} CV_{i,j,k+1/2} \left[h_{f,i,j,k+1} - Z_{i,j,k+1} + \frac{\rho_{i,j,k+1/2}}{\rho_f}(Z_{i,j,k+1} - TOP_{i,j,k+1}) \right].$$ (69)

The *RHS* accumulator is updated with the following equation to include this correction:

$$RHS_{i,j,k}^{new} = RHS_{i,j,k}^{old}$$
$$+ \hat{\rho}_{i,j,k+1/2} CV_{i,j,k+1/2} \left[h_{f,i,j,k+1} - Z_{i,j,k+1} + \frac{\rho_{i,j,k+1/2}}{\rho_f}(Z_{i,j,k+1} - TOP_{i,j,k+1}) \right].$$ (70)

To overcome the problem of having the principal variable within the correction term, the value for $h_{f,i,j,k+1}$ is taken from the preceding iteration of the flow equation, rather than from the current iteration.

In a similar manner, a correction term must also be applied to the cell that is being dewatered. In this case, the cell (i,j,k) is being dewatered and is receiving flow from the overlying cell $(i,j,k-1)$. In the standard finite-difference equations shown in Chapter 3, the mass flux computed for this situation would erroneously be calculated according to the following equation:

$$Q_{i,j,k-1/2}^m = \hat{\rho}_{i,j,k-1/2} CV_{i,j,k-1/2} \left[h_{f,i,j,k-1} - h_{f,i,j,k} + \frac{\rho_{i,j,k-1/2} - \rho_f}{\rho_f}(Z_{i,j,k-1} - Z_{i,j,k}) \right],$$ (71)

but the "actual" mass flux is:

$$Q_a^m = \hat{\rho}_{i,j,k-1/2} CV_{i,j,k-1/2} \left[h_{f,i,j,k-1} - Z_{i,j,k-1} + \frac{\rho_{i,j,k-1/2}}{\rho_f}(Z_{i,j,k-1} - TOP_{i,j,k}) \right].$$ (72)

The correction term, which is calculated by subtracting equation 72 from 71, is:

$$Q_c^m = \hat{\rho}_{i,j,k-1/2} CV_{i,j,k-1/2} \left[Z_{i,j,k} - h_{f,i,j,k} + \frac{\rho_{i,j,k-1/2}}{\rho_f}(TOP_{i,j,k} - Z_{i,j,k}) \right].$$ (73)

This correction for the dewatering cell is handled by modifying the *RHS* accumulator according to the following expression:

$$RHS_{i,j,k}^{new} = RHS_{i,j,k}^{old} + \hat{\rho}_{i,j,k-1/2} CV_{i,j,k-1/2} \left[Z_{i,j,k} - h_{f,i,j,k} + \frac{\rho_{i,j,k-1/2}}{\rho_f}(TOP_{i,j,k} - Z_{i,j,k}) \right].$$ (74)

As before, to overcome the problem of having the principal variable within the correction term, the value for $h_{f,i,j,k}$ is taken from the preceding iteration of the flow equation, rather than from the current iteration.

Variable-Density Flow for Water-Table Case

As previously shown, the general form of Darcy's law used by SEAWAT to calculate the mass flux between cell (i,j,k) and $(i+1, j, k)$ is:

$$Q_{i+1/2, j, k}^{m} = \hat{\rho}_{i+1/2, j, k} CC_{i+1/2, j, k}\left[h_{f, i+1, j, k} - h_{f, i, j, k} + \frac{\rho_{i+1/2, j, k} - \rho_{f}}{\rho_{f}}(Z_{i+1, j, k} - Z_{i, j, k})\right]. \qquad (75)$$

For the water-table case (fig. 9), however, equation 75 cannot accurately represent the mass flux between cell (i,j,k) and $(i+1, j, k)$ for two reasons. First, the concept of equivalent freshwater head does not apply when the evaluation point is above the water table. For example, when the center elevation of a model cell is above the water table, the equivalent freshwater head will decrease as fluid density increases (if the water table were to remain at the same elevation). This would suggest that for a fixed water-table elevation, if $\rho_{i,j,k}$ were to increase, then $Q_{i+1/2,j,k}$ would decrease, resulting in an inaccurate flow rate. The second reason that equation 75 is not appropriate for the water-table case relates to the elevation for which the equivalent freshwater head is evaluated. To accurately calculate flow between two cells, the equivalent freshwater head should be calculated halfway between the water-table elevation, h, and the bottom of the cell, BOT. This elevation is designated by $Z_{WT/2}$ and corresponds to the vertical midpoint between the water table and the bottom of the cell (fig. 9).
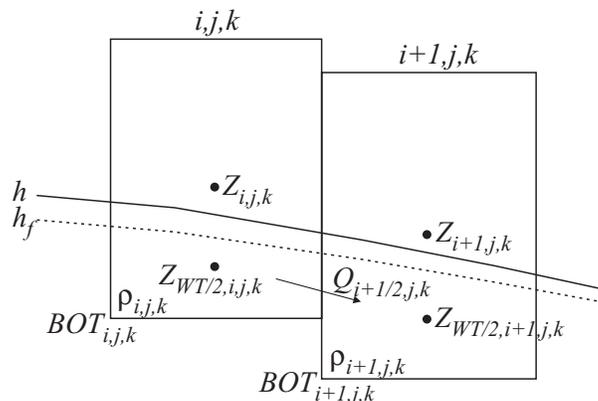
EXPLANATION

i,j,k Indices that refer to row, column, and layer, respectively, of a finite-difference model grid

h_f Equivalent freshwater head [L]

h Head [L]

Q Flow rate [L^3T^{-1}]

ρ Fluid density [ML^{-3}]

Z Elevation of cell water [L]

$Z_{WT/2}$ Elevation of vertical midpoint between the water table and the bottom of the model cell [L]

BOT

NOTE: L = length, M = mass, T = time

Figure 9. Conceptual representation of flow between two cells for the water-table case.

Based on this conceptual model for the water-table case, a better expression for the mass flux between cell (i,j,k) and $(i+1,j,k)$ is:

$$Q^m_{i+1/2,j,k} = \hat{\rho}_{i+1/2,j,k}CC_{i+1/2,j,k}\left[h_{f,WT/2,i+1,j,k}\right.$$

$$\left.-h_{f,WT/2,i,j,k}\right] + \frac{\rho_{i+1/2,j,k}-\rho_f}{\rho_f}(Z_{WT/2,i+1,j,k}-Z_{WT/2,i,j,k}), \tag{76}$$

where $h_{f,WT/2,i,j,k}$ and $h_{f,WT/2,i+1,j,k}$ are the equivalent freshwater heads at $Z_{WT/2,i,j,k}$ and $Z_{WT/2,i+1,j,k}$, respectively. These equivalent freshwater heads can be calculated from the equivalent freshwater heads at the cell centers by assuming hydrostatic conditions within the model cell:

$$h_{f,WT/2,i,j,k} = h_{f,i,j,k} + \frac{\rho_{i,j,k}-\rho_f}{\rho_f}(Z_{i,j,k}-Z_{WT/2,i,j,k}), \tag{77}$$

and:

$$h_{f,WT/2,i+1,j,k} = h_{f,i+1,j,k} + \frac{\rho_{i+1,j,k}-\rho_f}{\rho_f}(Z_{i+1,j,k}-Z_{WT/2,i+1,j,k}). \tag{78}$$

By substituting equations 77 and 78 into equation 76, the expression for flow between cell (i,j,k) and $(i+1,j,k)$ in terms of the equivalent freshwater head at the cell centers is:

$$Q^m_{i+1/2,j,k} = \hat{\rho}_{i+1/2,j,k}CC_{i+1/2,j,k}\left[h_{f,i+1,j,k} + \frac{\rho_{i+1,j,k}-\rho_f}{\rho_f}(Z_{i+1,j,k}-Z_{WT/2,i+1,j,k})\right.$$

$$\left.- h_{f,i,j,k} + \frac{-\rho_{i,j,k}-\rho_f}{\rho_f}(Z_{i,j,k}-Z_{WT/2,i,j,k}) + \frac{\rho_{i+1/2,j,k}-\rho_f}{\rho_f}(Z_{WT/2,i+1,j,k}-Z_{WT/2,i,j,k})\right]. \tag{79}$$

In SEAWAT, the method for using equation 79 to solve for the water-table case is similar to the correction method used by MODFLOW and SEAWAT for the dewatered case. If equation 75 represents the flow calculated by SEAWAT without any adjustments for the water-table case, a correction term can be calculated by subtracting the actual flow (eq. 79) from equation 75. The correction term can then be incorporated into the *RHS* accumulator to adjust for error that would result from using equation 75. Through algebraic manipulation, the water-table correction term for flow between cell (i,j,k) and $(i+1,j,k)$ is:

$$Q^m_c = \hat{\rho}_{i+1/2,j,k}CC_{i,j,k}\left[\frac{\rho_{i+1/2,j,k}-\rho_f}{\rho_f}(Z_{i+1,j,k}-Z_{i,j,k}+Z_{WT/2,i,j,k}-Z_{WT/2,i+1,j,k})\right.$$

$$\left.+ \frac{\rho_{i+1,j,k}-\rho_f}{\rho_f}(Z_{WT/2,i+1,j,k}-Z_{i+1,j,k}) + \frac{\rho_{i,j,k}-\rho_f}{\rho_f}(Z_{i,j,k}-Z_{WT/2,i,j,k})\right]. \tag{80}$$

The correction term is a function of $Z_{WT/2}$, which is:

$$Z_{WT/2} = \frac{h+BOT}{2}. \tag{81}$$

The addition of the correction term for the water-table case adds nonlinearity to the flow equation because head is a function of equivalent freshwater head. This problem is partially treated by using the equivalent

freshwater head from the previous iteration of the flow equation to solve for the $Z_{WT/2}$ terms prior to calculating the correction term.

This development of the correction term for the water-table case was presented for flow between cell (i,j,k) and $(i+1,j,k)$. For a two-dimensional water-table layer, there may be up to four correction terms, one for each horizontally adjacent cell. These correction terms are used to update the *RHS* accumulator according to the following expression:

$$
\begin{aligned}
RHS^{new}_{i,j,k} = RHS^{old}_{i,j,k} &+ \hat{\rho}_{i+1/2,j,k}CR_{i+1/2,j,k}\left[\frac{\rho_{i+1/2,j,k}-\rho_f}{\rho_f}(Z_{i+1,j,k}-Z_{i,j,k}+Z_{WT/2,i,j,k}-Z_{WT/2,i+1,j,k})\right.\\
&\left.+\frac{\rho_{i+1,j,k}-\rho_f}{\rho_f}(Z_{WT/2,i+1,j,k}-Z_{i+1,j,k})+\frac{\rho_{i,j,k}-\rho_f}{\rho_f}(Z_{i,j,k}-Z_{WT/2,i,j,k})\right]\\
&+ \hat{\rho}_{i-1/2,j,k}CR_{i-1/2,j,k}\left[\frac{\rho_{i-1/2,j,k}-\rho_f}{\rho_f}(Z_{i-1,j,k}-Z_{i,j,k}+Z_{WT/2,i,j,k}-Z_{WT/2,i-1,j,k})\right.\\
&\left.+\frac{\rho_{i-1,j,k}-\rho_f}{\rho_f}(Z_{WT/2,i-1,j,k}-Z_{i-1,j,k})+\frac{\rho_{i,j,k}-\rho_f}{\rho_f}(Z_{i,j,k}-Z_{WT/2,i,j,k})\right]\\
&+ \hat{\rho}_{i,j+1/2,k}CC_{i,j+1/2,k}\left[\frac{\rho_{i,j+1/2,k}-\rho_f}{\rho_f}(Z_{i,j+1,k}-Z_{i,j,k}+Z_{WT/2,i,j,k}-Z_{WT/2,i,j+1,k})\right.\\
&\left.+\frac{\rho_{i,j+1,k}-\rho_f}{\rho_f}(Z_{WT/2,i,j+1,k}-Z_{i,j+1,k})+\frac{\rho_{i,j,k}-\rho_f}{\rho_f}(Z_{i,j,k}-Z_{WT/2,i,j,k})\right]\\
&+ \hat{\rho}_{i,j-1/2,k}CC_{i,j-1/2,k}\left[\frac{\rho_{i,j-1/2,k}-\rho_f}{\rho_f}(Z_{i,j-1,k}-Z_{i,j,k}+Z_{WT/2,i,j,k}-Z_{WT/2,i,j-1,k})\right.\\
&\left.+\frac{\rho_{i,j-1,k}-\rho_f}{\rho_f}(Z_{WT/2,i,j-1,k}-Z_{i,j-1,k})+\frac{\rho_{i,j,k}-\rho_f}{\rho_f}(Z_{i,j,k}-Z_{WT/2,i,j,k})\right].
\end{aligned}
\tag{82}
$$

Modifications of MODFLOW Stress Packages

Modifications to the original package subroutines in MODFLOW were required because the flow equation in SEAWAT conserves mass, which means that all terms added to the *RHS* accumulator must be written as mass fluxes. Additionally, all terms added to the *HCOF* accumulator must be coefficients of freshwater head. Modifications to each of the stress packages in MODFLOW are described in the subsequent sections.

Well (WEL) Package

The WEL package is used to represent specified source or sink boundaries within the model domain. These specified flux boundaries may be injection wells or extraction wells. Original MODFLOW subroutines were modified to include the effects of injection and extraction wells. The *RHS* accumulator is updated by adding or subtracting the mass flux of the well. The mass flux is equal to the flow rate of the well, Q_{WELL}, multiplied by the appropriate fluid density, ρ_{WELL}. Conditional statements are used within the SEAWAT program to determine the density of the well fluid. If the well is an extraction well, the fluid density is equal to the density in the model cell. If the well is an injection well, the fluid density is calculated from the concentration of the well injection fluid. The concentration of injected fluid, C_{WELL}, is specified in the Source/Sink Mixing (SSM) package of MT3DMS. These steps are summarized with the following mathematical expressions:

For an extraction well ($Q_{well} < 0$):

$$\rho_{well} = \rho_{i, j, k} .$$ (83)

For an injection well ($Q_{well} > 0$):

$$\rho_{well} = \rho_f + C_{well} \cdot E .$$ (84)

Accordingly, the *RHS* accumulator is updated with the following expression:

$$RHS_{i, j, k}^{new} = RHS_{i, j, k}^{old} - \rho_{well} \cdot Q_{well} .$$ (85)

River (RIV) Package

The RIV package in MODFLOW is commonly used to approximate leakage to or from a stream or river. The conceptual model is based on the vertical leakage of water across river bottom sediments (fig. 10). The cross section of the river is assumed to be rectangular with impermeable vertical sides. Leakage into or out of the model cell is dependent on the stage in the river (h_{RIV}), the value of head in the model cell ($h_{i,j,k}$), and a conductance value. The conductance of the river is mathematically defined as:

$$COND_{RIV} = \frac{L \cdot w \cdot K_{seds}}{b_{seds}} ,$$ (86)

where:

$COND_{RIV}$ is the conductance of the riverbed [L^2T^{-1}],
    L is the length of the river segment in the model cell [L],
    w is the width of the river [L],
  K_{seds} is the hydraulic conductivity of the river bottom sediments [LT^{-1}], and
  b_{seds} is the thickness of the river bottom sediments [L].

The elevation of the base of the river bottom sediments is specified as *RBOT*, an input parameter for the RIV package. When the head in the model cell is above *RBOT*, river leakage (Q_{RIV}) is calculated using the following form of Darcy's law:

$$Q_{RIV} = COND_{RIV} \cdot (h_{RIV} - h_{i, j, k}) .$$ (87)

The sign convention used by MODFLOW treats ground-water sources as positive and sinks as negative. Q_{RIV}, therefore, is positive if the aquifer is receiving river leakage and negative if the aquifer is providing baseflow to the river. If $h_{i,j,k}$ falls below *RBOT*, the RIV package uses a slightly different equation for leakage:

$$Q_{RIV} = COND_{RIV} \cdot (h_{RIV} - RBOT) .$$ (88)

This approach restricts the maximum leakage rate and is a reasonable approximation for leakage when the water table falls below the base of a saturated river bottom deposit.

To incorporate river leakage into the system of MODFLOW equations, the *RHS* and *HCOF* accumulators are updated using the following conditions and expressions:

For $h_{i,j,k} > RBOT$:
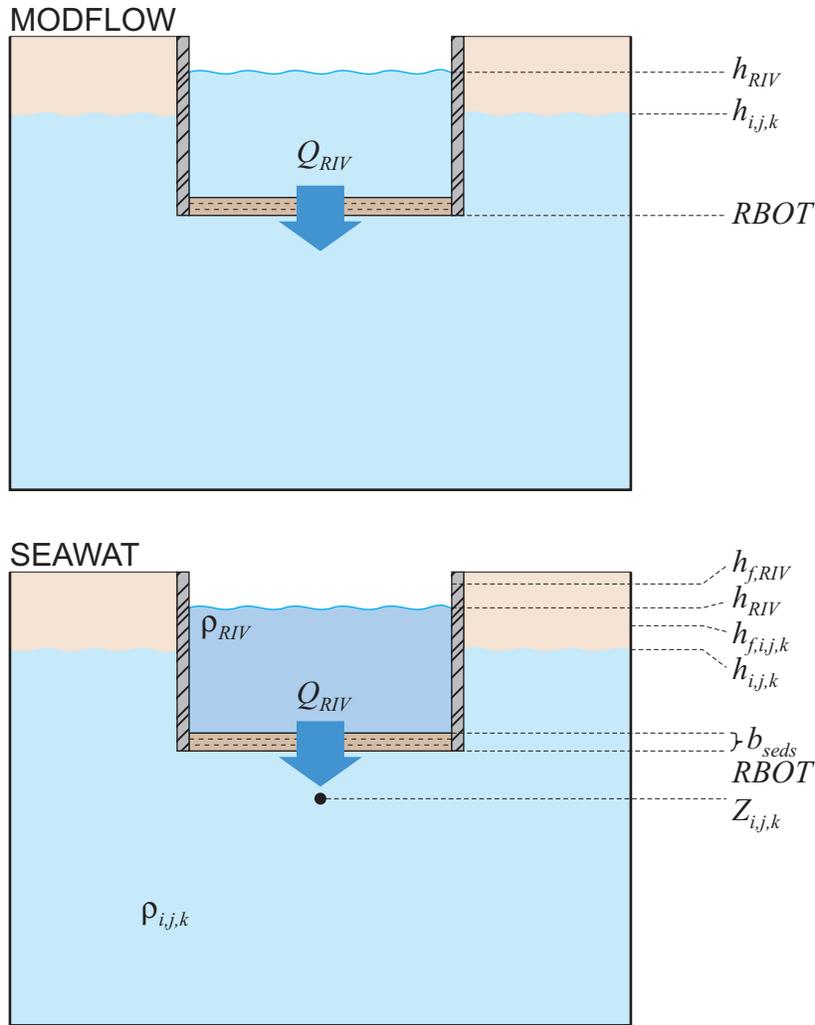
EXPLANATION

h_{RIV}	Head in the river [L]
$h_{i,j,k}$	Head in the model cell [L]
$RBOT$	Bottom elevation of the river bed sediments [L]
$h_{f,RIV}$	Equivalent freshwater head in the river relative to the top of the river bed [L]
$h_{f,i,j,k}$	Equivalent freshwater head in the model cell [L]
b_{seds}	Thickness of river bed sediments [L]
$Z_{i,j,k}$	Elevation of the center of the model cell [L]
ρ_{RIV}	Density of the river water [ML^{-3}]
$\rho_{i,j,k}$	Density of the water in the model cell [ML^{-3}]
Q_{RIV}	Flux of water from the river to the aquifer [L^3T^{-1}]

NOTE: L = length, M = mass, T = time

Figure 10. Conceptual model and variable description for river leakage in MODFLOW and SEAWAT.

$$HCOF_{i,j,k}^{new} = HCOF_{i,j,k}^{old} - COND_{RIV}, \tag{89}$$

and:

$$RHS_{i,j,k}^{new} = RHS_{i,j,k}^{old} - COND_{RIV} \cdot h_{RIV}. \tag{90}$$

For $h_{i,j,k} \leq RBOT$:

$$RHS_{i,j,k}^{new} = RHS_{i,j,k}^{old} - COND_{RIV}(h_{RIV} - RBOT). \tag{91}$$

In SEAWAT, the mathematical treatment of river leakage is more complicated because a variable-density form of Darcy's law is required. Additionally, the river leakage must be converted from a volumetric flux to a mass flux using the appropriate fluid density. The conceptual model of variable-density river leakage is shown in figure 10. To provide the reader with an understanding of how to incorporate a head-dependent, variable-density package into SEAWAT, the development of the river leakage equations is presented in detail.

The conceptual model for variable-density river leakage is based on vertical flow across river bottom sediments. The general form of Darcy's law for variable-density vertical flow is:

$$Q_z = -A\frac{k}{\mu}\left[\frac{dP}{dz} + \rho g\right]. \tag{92}$$

In this form, positive flow is in the positive z direction (upward).

The objective of the following steps is to rewrite equation 92 into a form that can be added to the *RHS* and *HCOF* accumulators in SEAWAT. This means that pressure will be replaced with freshwater head, the conceptual model for river leakage will be used to reformulate the equation, and leakage will be converted from volumetric flux to mass flux.

The equation for pressure (eq. 23) is substituted into equation 92, which is then rearranged to give:

$$Q_z = -A\frac{k\rho_f g}{\mu}\left[\frac{dh_f}{dz} + \frac{\rho - \rho_f}{\rho_f}\right]. \tag{93}$$

The equivalent freshwater hydraulic conductivity, K_f, is defined as:

$$K_f = \frac{k\rho_f g}{\mu_f}. \tag{94}$$

Substituting equation 94 into equation 93 gives:

$$Q_z = -AK_f\frac{\mu_f}{\mu}\left[\frac{dh_f}{dz} + \frac{\rho - \rho_f}{\rho_f}\right]. \tag{95}$$

As previously discussed, the dynamic viscosity of water is slightly dependent on the concentration of dissolved constituents, but for many applications it can be assumed that μ_f/μ is one. With this simplification, equation 95 reduces to:

$$Q_z = -\frac{AK_f}{dz}\left[dh_f + \frac{\rho - \rho_f}{\rho_f}dz\right]. \tag{96}$$

Equation 96 is one form of the equation for vertical, variable-density ground-water flow. In applying this equation to the RIV package in SEAWAT, it was assumed that energy (pressure and elevation) losses associated with the vertical flow occur primarily across the river bottom materials, and that losses across the upper part of the model cell underlying the river are small by comparison. It was further assumed that fluid density is essentially uniform within the cell. Under these assumptions the head, expressed in terms of the cell fluid, does not vary with vertical distance through the cell; thus, the value for head is the same at *RBOT* and the cell center. However, the values of freshwater head at *RBOT* and at the cell center must differ under these conditions and are related by:

$$h_{f, RBOT} = h_{f, i, j, k} + \frac{\rho_{i, j, k} - \rho_f}{\rho_f}(Z_{i, j, k} - RBOT), \tag{97}$$

and the equation for river leakage is:

$$Q_{RIV} = -\frac{AK_{f, seds}}{b_{seds}}\left[h_{f, RIV} - h_{f, RBOT} + \frac{\bar{\rho} - \rho_f}{\rho_f}b_{seds}\right], \tag{98}$$

where $\bar{\rho}$ is the average fluid density of the river and the model cell. By substituting equation 97 into equation 98, and introducing a new term called the equivalent freshwater river conductance, $COND_{f,RIV}$, where:

$$COND_{f, RIV} = \frac{AK_{f, seds}}{b_{seds}}, \tag{99}$$

the equation for river leakage (changing the sign to the MODFLOW sign convention of positive into the model cell) becomes:

$$Q_{RIV} = -COND_{f, RIV} \cdot h_{f, i, j, k} + COND_{f, RIV}\left[h_{f, RIV} - \frac{\rho_{i, j, k} - \rho_f}{\rho_f}(Z_{i, j, k} - RBOT) + \frac{\bar{\rho} - \rho_f}{\rho_f}b_{seds}\right]. \tag{100}$$

The volumetric river leakage, Q_{RIV}, is converted to a mass river leakage by multiplying Q_{RIV} by the upstream fluid density $\hat{\rho}$, where $\hat{\rho}$ is equal to $\rho_{i,j,k}$ if flow is out of the cell or ρ_{RIV} if flow is into the model cell.

The following expressions are used to add the river leakage to the *RHS* and *HCOF* accumulators. Note that the actual head in the model cell $h_{i,j,k}$ is used in the conditional statements rather than the equivalent freshwater head $h_{f,i,j,k}$.

For $h_{i,j,k} > RBOT$:

$$HCOF_{i, j, k}^{new} = HCOF_{i, j, k}^{old} - \hat{\rho} \cdot COND_{f, RIV}, \tag{101}$$

and:

$$RHS_{i, j, k}^{new} = RHS_{i, j, k}^{old} - \hat{\rho} \cdot COND_{RIV}\left[h_{f, RIV} - \frac{\rho_{i, j, k} - \rho_f}{\rho_f}(Z_{i, j, k} - RBOT) + \frac{\bar{\rho} - \rho_f}{\rho_f}b_{seds}\right]. \tag{102}$$

For $h_{i,j,k} \leq RBOT$:

$$RHS_{i, j, k}^{new} = RHS_{i, j, k}^{old} - \rho_{RIV} \cdot COND_{f, RIV}\left[h_{f, RIV} - RBOT + \frac{\rho_{RIV} - \rho_f}{\rho_f}b_{seds}\right]. \tag{103}$$

For the constant-density case simulated by MODFLOW, the thickness of the river bottom sediments is lumped into the conductance term. In the variable-density equations for river leakage, however, b_{seds} is in the conductance term ($COND_{f,RIV}$) and the leakage equation. This means that b_{seds} must be specified by the user for SEAWAT to appropriately include the effects of variable-density river leakage.

Drain (DRN) Package

The DRN package in MODFLOW uses a head-dependent flux condition to withdraw water from a model cell if the head in the model cell is higher than the drain elevation (fig. 11). The equations used by MODFLOW are as follows:

For $h_{i,j,k} > h_{DRN}$:

$$Q_{DRN} = COND_{DRN} \cdot (h_{DRN} - h_{i,j,k}).$$
(104)

For $h_{i,j,k} < h_{DRN}$:

$$Q_{DRN} = 0,$$
(105)

where:

Q_{DRN} is the volumetric flux to the drain [L^3T^{-1}],

$COND_{DRN}$ is the conductance of the drain [L^2T^{-1}], and

h_{DRN} is the control stage of the drain [L].

With the above formulation, the *RHS* and *HCOF* accumulators are updated according to the following condition and expressions:

For $h_{i,j,k} > h_{DRN}$:

$$HCOF_{i,j,k}^{new} = HCOF_{i,j,k}^{old} - COND_{DRN},$$
(106)

and:

$$RHS_{i,j,k}^{new} = RHS_{i,j,k}^{old} - COND_{DRN} \cdot h_{DRN}.$$
(107)

In adapting the DRN package to SEAWAT, it was assumed that the density of water in the drain would be equal at all times to that in the model cell (i,j,k) to which the drain is connected, and that the level of water in the drain would remain fixed by engineered or natural controls at a head level, h_{DRN} (fig. 11). Under these assumptions, the volumetric flow from the cell into the drain is given by the equations used by MODFLOW (eqs. 104 and 105), where $COND_{DRN}$ is the drain conductance for water of density, $\rho_{i,j,k}$, which is the density of the water present in the cell. The drain conductance term, $COND_{DRN}$, is related to the drain conductance for freshwater, $COND_{f,DRN}$, by:

$$COND_{f,DRN} = COND_{DRN} \frac{\rho_f}{\rho_{i,j,k}}.$$
(108)

MODFLOW

Q_{DRN}

$h_{i,j,k}$
h_{DRN}

SEAWAT

Q_{DRN} $\rho_{i,j,k}$

$\rho_{i,j,k}$

$h_{f,i,j,k}$
$h_{f,DRN}$
$h_{i,j,k}$
h_{DRN}
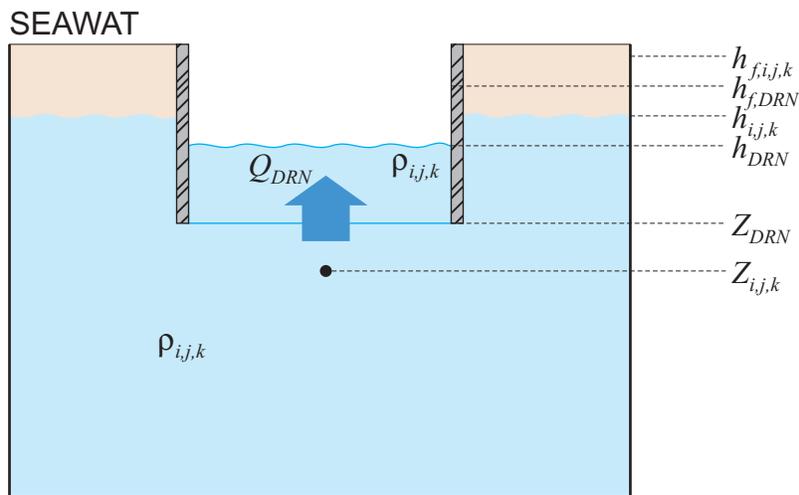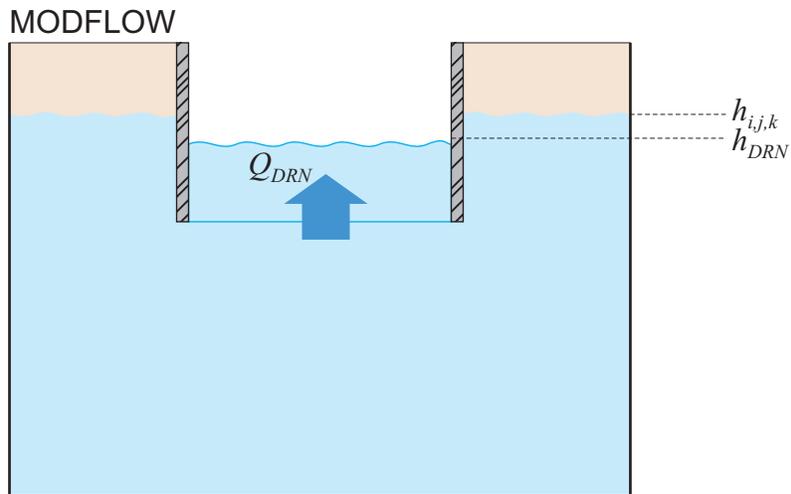
Z_{DRN}
$Z_{i,j,k}$

EXPLANATION

$h_{i,j,k}$ Head in the model cell [L]

h_{DRN} Head in the drain [L]

$h_{f,i,j,k}$ Equivalent freshwater head in the model cell [L]

$h_{f,DRN}$ Equivalent freshwater head in the drain [L]

Z_{DRN} Elevation of the drain bottom [L]

$Z_{i,j,k}$ Elevation of the center of the model cell [L]

$\rho_{i,j,k}$ Density of the water in the model cell [ML^{-3}]

Q_{DRN} Flux of water from the aquifer to the drain [L^3T^{-1}]

NOTE: L = length, M = mass, T = time

Figure 11. Conceptual model and variable description for drain leakage in MODFLOW and SEAWAT.

Applying equation 4 to the drain, where again the density of water in the drain is the same as that in the model cell, $\rho_{i,j,k}$, gives:

$$h_{DRN} = \frac{\rho_f}{\rho_{i,j,k}} h_{f,DRN} + \frac{\rho_{i,j,k} - \rho_f}{\rho_{i,j,k}} Z_{DRN}, \tag{109}$$

where, as shown in figure 11, Z_{DRN} is the elevation of the bottom of the drain. Substituting equations 65, 108, and 109 into 104 yields:

$$Q_{DRN} = COND_{f,DRN} \cdot \left[h_{f,DRN} - h_{f,i,j,k} - \frac{\rho_{i,j,k} - \rho_f}{\rho_f} (Z_{i,j,k} - Z_{DRN}) \right]. \tag{110}$$

Equation 110 is multiplied by $\rho_{i,j,k}$ to obtain an expression for mass flux into the drain.

To incorporate the effects of the drain into SEAWAT, the *HCOF* and *RHS* accumulators are updated according to the following expressions:

For $h_{i,j,k} > h_{DRN}$:

$$HCOF_{i,j,k}^{new} = HCOF_{i,j,k}^{old} - COND_{f,DRN} \cdot \rho_{i,j,k}, \tag{111}$$

and:

$$RHS_{i,j,k}^{new} = RHS_{i,j,k}^{old} - \rho_{i,j,k} \cdot COND_{f,DRN} \left[h_{f,DRN} - \frac{\rho_{i,j,k} - \rho_f}{\rho_f} (Z_{i,j,k} - Z_{DRN}) \right]. \tag{112}$$

In the constant-density case simulated by MODFLOW, the user need only specify the stage within the drain and the conductance. Because the drain formulation in SEAWAT is written for the variable-density case, the user also needs to specify the elevation of the drain bottom, Z_{DRN}.

Recharge (RCH) Package

The RCH package in MODFLOW is used to add aerial recharge to a model. If the recharge rates are negative, the RCH package also can be used to withdraw ground water from a model. In the input data sets, the recharge rate (*RECH*) is entered in dimensions of [LT⁻¹], but is converted to a volumetric flux (Q_{RCH}) by multiplying by the cell area. A positive value for *RECH* adds water to a model cell; a negative value for *RECH* withdraws ground water from a model cell. The recharge quantity is included in the MODFLOW system of equations by subtracting the volumetric flux from the *RHS* accumulator. The expression is:

$$RHS_{i,j,k}^{new} = RHS_{i,j,k}^{old} - Q_{RCH}. \tag{113}$$

SEAWAT uses this same approach, except the volumetric flux is converted to a mass flux. If Q_{RCH} is positive, the recharge density is calculated from the concentration of the recharge fluid specified in the MT3DMS data sets. If Q_{RCH} is negative, the recharge density is set equal to the fluid density of that model cell, which is the approach used by MT3DMS for negative recharge. Therefore, the expressions for determining the appropriate recharge density, ρ_{RCH}, are as follows:

For *RECH* > 0:

$$\rho_{RCH} = \rho_f + C_{RCH} \cdot E. \tag{114}$$

For *RECH* < 0:

$$\rho_{RCH} = \rho_{i,j,k}, \tag{115}$$

where C_{RCH} is the concentration of the recharge fluid [ML^{-3}]. Accordingly, the *RHS* accumulator is updated with the following expression:

$$RHS_{i,j,k}^{new} = RHS_{i,j,k}^{old} - \rho_{RCH} \cdot Q_{RCH}. \tag{116}$$

Evapotranspiration (EVT) Package

The EVT package in MODFLOW is used to simulate ground-water withdrawals from an aquifer. The rate of ground-water withdrawal (Q_{EVT}) is dependent on the depth from a user-specified surface, *SURF*, to the position of the water table. When the water table is below the extinction depth, *EXTD*, the evapotranspiration rate is equal to zero. When the water table is above *SURF*, Q_{EVT} is equal to the maximum evapotranspiration rate (Q_{MAX}). Values of Q_{MAX} are positive in the input data sets, but the values of Q_{EVT} that result from the equations are negative. In the input data sets, Q_{MAX} is expressed as [LT^{-1}] but is multiplied by the area of the model cell to convert to a volumetric flux. When the water table is between *SURF* and *EXTD*, Q_{EVT} is linearly interpolated between Q_{MAX} and zero, depending on the depth to the water table.

Mathematically, the conceptual model for evapotranspiration is written with the following conditions and expressions:
For $h_{i,j,k}$ > *SURF*:

$$Q_{EVT} = -Q_{MAX}. \tag{117}$$

For $h_{i,j,k}$ < (*SURF* – *EXTD*):

$$Q_{EVT} = 0. \tag{118}$$

For (*SURF* – *EXTD*) < $h_{i,j,k}$ < *SURF*:

$$Q_{EVT} = \frac{-Q_{MAX}}{EXTD} h_{i,j,k} - Q_{MAX} + \frac{Q_{MAX} \cdot SURF}{EXTD}. \tag{119}$$

MODFLOW incorporates these conditions into the *RHS* and *HCOF* accumulators with the following equations:
For $h_{i,j,k}$ > *SURF*:

$$RHS_{i,j,k}^{new} = RHS_{i,j,k}^{old} + Q_{MAX}. \tag{120}$$

For $h_{i,j,k}$ < (*SURF* – *EXTD*):

$$\text{No change in } RHS \text{ or } HCOF.$$

For (*SURF* – *EXTD*) < $h_{i,j,k}$ < *SURF*:

$$HCOF_{i,j,k}^{new} = HCOF_{i,j,k}^{old} - \frac{Q_{MAX}}{EXTD}, \tag{121}$$

and:

$$RHS^{new}_{i,j,k} = RHS^{old}_{i,j,k} + Q_{MAX} - \frac{Q_{MAX} \cdot SURF}{EXTD}.$$ (122)

In SEAWAT, the ground-water flow equation is written in terms of freshwater head, $h_{f,i,j,k}$. The conceptual model for evapotranspiration, however, poses Q_{EVT} as a function of the water-table position ($h_{i,j,k}$). This means that the MODFLOW equations for Q_{EVT} are not appropriate for variable-density cases. Accordingly, the equations for Q_{EVT} in SEAWAT are adjusted by substituting an expression for the actual head $h_{i,j,k}$ into the original MODFLOW equations and rewriting in terms of freshwater head $h_{f,i,j,k}$.

When equation 65 is substituted into equation 119, the following equation results for Q_{EVT}:

$$Q_{EVT} = \frac{-Q_{MAX}}{EXTD}\frac{\rho_f}{\rho_{i,j,k}}h_{i,j,k} - \frac{Q_{MAX}}{EXTD}Z_{i,j,k}\frac{\rho_{i,j,k}-\rho_f}{\rho_{i,j,k}} - Q_{MAX} + \frac{Q_{MAX} \cdot SURF}{EXTD}.$$ (123)

In SEAWAT, the *RHS* and *HCOF* accumulators are updated using the following conditions and equations. The conditional statements use the actual head $h_{i,j,k}$ rather than the freshwater head $h_{f,i,j,k}$, and evapotranspiration is expressed as a mass flux rather than volumetric flux by multiplying by the density of the evapotranspiration fluid ρ_{EVT}. The expressions are:

For $h_{i,j,k} > SURF$:

$$RHS^{new}_{i,j,k} = RHS^{old}_{i,j,k} + \rho_{EVT} \cdot Q_{MAX}.$$ (124)

For $h_{i,j,k} < (SURF - EXTD)$:

No change in *RHS* or *HCOF*.

For $(SURF - EXTD) < h_{i,j,k} < SURF$:

$$HCOF^{new}_{i,j,k} = HCOF^{old}_{i,j,k} - \rho_{EVT} \cdot \frac{Q_{MAX}}{EXTD}\frac{\rho_f}{\rho_{i,j,k}},$$ (125)

and

$$RHS^{new}_{i,j,k} = RHS^{old}_{i,j,k} + \rho_{EVT}\left[\frac{Q_{MAX}}{EXTD}Z_{i,j,k}\frac{\rho_{i,j,k}-\rho_f}{\rho_{i,j,k}} + Q_{MAX} - \frac{Q_{MAX} \cdot SURF}{EXTD}\right].$$ (126)

With MT3DMS, users are allowed to specify the concentration of the evapotranspiration fluid withdrawn from a cell. The conversion from volumetric to mass flux uses ρ_{EVT}, which is calculated from the concentration of the evapotranspiration water, C_{EVT}, using the following equation:

$$\rho_{EVT} = \rho_f + C_{EVT} \cdot E.$$ (127)

If the concentration of the evapotranspiration fluid is not specified, the density of freshwater is used to convert the volumetric evapotranspiration rate to a mass flux.

General-Head Boundary (GHB) Package

The GHB package in MODFLOW is one of the more robust packages available for simulating a wide range of boundary conditions. General-head boundaries are head-dependent boundaries where the volumetric flux, Q_{GHB}, is proportional to the head difference. The form of Darcy's law used to characterize the flux is:

$$Q_{GHB} = COND_{GHB} \cdot (h_{GHB} - h_{i,j,k}), \tag{128}$$

where:

$COND_{GHB}$ is the conductance of the GHB [L^2T^{-1}], and

h_{GHB} is the head value for the GHB.

MODFLOW incorporates this type of boundary condition into the system of equations by updating the *RHS* and *HCOF* accumulators with the following expressions:

$$HCOF_{i,j,k}^{new} = HCOF_{i,j,k}^{old} - COND_{GHB}, \tag{129}$$

and:

$$RHS_{i,j,k}^{new} = RHS_{i,j,k}^{old} - COND_{GHB} \cdot h_{GHB}. \tag{130}$$

For constant-density simulations, equation 128 is valid for horizontal or vertical flow between the model domain and the general-head boundary. In SEAWAT simulations, however, the variable-density form of Darcy's law is dependent on elevation as well as the head difference, which means that the elevation of the general-head boundary reservoir is important. The GHB package in SEAWAT was designed so that reservoirs for the general-head boundaries could be located anywhere around the cell. Accordingly, the following equation is used to quantify the volumetric flux between a general-head boundary and a model cell:

$$Q_{GHB} = COND_{f,GHB} \cdot \left[h_{f,GHB} - h_{f,i,j,k} + \frac{\bar{\rho} - \rho_f}{\rho_f}(Z_{GHB} - Z_{i,j,k}) \right], \tag{131}$$

where:

$COND_{f,GHB}$ is the equivalent freshwater conductance of the general-head boundary [L^2T^{-1}],

$h_{f,GHB}$ is the equivalent freshwater head of the general-head boundary [L],

$\bar{\rho}$ is the average fluid density of the general-head boundary reservoir and the model cell [ML^{-3}], and

Z_{GHB} is the elevation of the base of the general-head boundary reservoir [L].

SEAWAT incorporates the effects of the general-head boundary into the system of equations by updating the *HCOF* and *RHS* accumulators with the appropriate mass flux:

$$HCOF_{i,j,k}^{new} = HCOF_{i,j,k}^{old} - \hat{\rho} \cdot COND_{f,GHB}, \tag{132}$$

and:

$$RHS_{i,j,k}^{new} = RHS_{i,j,k}^{old} - \hat{\rho} \cdot COND_{f,GHB} \cdot \left[h_{f,GHB} + \frac{\bar{\rho} - \rho_f}{\rho_f}(Z_{GHB} - Z_{i,j,k}) \right], \tag{133}$$

where: $\hat{\rho}$ is the upstream-weighted fluid density with a value of ρ_{GHB} if flow is into the model cell, and $\rho_{i,j,k}$ if flow is out of the model cell. The value for ρ_{GHB} is calculated from the concentration of the general-head boundary specified in the MT3DMS input data set.

The elevation of the general-head boundary (Z_{GHB}) is not standard input for the general-head boundary package. If this information is omitted from the GHB package, SEAWAT assumes the reservoir for the general-head boundary is at the same elevation as the center elevation for the model cell.

Time-Varying Constant Head (CHD) Package

The CHD package allows the values for constant head cells to change during a stress period. Users enter a starting and ending head value for each constant head cell, and the program linearly interpolates a head value at the appropriate times based on the elapsed time within the stress period. The CHD package was modified to allow SEAWAT users the option to enter either equivalent freshwater heads or heads. If the user enters equivalent freshwater heads, SEAWAT linearly interpolates an equivalent freshwater head value for the end of the timestep. If the user enters heads, however, SEAWAT converts the head value that was linearly interpolated to an equivalent freshwater head using equation 3 and the fluid density calculated for that cell. Therefore, if the solute concentration in the CHD cell changes during the simulation, the user has the option to specify the head (or stage if the CHD cell represents a surface-water feature) rather than equivalent freshwater head.

Modification of MODFLOW Solver Packages

There are no modifications to the source code of the solver packages, but there are changes in the main program where the statements call the solvers. SEAWAT passes the arrays *RHOCC*, *RHOCR*, and *RHOCV* into the solvers, which are the conductance arrays multiplied by the upstream-weighted fluid density. The *RHOCC*, *RHOCR*, and *RHOCV* arrays are updated during each iteration of the flow equation with the current upstream-weighted fluid density. These mass conductances are passed to the solvers because all terms in the *HCOF* and *RHS* accumulators are written as mass terms rather than as volumetric terms.

MODFLOW-MT3DMS Link Package and Modifications to MT3DMS

The link package passes advective fluxes for the model domain and boundaries, along with saturated cell thicknesses, from the flow model component to the transport model component. The link subroutines, which include one subroutine for each stress package, were updated with the appropriate variable-density flow equations for the different boundary conditions so that the link package is consistent with the variable-density equations previously discussed.

There are only minor modifications to MT3DMS. These modifications do not change the way the transport equation is solved, but only facilitate the mechanics of running MODFLOW and MT3DMS within a single code. For this reason, a description of the relatively minor changes to MT3DMS is not presented in this document.

CHAPTER 6
INSTRUCTIONS FOR USING SEAWAT

A principal advantage in using SEAWAT is that the program reads and writes standard MODFLOW and MT3DMS data sets. Users of MODFLOW and MT3DMS can easily apply SEAWAT to problems involving variable-density ground-water flow; however, users not familiar with MODFLOW and MT3DMS should accustom themselves with these programs before using SEAWAT. The MODFLOW and MT3DMS manuals provide detailed instructions for selecting simulation options, creating input files, and processing model results. This chapter assumes that SEAWAT users have access to these manuals and are familiar with the concepts and limitations of the programs. Users should also recognize that solute-transport modeling presents additional considerations and requirements in addition to those for flow modeling (Zheng and Bennett, 1995). For example, the quasi three-dimensional approach should not be used with SEAWAT. Instead, a true three-dimensional approach with an increased level of vertical discretization may be required to accurately simulate solute-transport and variable-density flow patterns.

In the next sections, instructions for preparing input files for individual MODFLOW and MT3DMS packages for use in SEAWAT are explained. Input files for the packages are divided into records. In most cases, records used for SEAWAT are the same as records for MODFLOW and MT3DMS. Information for these identical records is not included in this chapter. If, however, a record contains additional information that is specific to SEAWAT, then this information is included in this chapter. An input variable within a record that is highlighted in bold indicates that the variable is specific to SEAWAT or that a change has been made to facilitate data entry for SEAWAT.

Preparation of MODFLOW Input Packages for SEAWAT

The MODFLOW input packages for SEAWAT are:

- Basic (BAS) package
- Output Control (OC) option
- Block-Centered Flow (BCF) package
- Well (WEL) package
- Drain (DRN) package
- River (RIV) package
- Evapotranspiration (EVT) package
- General-Head Boundary (GHB) package
- Recharge (RCH) package
- Time-Varying Constant Head (CHD) package
- Solver packages, including Strongly Implicit Procedure (SIP), Successive Over-Relaxation (SOR), and Preconditioned Conjugate Gradient (PCG)

Basic (BAS) Package

For a SEAWAT simulation, the user is required to develop an input file for the BAS package.

Record 4   Data: IUNIT(24)

   Format: 24I3

   SEAWAT uses the IUNIT array (like MODFLOW) to determine which stress packages and solver are used for the flow portion of the variable-density simulation. Packages are activated by entering a positive integer into the appropriate position in the IUNIT array.

The value of the integer is the FORTRAN unit number that will be used to open the input file for that package. The list below shows the location of the particular packages within the IUNIT array.

1	2	3	4	5	6	7	8	9	10	11	12
BCF	WEL	DRN	RIV	EVT	XXX	GHB	RCH	SIP	XXX	SOR	OC

13	14	15	16	17	18	19	20	21	22	23	24
PCG	XXX	XXX	XXX	XXX	XXX	XXX	CHD	XXX	LKMT	XXX	XXX

IMPORTANT: FORTRAN unit numbers 1, 6, and 35 to 49 are reserved for SEAWAT files. These numbers should not be used by the user for MODFLOW input or output files.

Record 8   Data: SHEAD(NCOL,NROW)

Module: U2DREL (one array for each layer in grid)

The starting heads entered in this record should represent equivalent freshwater heads.

Record 9   Data: PERLEN, NSTP, TSMULT

Format: F10.0, I10, F10.0

Information in record 9 is required for the BAS package, but SEAWAT does not use this information. These same parameters are also required for the MT3DMS Basic Transport (BTN) package. SEAWAT uses the time parameters from the BTN package to determine stress period information.

Output Control (OC) Option

The output control (OC) option is used to control the results that are saved from the flow portion of the variable-density simulation. Results pertaining to flow include heads, drawdowns, cell-by-cell flow terms, and budget information. Concentrations and other solute-transport results are saved according to the standard MT3DMS instructions.

Block-Centered Flow (BCF) Package

The user is required to develop an input file for the BCF package. This file contains information about spatially distributed input parameters such as hydraulic conductivity, aquifer tops and bottoms, and storage coefficients.

Record 1   Data: ISS, IBCFCB, HDRY, IWDFLG, WETFCT, IWETIT, IHDWET, **IWTABLE**

Format: 2I10, F10.0, I10, F10.0, 2I10, **I10**

ISS is the steady-state flag. When ISS is set to one, SEAWAT will solve the steady-state form of the flow equation. This does not mean that the solute-transport part of the model will automatically run to steady state. For most applications, the user should specify transient flow conditions (ISS equal to zero) because the redistribution of salt in the aquifer may affect flow patterns.

The input variable, **IWTABLE**, determines if the corrections for the variable-density water-table case will be included in the solution to the flow equation. If **IWTABLE** is zero (or not specified), SEAWAT will *not* use equation 82 to correct for variable-density flow under

water-table conditions. If **IWTABLE** is greater than zero, SEAWAT will use equation 82 to correct for variable-density flow. Because equation 82 adds nonlinearity to the flow equation, the solvers may not converge for complicated water-table conditions. The user, therefore, has the option to run SEAWAT with or without the corrections.

Record 6   Data: SF1(NCOL,NROW)

           Format: U2DREL

           SF1 is the primary storage coefficient. Values for SF1 should be entered as equivalent freshwater storage coefficients.

Record 7   Data: TRAN(NCOL,NROW)

           Format: U2DREL

           TRAN is the transmissivity along rows. Values for TRAN should be entered as equivalent freshwater transmissivity values.

Record 8   Data: HY(NCOL,NROW)

           Format: U2DREL

           HY is the hydraulic conductivity along rows and should be entered as equivalent freshwater hydraulic conductivity.

Record 10 Data: VCONT(NCOL,NROW)

           Format: U2DREL

           VCONT is the vertical hydraulic conductance and should be entered in equivalent freshwater terms.

Record 11 Data: SF2(NCOL,NROW)

           Format: U2DREL

           SF2 is the secondary storage coefficient. Values for SF2 should be entered as equivalent freshwater storage coefficients.

Well (WEL) Package

As in a standard MODFLOW simulation, an input file for the WEL package is required for a SEAWAT simulation if a nonzero integer is entered in position 2 of the IUNIT array in the BAS package.

Record 3   Data: K, I, J, Q_{well}

           Format: 3I10, F10.0

           For extraction wells, the pumping rate (Q_{well}) is less than zero, and the concentration of the fluid withdrawn from the aquifer is equal to the concentration of the model cell that contains the extraction well. For injection wells, Q_{well} is greater than zero. If the concentration of the injection fluid is greater than zero, the user specifies this information in the MT3DMS source/sink mixing (SSM) package. The user cannot specify different concentrations for two injection wells in the same model cell. This limitation is described in more detail later.

Drain (DRN) Package

An input file for the DRN package is required for a SEAWAT simulation if a nonzero integer is entered in location 3 of the IUNIT array in the BAS package.

Record 1   Data: MXDRN, IDRNCB, **IDRNELEV**

           Format: 3I10

To accurately simulate the flow of variable-density ground water to a drain, the elevation of the drain bottom also is required. A positive value for the flag, **IDRNELEV**, indicates that drain bottom elevations are included in record 3 for each drain. If **IDRNELEV** is equal to zero, SEAWAT sets the elevation of the drain bottom to the elevation of the center of the model cell.

Record 3   Data: $K, I, J, h_{f,DRN}, COND_{f,DRN}, \boldsymbol{Z_{DRN}}$

Format: 3I10, 3F10.0

The variable $h_{f,DRN}$ represents the equivalent freshwater stage within the drain. The variable $COND_{f,DRN}$ is the equivalent freshwater conductance of the drain sediments. The variable $\boldsymbol{Z_{DRN}}$ is the bottom elevation of the drain.

River (RIV) Package

An input file for the RIV package is required for a SEAWAT simulation if a nonzero integer is entered in location 4 of the IUNIT array in the BAS package.

Record 1   Data: MXRIVR, IRIVCB, **IRBDTHK**

Format: 3I10

To accurately simulate the flow of variable-density ground water to a river, the thickness of the river bottom sediments is required. A positive value for the flag, **IRBDTHK**, indicates that river bottom thicknesses are included in record 3 for each river. If **IRBDTHK** is equal to zero, SEAWAT sets the thickness of the river bottom sediments (b_{seds}) equal to the distance between the river bottom ($RBOT$) and the vertical center of the cell ($Z_{i,j,k}$).

Record 3   Data: $K, I, J, h_{f,RIV}, COND_{f,RIV}, RBOT, \boldsymbol{b_{seds}}$

Format: 3I10, 3F10.0

The variable $h_{f,RIV}$ is the equivalent freshwater head of the river. The variable $COND_{f,RIV}$ is the equivalent freshwater conductance of the river bottom sediments. The variable $RBOT$ is the elevation of the river bottom. The variable $\boldsymbol{b_{seds}}$ is the thickness of the river bottom sediments (distance over which the resistance to flow occurs).

The concentration of river water is specified in the MT3DMS SSM package. The user cannot specify different concentrations for two river boundaries in the same model cell. This limitation is described in more detail later.

Evapotranspiration (EVT) Package

An input file for the EVT package is required for a SEAWAT simulation if a nonzero integer is entered in location 5 of the IUNIT array in the BAS package.

Record 1   Data: NEVTOP, IEVTCB

Format: 2I10

Another evapotranspiration option, originally developed by Swain and others (1996), was added to the SEAWAT code. If NEVTOP is equal to 3, evapotranspiration is withdrawn from the highest active cell in the model. This option is not included in the standard version of MODFLOW.

SEAWAT allows a nonzero concentration for the evapotranspiration fluid withdrawn from the model. The concentration value is specified in the MT3DMS SSM package.

General-Head Boundary (GHB) Package

An input file for the GHB package is required for a SEAWAT simulation if a nonzero integer is entered in location 17 of the IUNIT array in the BAS package.

Record 1   Data: MXGHB, IGHBCB, **IGHBELEV**

                 Format: 3I10

To accurately simulate the flow of variable-density ground water to general-head boundaries, the elevation of the general-head boundary is required. A nonzero value for the flag, **IGHBELEV**, indicates that elevations for the general-head boundaries are included in record 3 for each boundary. If **IGHBELEV** is equal to zero, SEAWAT sets the elevation of the general-head boundary (Z_{GHB}) to the center elevation of the model cell ($Z_{i,j,k}$). In this case, flow between the general-head boundary and the model cell is calculated with the equation for horizontal ground-water flow.

Record 3   Data: K, I, J, $h_{f,GHB}$, $COND_{f,GHB}$, $\boldsymbol{Z_{GHB}}$

                 Format: 3I10, 3F10.0

The variable $h_{f,GHB}$ is the equivalent freshwater head within the general-head boundary. The variable $COND_{f,GHB}$ is the equivalent freshwater conductance of the general-head boundary. The variable $\boldsymbol{Z_{GHB}}$ is the elevation of the general-head boundary from which the equivalent freshwater head ($h_{f,GHB}$) is calculated.

The concentration of source water is specified in the MT3DMS SSM package. The user cannot specify different concentrations for two general-head boundaries in the same model cell. This limitation is described in more detail in the description of the MT3DMS SSM input instructions.

Recharge (RCH) Package

There are no special considerations, in terms of data input, for using the RCH package in SEAWAT. Recharge rates can be positive or negative. If a positive recharge value is specified, the concentration of the recharge fluid can be specified in the MT3DMS SSM package. If a negative value is specified for recharge, fluid is withdrawn from the model at the concentration and density of the model cell.

Time-Varying Constant Head (CHD) Package

An input file for the CHD package is required for a SEAWAT simulation if a nonzero integer is entered in location 20 of the IUNIT array in the BAS package.

Record 1   Data: MXCHD, **ICHDSALT**

                 Format: 2I10

If the CHD input package contains head values in terms of equivalent freshwater heads (default), **ICHDSALT** must be zero. If the CHD input package contains head values, **ICHDSALT** must be greater than zero.

Record 3   Data: K, I, J, SHEAD, EHEAD

                 Format: 2I10

The head values in record 3 represent the starting and ending head values for the stress period, where SHEAD represents the head and the start of the stress period and EHEAD represents the head at the end of the stress period. Users may enter SHEAD and EHEAD as either equivalent freshwater heads or heads, depending on the value of **ICHDSALT**. If head values are entered, SEAWAT calculates an equivalent freshwater value during the simulation using the calculated fluid density in the CHD model cell.

Solver (SIP, SOR, PCG) Packages

Users may select one of the three solver packages implemented in MODFLOW to solve the variable-density ground-water flow equation. These solver packages are Strongly Implicit Procedure (SIP), Successive Over-Relaxation (SOR), and Preconditioned Conjugate Gradient (PCG).

When setting input parameters for the solver packages, convergence criteria for head should be more tightly specified for variable-density simulations. For example, the criteria for head convergence (HCLOSE) may have to be set about four to six orders of magnitude lower than for constant density simulations.

The RCLOSE parameter, specified for the PCG solver, has dimensions of mass flux instead of volumetric flux. This means that the RCLOSE parameter may be set higher than for a constant density simulation, by a factor of the average fluid density.

Preparation of MT3DMS Input Packages for SEAWAT

In the subsequent sections, instructions for preparing individual MT3DMS packages for SEAWAT are explained. An input variable highlighted in bold indicates that it is specific to SEAWAT, or a change has been made to facilitate data entry for SEAWAT. The MT3DMS packages for SEAWAT are:

- Basic transport (BTN) package
- Advection (ADV) package
- Dispersion (DSP) package
- Source/Sink Mixing (SSM) package
- Reaction (RCT) package
- Generalized Conjugate Gradient (GCG) solver package

There are no special considerations for designing DSP, RCT, and GCG packages to run with SEAWAT. Thus, no information for these packages is presented.

Basic Transport (BTN) Package

The basic transport (BTN) package is required for a SEAWAT simulation. Users should ensure that input parameters in the BTN are consistent with input parameters in the MODFLOW input files.

A2   Record: NLAY, NROW, NCOL, NPER, NCOMP, MCOMP

     Format: 6I10

       The version of MT3DMS used in SEAWAT can be used to simulate the transport of more than one chemical species. In SEAWAT, the first species (NCOMP = 1) is used to relate concentration to fluid density. The transport of other species also may be simulated with SEAWAT, but the concentrations of those species will not affect density.

A4   Record: TUNIT, LUNIT, MUNIT

     Format: 3A4

       The equation of state, which relates fluid density to the solute concentration, is embedded in the SEAWAT program. The equation of state used in SEAWAT requires that the dimensions of concentration be the same as the dimensions of density [ML^{-3}]. Additionally, the units of solute concentration used in the simulation must be the same as the units of density. To use the correct value for freshwater density, the SEAWAT program requires that the units for length and mass be specified in an input file. To minimize the difference in input from a standard MODFLOW/MT3DMS application, SEAWAT uses the units of mass and length specified in the input file for the BTN package.

These units are used to select the equation of state that relates solute concentration to fluid density. In standard MT3DMS applications, the entries for simulation time (TUNIT), length (LUNIT), and mass (MUNIT) are used only as labels in the output file and do not affect the calculation results. SEAWAT can use either metric or English units for concentration and density, but only one of the two units may be used to describe the problem.

If the international metric system is preferred, the specified unit of length must be meters and the unit of mass must be kilograms. Thus, the entries for the units of length and mass must be "M" or "m" and "KG" or "kg." For example, the input line may look like:

DAY   M   KG

SEAWAT will read this record, and automatically assign the density of freshwater as 1,000 kg/m^3 and the density of seawater as 1,025 kg/m^3.

If the English system is preferred, the unit of length must be feet and the unit of mass must be pounds. Thus, the entries for units of length and mass must be "FT" or "ft" and "LB" or "lb." For example, the input line may look like:

DAY   FT   LB

SEAWAT will read these entries and automatically assign the freshwater density as 62.44 lb/ft^3 (pounds per cubic feet) and the density of seawater as 64.00 lb/ft^3.

SEAWAT uses the units of length and mass specified in the BTN package to select the appropriate equation of state for fluid density. SEAWAT also assumes that all values of concentration listed in the input files (such as initial concentration) have the same units of mass per cubic length as specified in the BTN units list. Additionally, the unit of the length specified here must be consistent with the unit of length used in MODFLOW.

A9   Array: HTOP(NCOL,NROW)

         Reader: RARRAY

For models with an unconfined layer, it is important to specify HTOP slightly higher than the highest expected elevation of the water table. HTOP is used to calculate the center elevation for each cell in the upper layer.

A21   Record: PERLEN, NSTP, TSMULT, **INITIALDT**

         Format: F10.0, I10, 3F10.0

PERLEN is the length of the stress period. In a standard MODFLOW simulation, the user specifies the number and lengths of timesteps for the flow solution, but in SEAWAT the program determines the lengths of timesteps unless the GCG solver is used. The input variables, NSTP and TSMULT, can be used in SEAWAT to select times for output of flow information according to the values set in the OC option. NSTP and TSMULT also can be used to force shorter timesteps at the beginning of a stress period. SEAWAT calculates the lengths of timesteps according to stability criteria, but also decreases the length of a timestep according to output times requested by the user. Therefore, if the flow field is changing rapidly due to a pumping well, for example, the user can decrease the lengths of timesteps at the beginning of the stress period by setting appropriate values for NSTP and TSMULT.

As discussed in Chapter 4, a short initial timestep is required to start each stress period. The user specifies the length of the initial timestep (**INITIALDT**). If **INITIALDT** is not included in the input file, SEAWAT uses a default value of 0.01 time units as the initial timestep for that stress period. SEAWAT will print a warning message on the screen if the length of the second timestep, which is calculated by SEAWAT, is smaller than the length of the first timestep. Users receiving this warning should decrease the value of **INITIALDT** so that errors do not result from the initial velocity field used to start the stress period.

Note that **INITIALDT** is entered for each stress period. This means that **INITIALDT** can change during the simulation from stress period to stress period.

A23   Record: DT0, MXSTRN, TTSMULT, TTSMAX

        Format: 8F10.0

Due to restrictions in the length of a transport step, SEAWAT may require a substantial number of transport steps to complete a stress period. For this reason, MXSTRN should be set large enough to avoid the possibility of the program stopping because too many transport steps were required to finish the stress period. The user also may want to try different values for DT0. The maximum length of a transport step will be calculated by SEAWAT based on restrictions in solving the transport equation. These restrictions, however, do not include a restriction based on the timestep lag between the solution to the transport equation and the solution to the flow equation. Therefore, the user may want to verify that the one step lag used in SEAWAT does not affect the model results by rerunning SEAWAT with a small value for DT0. For most cases, the results from a run with a small value of DT0 will compare well with the results from a simulation in which SEAWAT calculates the length of the transport step.

Advection (ADV) Package

The ADV package contains simulation options for representing the advection part of the solute-transport equation.

B1   Record: MIXELM, PERCEL, MXPART, NADVFD, **NSWTCPL**, **DNSCRIT**

        Format: I10, F10.0, 2I10, **I10, F10.0**

To activate the implicit coupling between the flow and transport equations in SEAWAT, two additional parameters are required within the ADV package. **NSWTCPL** is the maximum number of coupling iterations that SEAWAT will perform. **DNSCRIT** is the convergence parameter for the coupling between flow and transport and has units of fluid density. If the maximum density difference between two consecutive 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 exceeded.

Much effort is required in determining the appropriate method and parameters for solving the solute-transport equation. Most of these options and parameters are found in the ADV package. Users are strongly encouraged to obtain a firm understanding of these different parameters and methods implemented in MT3DMS for solving the solute-transport equation. Without an accurate solution to the solute-transport equation, SEAWAT cannot produce accurate results.

Source/Sink Mixing (SSM) Package

Source concentrations in the SSM package are entered using the same units as specified in the BTN package. There cannot be more than one source of the same boundary type in the same cell unless the source concentrations are equal for both boundaries. For example, there cannot be two RIV boundaries with different concentrations in the same model cell. SEAWAT does not give an error if this situation occurs and will proceed by assigning the first source concentration in the SSM package to all of the boundaries of that type in that cell.

Running SEAWAT

       SEAWAT runs in a similar manner as MODFLOW-88. Perhaps the best method with a personal computer is to open a DOS window and change directories to the subdirectory that contains the input files. The SEAWAT executable is then initiated by typing the path name (if necessary) and the name of the SEAWAT executable. After the executable is initiated from the DOS window, SEAWAT prompts the user for filenames of the different packages and the names of the output files to create. An example is presented below with the user responses in bold.

```
    SEAWAT: A COMPUTER PROGRAM FOR SIMULATION OF THREE-DIMENSIONAL
                 VARIABLE-DENSITY GROUND-WATER FLOW
                          VERSION 2.10
                         February 2002
                          written by:


                          WEIXING GUO
                          CDM Missimer


                       CHRISTIAN LANGEVIN
                       U.S. Geological Survey

This program is public domain and is released on the condition that
neither the U.S. Geological Survey nor the United States Government
may be held liable for any damages resulting from their authorized or
unauthorized use.


 Enter Name for SEAWAT Output Listing File:
seawat.out
 Enter Name for MODFLOW BAS Input File:
seawat.bas
 Enter Name for MODFLOW BCF Input File:
seawat.bcf
 Enter Name for MODFLOW WEL Input File:
seawat.wel
 Enter Name for MODFLOW RIV Input File:
seawat.riv
 Enter Name for MODFLOW EVT Input File:
seawat.evt
 Enter Name for MODFLOW GHB Input File:
seawat.ghb
 Enter Name for MODFLOW RCH Input File:
seawat.rch
 Enter Name for MODFLOW PCG Input File:
seawat.pcg
 Enter Name for MODFLOW OpC Input File:
seawat.oc
 Enter Name for MT3DMS BTN Input File:
seawat.btn
 ***** Density of Fresh Water is 1000 kg/m3
```

```
 Enter Name for MT3DMS ADV Input File:
seawat.adv
 Enter Name for MT3DMS DSP Input File:
seawat.dsp
 Enter Name for MT3DMS SSM Input File:
seawat.ssm
 Enter Name for MODFLOW Unformatted Head File:
seawat.hds
 Enter Name for MODFLOW Unformatted Flow File:
seawat.cbb
```

      To expedite the initiation of a SEAWAT simulation, a batch file that calls the SEAWAT executable can be used to "pipe in" a response file. This eliminates the need for the user to type a filename after each prompt. A typical batch file, which can be created with an ASCII text editor, might contain a single line as follows:

..\exe\seawat2_1.exe < seawat.dat

The seawat.dat file contains a list of filenames in the same order requested by the SEAWAT code. For the above example, the seawat.dat file would contain the following lines:

```
seawat.out
seawat.bas
seawat.bcf
seawat.wel
seawat.riv
seawat.evt
seawat.ghb
seawat.rch
seawat.chd
seawat.pcg
seawat.oc
seawat.btn
seawat.adv
seawat.dsp
seawat.ssm
seawat.hds
seawat.cbb
```

      Changes to the BAS, OC, or BTN packages that include or eliminate input packages or output files require modifications to the response file (for example, seawat.dat). Additionally, note that the order of the filenames in seawat.dat must follow the same prompting order of the SEAWAT executable, and there must be a line return after the last filename entry.

Output Files and Post Processing

Output files from a SEAWAT simulation generally consist of standard MODFLOW output files and standard MT3DMS output files. There are, however, several differences in the output files that are unique to SEAWAT. These differences include the following.

- The listing file, which contains general information about a simulation, consists of MODFLOW and MT3DMS output.
- The listing file may become very large if the user chooses to print information such as heads, drawdowns, dispersion coefficients, and so forth.
- Heads and drawdowns are written in terms of equivalent freshwater values.
- SEAWAT uses a temporary file, called $file.umt, to store advective fluxes for the current timestep. The user may delete this file at the end of a simulation.
- The flow terms in the cell-by-cell flow file are expressed as volumetric fluxes rather than mass fluxes. This file, therefore, can be subsequently used for particle tracking or generating fluid-budget information for zones within the model domain.
- The cell-by-cell flow file also can contain an additional array identified by the text string "DCDT." The DCDT array stores the rate change in fluid volume due to the change in concentration. The DCDT array is written at the same times as data from the BCF package. Users should refer to descriptions of the input parameters ICBCFL and IBCFCB within the BCF input file for more information.

Calculation of Equivalent Freshwater Head

In a conventional MODFLOW application, boundary heads typically are assigned by interpolating between measured values of head in the available observation wells. In a SEAWAT application, the measured heads presumably represent values of h, which must be converted to freshwater heads through equation 3 to serve as MODFLOW boundary heads under SEAWAT. This implies that the monitoring wells must be tightly cased piezometers open to only a short vertical interval. Additionally, the density of the water in the casing of each well must be uniform and equal to the density of the ground water outside the well screen, and this density must be known with reasonable certainty for each monitoring well. To the extent that data are available, therefore, the assignment of boundary heads generally is made by converting observed water levels in the field to equivalent freshwater heads using equation 3, and interpolating among the calculated values.

In any three-dimensional MODFLOW simulation, uncertainty arises where a monitoring well actually has a lengthy screen. (The measured water level is then a composite value for the interval penetrated by the screen, rather than a point measurement that can be associated with a particular depth.) With SEAWAT, the uncertainty associated with a long screen is increased by the possibility that density (in addition to the variation in pressure and elevation) may vary with depth through the screened interval. Even in wells that have a short screen, density variation with depth may occur within the well casing, particularly where the salinity of the ground water opposite the well screen has greatly varied with time in the period prior to measurement or where the well was not fully purged after drilling. In these instances and if data are available on the vertical distribution of salinity within the casing, an average density for the water, ρ_{av}, in the casing may be calculated as:

$$\rho_{av} = \frac{1}{Z_W - Z_S} \int_{Z_S}^{Z_W} \rho(Z) dZ, \tag{134}$$

where:

Z_w is the elevation of the water level in the well,

Z_s is the elevation of the top of the well screen, and

$\rho(Z)$ represents the density of the water in the casing expressed as a function of elevation.

The variable, ρ_{av}, then can be used in place of ρ in equation 3 to calculate the equivalent freshwater head at the screened depth of the well.

Comparison of calculated and observed water levels in model calibration under SEAWAT must generally be carried out after first converting the calculated freshwater heads to water levels corresponding to field densities through equation 4 or converting the observed water levels to equivalent freshwater heads through equation 3. Interpretation of calculated results to predict field water levels similarly requires conversion of calculated freshwater heads to heads expressed in terms of the aquifer water using equation 4.

Tips for Designing SEAWAT Models

Getting started with any new modeling software requires an investment of time and effort to become familiar with the intricacies of that particular program. Although SEAWAT was designed to be relatively easy to use, new users may encounter some problems in getting the code to work properly. The purpose of this section is to discuss some of the potential problems that users may face when designing a SEAWAT model and provide tips for avoiding the most common errors.

Perhaps the best approach for designing a new SEAWAT model is to start with a simple cross-sectional model that runs relatively quickly. Initially, the simple model should only contain a few flow packages and have only a single transport mechanism, such as advection. By designing a model in this manner, the user creates a simple tool that can be used to quickly evaluate appropriate grid resolution, aquifer parameters, hydrologic stresses, numerical dispersion, computer run times, solver limitations, and transport options. The simple cross-sectional model can then be used throughout the development of larger, more-detailed models of increasing complexity. Development of a simple cross-sectional model is particularly recommended for first-time users of SEAWAT.

As previously stated, one of the benefits of SEAWAT is that it uses standard MODFLOW and MT3DMS input files with minor optional modifications. This benefit, however, can lead to runtime errors or erroneous model results if the MODFLOW input files are not consistent with the MT3DMS input files. For example, the number of rows, columns, and layers must be included in both the MODFLOW BAS and MT3DMS BTN input files. In the current version, SEAWAT does not check for consistency between input files, and thus, unexpected model results may occur if the input files are not properly constructed. One of the best ways to avoid this type of error is to use a thoroughly tested preprocessor to create the input files.

One very important consideration in the design of a variable-density ground-water flow model is the selection of appropriate grid resolution. Appropriate grid resolution in a horizontal direction can often be determined by following the guidelines for constant-density simulation of flow and solute transport (Anderson and Woessner, 1992; Zheng and Bennett, 1995). The grid resolution in the vertical direction, however, often requires a much greater level of detail to represent the complex flow patterns near areas of high concentration gradients. At present, there is no way to determine the required level of resolution prior to performing a simulation. Experience suggests that 10 model layers per aquifer unit seem to be adequate, but users are encouraged to perform numerical experiments with different levels of grid resolution in order to determine the most appropriate number of layers. Experience also has shown that models designed with spatially uniform cell volumes are less prone to numerical instabilities than models designed with variable cell volumes. These requirements for grid design can have important implications for converting an existing, constant-density flow model into a variable-density SEAWAT model. Many constant-density flow models are designed with variable cell volumes so that the tops and bottoms of a model layer follow the tops and bottoms of an aquifer unit. The grid resolution for these models, particularly in the vertical direction, must commonly be increased before a simulation with SEAWAT will give accurate results.

In general, there are two options for treating the lengths of timesteps; they can be calculated by SEAWAT according to the criteria discussed in Chapter 4, or they can be specified by the user if the implicit finite-difference method is used to solve the solute-transport equation. If the timestep lengths are calculated by SEAWAT during runtime, there can be circumstances when the timestep lengths are too short to allow reasonable simulation times. The user usually has a number of options for lengthening the timesteps when this situation occurs. First, the user should open the listing file, and search for the sections that list the maximum step sizes. MT3DMS, and thus SEAWAT, list the maximum step size for the different criteria; the shortest timestep is the one used for the calculation. Included in this section of the listing file is the model cell (layer, row, and column) where the limitation in timestep length occurs. In many instances, experience has shown that there is an error (possibly conceptual) in aquifer parameters, boundary conditions, or initial conditions near the limiting model cell. Often times, when the error is corrected, the calculated timestep lengths will be substantially longer. Another option for lengthening the timesteps is to increase the value of PERCEL (the courant number)–the fraction of a model cell in which advection can occur in any one direction. Whereas increases in PERCEL may increase the timestep lengths, the resulting solution may be less accurate compared to a run with a smaller value for PERCEL.

The concept of steady-state or transient conditions can be confusing when referring to variable-density models because of the coupled flow and solute-transport components. Flow is considered at steady state when the heads do not change with time; transport is at steady state when the concentrations do not change with time. In designing a SEAWAT model, the flow portion should be specified as transient for most problems (ISS set to zero in the MODFLOW BCF input file). SEAWAT will work when the steady-state option is activated, but in some instances, the flow portion of the model will not converge. There is no option to run the transport model as steady state, so most SEAWAT simulations will be transient with respect to flow and solute transport.

One of the most common simulations that users may perform with SEAWAT is one in which the model is run with constant hydrologic stresses until heads and concentrations do not change with time. At this point, the model has come to steady state with respect to flow and transport. Although there are a number of ways to determine when the model has reached steady state, perhaps the easiest way is to plot the total solute mass in the model as a function of time. This information is available in a file called, mt3d001.mas. In most long-term simulations, the SEAWAT model reaches steady state when the total solute mass in the model does not change with time. An exception to this is the case where a plume of solute moves through the model domain, and no solute is lost to internal or external boundaries.

In many variable-density simulations, the goal is to evaluate temporal changes in concentration and head. For most of these types of simulations, it is important that the initial heads and concentrations are at equilibrium with one another and that they have come to equilibrium with the imposed hydrologic stresses. It is also important that the initial heads are represented as equivalent freshwater values and that concentrations are represented as total dissolved solids. If initial heads and concentrations are not at equilibrium, they may not be solutions to the variable-density ground-water flow equation, and thus, they may change at the start of the simulation for reasons other than expected. Two types of simulations can be used to produce appropriate initial conditions for this type of transient model. The first is a SEAWAT model that has been run to steady state using representative hydrologic conditions from that time period or one hydrologically similar. The other is a transient SEAWAT model with temporally varying stresses that has been run repeatedly, each time with the initial conditions set from the results of the previous run, until the model produces the same results each time. The user should determine the best approach for the particular problem.

MT3DMS contains powerful options for solving the solute-transport equation. Selection of the best method depends primarily on the particular problem and usually involves a compromise between accuracy and length of computer runtime. For example, the implicit finite-difference solver can, in many circumstances, allow SEAWAT to take long timesteps, but the numerical dispersion resulting from this method can pose severe limitations for problems involving sharp fronts with large concentration gradients. The total-variation-diminishing (TVD) solver will often provide accurate solutions for problems with sharp fronts and uniform cell volumes, but may require relatively short timesteps. The method of characteristic (MOC)

schemes, which can be computationally intensive, will often provide acceptable answers when many of the other methods will not work. Users should experiment with all of the methods and options to find the one that provides the most accurate results with the shortest runtimes.

One of the most time-consuming problems that some users may encounter is trying to achieve convergence with the flow portion of the SEAWAT model. In many instances, convergence problems are due to errors in the input files, but once found the errors can be easily corrected. Some of the most common errors in the input files are often the result of failing to convert boundary heads to equivalent freshwater heads or using inconsistent units, inappropriate storage coefficients, a value of zero specified for porosity in the MT3DMS BTN input file, or a flow residual in the PCG input file that was not converted to a mass flux. Complex models and conceptual errors in model design can also cause problems with convergence. For example, problems with wetting and drying, which are difficult for many constant-density models to solve, will often cause convergence problems for SEAWAT, as will some water-table problems and conditions with layer conversions from confined to unconfined. Some common conceptual errors that may cause convergence problems include using inappropriate initial conditions, applying rapidly changing boundary conditions with insufficient temporal discretization, or assigning drastically different values to adjacent zones of aquifer properties.

The SEAWAT results that are typically evaluated at the end of a run include the ASCII output listing file and binary files that contain equivalent freshwater heads, solute concentrations, and cell-by-cell flows. When the appropriate input options are specified, the ASCII output listing file provides useful information about the fluid mass balance and the solute mass balance (also included in mt3d001.mas). Users should verify that mass-balance errors are within an acceptable range. Users also should plot contours or color floods (color gradations) of equivalent freshwater heads and solute concentrations for selected simulation times. When a model has been designed properly and SEAWAT produces an accurate solution, users should expect to see values of equivalent freshwater head that rapidly increase with depth compared to contours from a similar simulation of a constant-density system. This rapid increase will only be observed in areas of the model that have solute concentrations greater than freshwater. Users should remember that for most variable-density models, flow lines will not be perpendicular to contours of equivalent freshwater head, even with a system that is isotropic with respect to permeability. Perhaps the best way to evaluate flow directions from a SEAWAT run is to plot the vectors of discharge, which can be calculated from data in the cell-by-cell flow file. Users also should closely evaluate plots of solute concentration. In addition to providing useful information about the flow system, plots of solute concentration can indicate areas of numerical dispersion or numerical instabilities.

CHAPTER 7
BENCHMARK PROBLEMS

SEAWAT was verified by running four different problems and comparing the results to those from other variable-density codes. Voss and Souza (1987) suggest that new variable-density codes should be tested and verified by running four or five benchmark problems that vary in complexity. These benchmark problems are listed below with the reference that describes the problem.

- Box problems (Voss and Souza, 1987)
- Henry problem (Voss and Souza, 1987)
- Elder problem (Voss and Souza, 1987)
- HYDROCOIN problem (Konikow and others, 1997)

This chapter presents the development and results for the above referenced benchmark problems. For each of the four problems evaluated, the results from SEAWAT compare well with the results from other numerical codes.

Box Problems

The purpose of the box problems is to verify that fluid velocities are properly calculated by SEAWAT. While inconsistent approximations for velocity are more likely to occur with finite-element models, the box problems also provide a good test for the finite-difference approximation used by SEAWAT. There are two different cases of the box problem (Voss and Souza, 1987). In the first case, SEAWAT is tested by simulating flow within a two-dimensional, vertical cross-sectional model with no-flow boundaries on all sides. The size of the model domain and values for hydraulic conductivity and porosity are inconsequential. Longitudinal dispersivity values should be set to a length similar in size to the length of a model cell, and the diffusion coefficient and transverse dispersivity value should be set to zero. The initial conditions within the box consist of a layer of freshwater overlying a layer of saltwater–a stable configuration for fluid density. When this model is run with steady-state conditions, the interface between freshwater and saltwater should remain in the same layer of the model. For the second case, horizontal flow is induced by specifying different, but hydrostatic constant heads on the left and right sides of the box. Descriptions of these two cases are provided in the subsequent sections.

Case 1

For the first case, SEAWAT was used to simulate flow for 50,000 days. The model simulates variable-density ground-water flow in a two-dimensional cross section with 1 row, 20 columns, and 20 layers. The size for each model cell is 100-m horizontal by 100-m vertical. No-flow boundaries surround the model on all sides. The initial concentrations were based on freshwater overlying seawater. Initial concentrations are 0 kg/m^3 for layers 1 to 17 and 35 kg/m^3 for layers 18 to 20. Initial freshwater heads were calculated to achieve hydrostatic conditions (no vertical flow). A uniform and isotropic value for hydraulic conductivity was set to 100 m/d; the porosity was set to 0.01, and the value for longitudinal dispersivity was set to 100 m (the length of the cell dimensions). The transverse dispersivity value was set to zero.

The SIP and PCG packages of MODFLOW and the GCG package with the finite-difference option of MT3DMS were used for case 1, and there was no vertical mixing, provided that the tolerances were set properly. The SIP solver was used with a head convergence criterion of 1 x 10^{-8} m to solve the flow equation. Larger values for the head convergence criterion produced erroneous vertical flow patterns that caused mixing of the fluid layers. The PCG solver would not converge for this first case probably because the model is surrounded by no-flow boundaries and does not have a specified head value within the model domain. The GCG solver was used with a courant number (number of cells or fraction of a cell that a parcel of water can advect during one timestep) of 1.0 to solve the solute-transport equation.

Case 2

The same dimensions, initial conditions, and aquifer properties used for case 1 were used in case 2; however, the boundary conditions and solution parameters were different between the two cases. For columns 1 and 20, constant heads were specified to induce flow in the positive x-direction. These heads (1.0 m for column 1 and 0.0 m for column 20) were adjusted to equivalent freshwater heads using vertical hydrostatic conditions and the initial concentrations as specified for the first case. The PCG solver was successfully used with a head convergence criterion of 1 x 10^{-7} m and a flow residual of 10 kg/d. Case 2 was run for 50,000 days, and no dispersion or vertical mixing was simulated between the freshwater and salt-water. With these aquifer parameters and boundary conditions, the flow velocity is 5 m/d, which means that a fluid particle travels across the model 125 times during the simulation. This suggests that the simulation time is sufficiently long to ensure that SEAWAT adequately simulates this test problem.

Henry Problem

Henry (1964) presented an analytical solution for a problem of ground water flowing toward a seawater boundary. Because an analytical solution was available for the Henry problem, many numerical codes have been evaluated and tested with the Henry solution. Segol (1993) showed, however, that the Henry solution was not exact because Henry (1964) eliminated, for computational reasons, mathematical terms from the solution that he thought to be insignificant. When Segol (1993) recalculated Henry's solution with the additional terms, the improved answer was slightly different from the original solution. With the new solution, Segol (1993) showed that numerical codes, such as SUTRA (Voss, 1984), could reproduce the correct answer for the Henry problem.

The basic design of the Henry problem is shown in figure 12. The cross-sectional box is 2-m long, by 1-m high, and by 1-m wide. A constant flux of fresh ground water is applied to the left boundary at a rate (Q_{in}) of 5.702 m^3/d per meter with a concentration (C_{in}) equal to zero. A constant head boundary is applied to the right side of the box to represent seawater hydrostatic conditions. The right boundary represents seawater hydrostatic conditions. The upper and lower model boundaries are no flow.
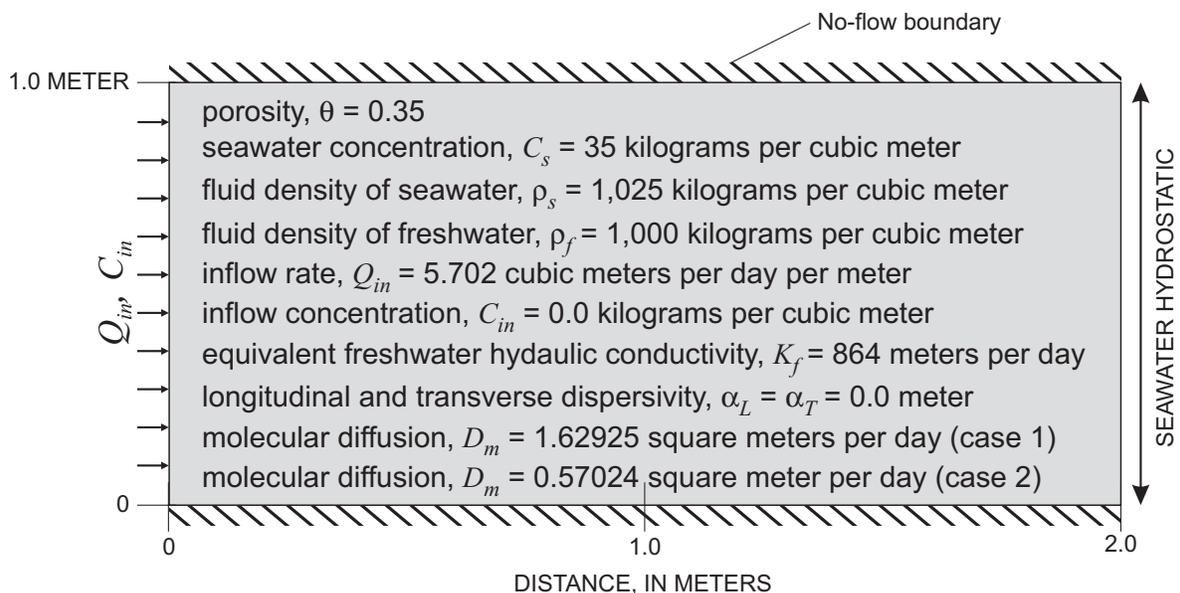

Figure 12. Boundary conditions and model parameters for the Henry problem.

The Henry problem caused further confusion among the modeling community because some researchers attempting to verify numerical codes calculated an erroneous value for molecular diffusion that did not correlate with the original value used by Henry (Voss and Souza, 1987). For this reason, some researchers consider there to be two cases of the Henry problem: one in which the value for molecular diffusion (D_m) is 1.62925 m^2/d and another with a value of 0.57024 m^2/d.

The finite-difference model grid used to discretize the problem domain consists of 1 row with 21 columns and 10 layers. Each cell, with the exception of the cells in column 21, is 0.1 by 0.1 m in size. Cells in column 21 are 0.01-m horizontal by 0.1-m vertical. The narrow column of cells in column 21 was used to more precisely locate the seawater hydrostatic boundary at a distance of 2 m. The WEL package was used to assign injection wells, with constant inflow rates of 0.5702 m^3/d to each cell of column 1. Constant fresh-water heads were assigned to the cells in column 21 using a head value of 1.0 m and a concentration of 35 kg/m^3. The concentration for inflow from these constant head cells was specified at 35 kg/m^3.

For both cases of the Henry problem, the implicit finite-difference solver (GCG) with the upstream-weighting scheme was used to solve the transport equation. The initial timestep was specified as 0.001 day, and a timestep multiplier of 1.9 was used to increase subsequent timesteps. For both cases, 23 timesteps were required to run the 1-day simulation period. The comparison between SEAWAT results and results from SUTRA (Segol, 1993) are shown for the Henry problem in figure 13. Contours of relative salinity concentration are in good agreement for both cases.
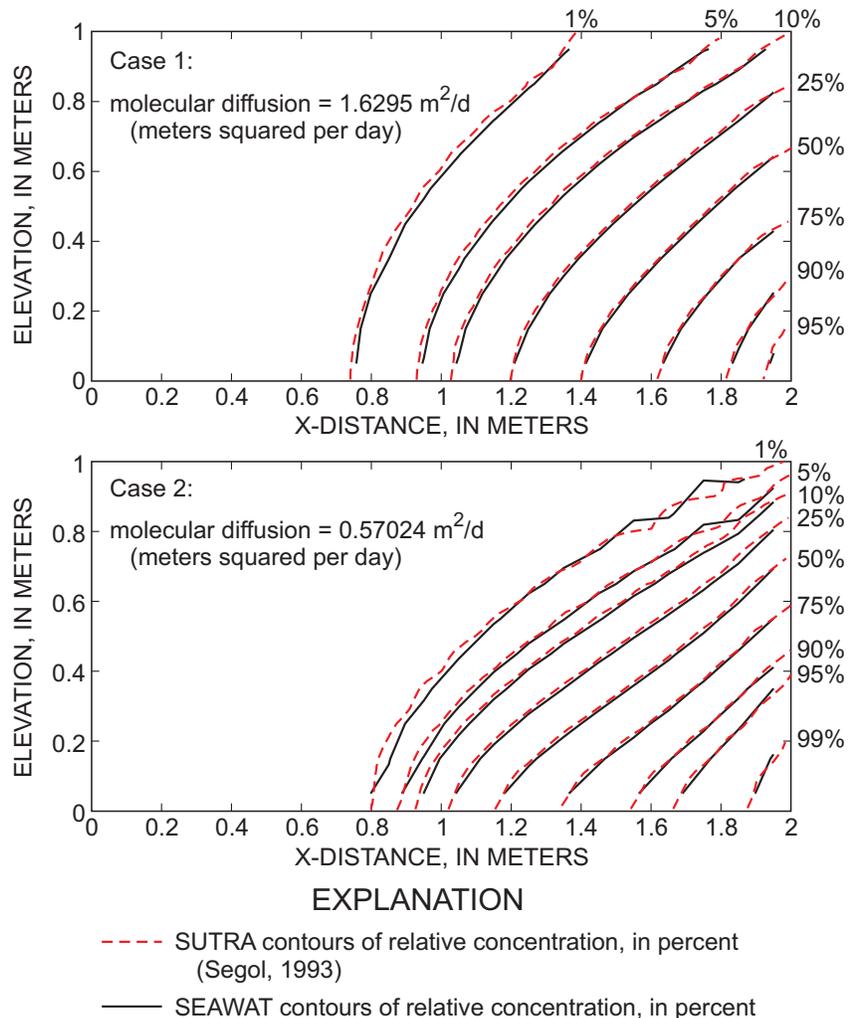

Figure 13. Comparison between SEAWAT and SUTRA for the Henry problem.

Elder Problem

The Elder problem was originally designed for heat flow (Elder, 1967), but Voss and Souza (1987) recast the problem as a variable-density ground-water problem in which fluid density is a function of salt concentration. The Elder problem is commonly used to verify variable-density ground-water codes. The geometry and boundary conditions for the problem are shown in figure 14. A constant-concentration boundary is specified for a portion of the upper boundary. Molecular diffusion is the sole mechanism for hydrodynamic dispersion during the simulation, which runs for 20 years. Salt from the constant-concentration boundary diffuses into the model domain and initiates complex vortices that redistribute the salt mass throughout the model. A constant-concentration boundary with a value of zero is specified for the lowest layer in the model. Two outlet cells with constant head values of zero are specified for the upper left and right boundaries. These constant head cells allow salt to diffuse into the model by providing an outlet for fluid and salt mass.
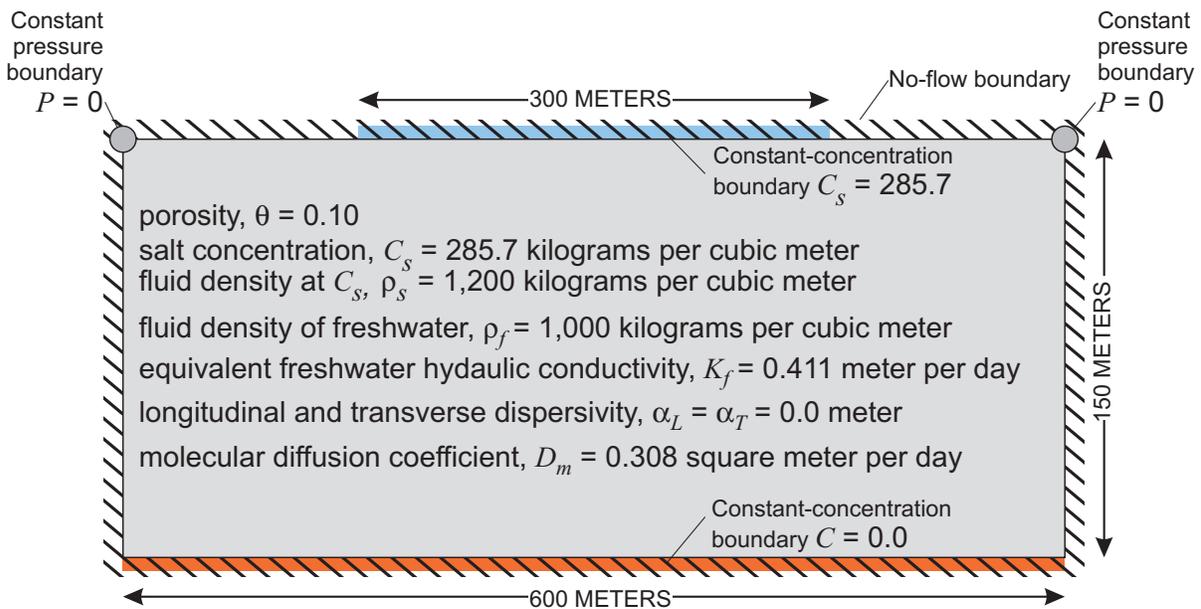
Figure 14. Boundary conditions and model parameters for the Elder problem.

The finite-difference grid used with SEAWAT to simulate the revised Elder problem (fig. 15) is similar in resolution to the finite-element grid used by Voss and Souza (1987). The SEAWAT grid consists of 1 row with 44 columns and 27 layers. Each cell is 13.63-m horizontal by 6-m vertical. For layer 1, cells in columns 1 to 11 and 34 to 44 are inactive. Cells in layer 1 from columns 12 to 33 are designated as constant concentration with a value of 285.7 kg/m^3. Using the equation of state in SEAWAT, this concentration value corresponds to the appropriate fluid density of 1,200 kg/m^3. In layer 2, constant heads are specified with a value of 150.0 m for the first and last columns, which provide a fluid outlet. For layers 2 to 27, the first and last columns are bounded by no-flow conditions. All of the cells in layer 27 also have a specified concentration of 0.0 kg/m^3, and there are no-flow conditions along the bottom face.

Initial concentrations within the model domain are set to zero, except for those in layer 1, which are set to 285.7 kg/m^3. Initial heads are set everywhere to zero. Hydraulic conductivity generally is uniform and isotropic with a value of 0.411 m/d. For layers 1 and 27, however, the horizontal and vertical hydraulic conductivities are set to 1 x 10^{-5} m/d to restrict flow within the top and bottom layers. The storage coefficient is uniformly set to zero, and the porosity value is uniformly set to 0.1. A value of 0.308 m^2/d is used as the coefficient of molecular diffusion.

Figure 15. Finite-difference grid used to simulate the Elder problem.

The PCG solver was used with a head convergence criterion of 1 x 10^{-7} m and a flow convergence of 1 kg/d. For the transport equation, the GCG solver was used with a courant number of 0.1 to limit the size 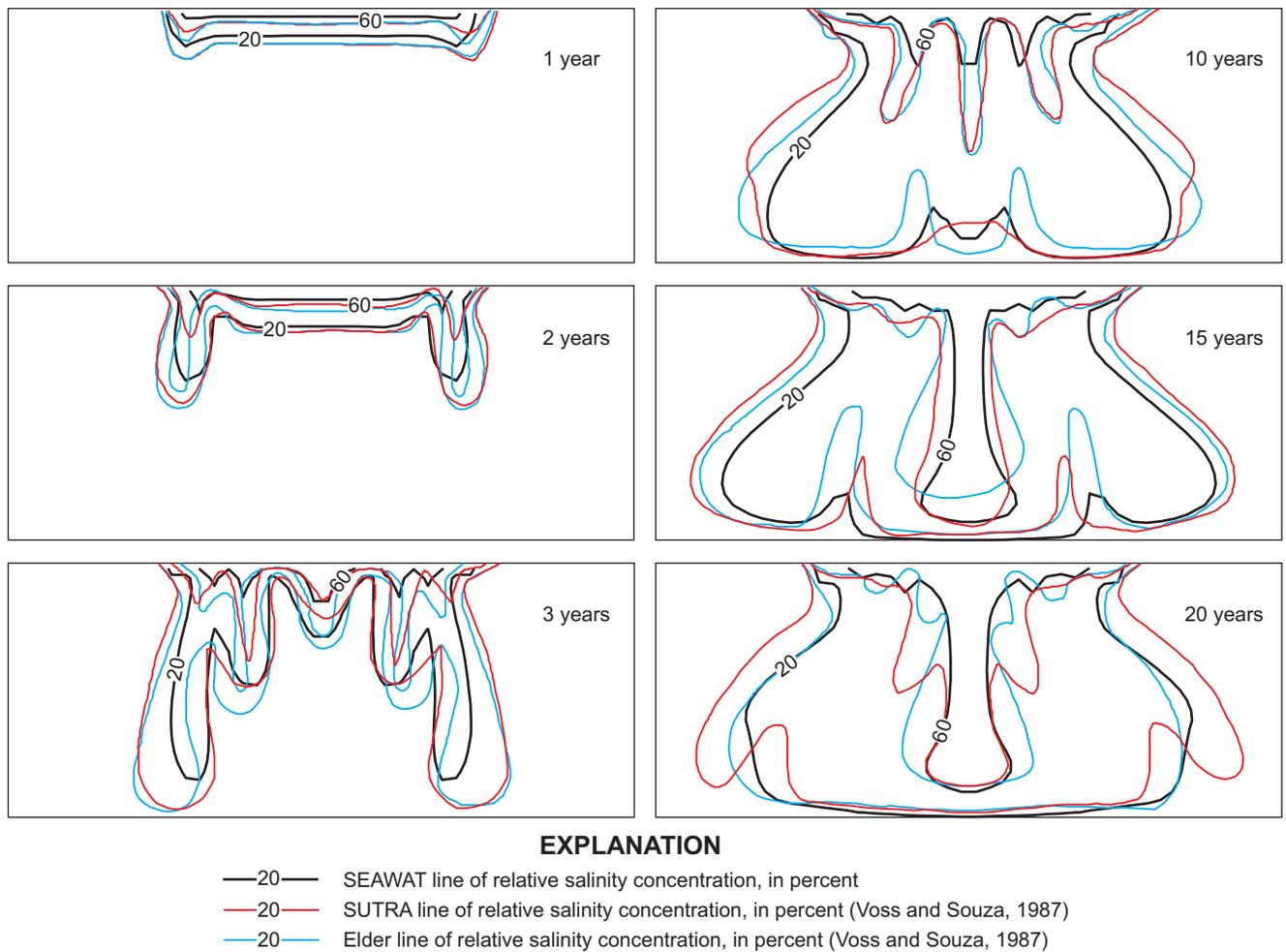of the timesteps. The average size of the timesteps was about 3 days, taking 2,321 timesteps to run the 20-year simulation. Relative salinity concentrations from SEAWAT are compared with results from SUTRA (Voss and Souza, 1987) and the original documentation results from Elder (1967) for six different times (fig. 16). Although some differences are evident, there appears to be a reasonably good match between the patterns from SEAWAT and those of SUTRA (Voss and Souza, 1987) and Elder (1967).

HYDROCOIN Problem

The purpose of the Hydrologic Code Intercomparison (HYDROCOIN) project was to evaluate the accuracy of selected ground-water modeling codes. One of the problems used for testing is the HYDRO-COIN problem. The problem presented here is based on case 5 that was reevaluated with the MOCDENSE code by Konikow and others (1997). The general geometry and boundary conditions for the HYDROCOIN problem are shown in figure 17. A sloping pressure boundary is imposed across the top of the box that is surrounded on the sides and bottom by no-flow conditions. Along the base of the middle part of the model, a constant-concentration condition is applied to represent the top of a salt dome. As ground water flows along the bottom boundary and over the salt dome, salt disperses into the system and collects in the lower right corner of the model domain.

The finite-difference grid used by SEAWAT (and MOCDENSE) consists of 1 row with 45 columns and 76 layers. Each cell is 20-m horizontal by 4-m vertical. The head values for the sloping constant-head boundary vary linearly between 10.080 m at the center of the first column and 0.113 m at the center of the last column (column 45). Fluid that enters the model domain from this upper boundary has a concentration

EXPLANATION

——20—— SEAWAT line of relative salinity concentration, in percent

——20—— SUTRA line of relative salinity concentration, in percent (Voss and Souza, 1987)

——20—— Elder line of relative salinity concentration, in percent (Voss and Souza, 1987)

Figure 16. Comparison between SEAWAT, SUTRA, and Elder's solution for the Elder problem over time.

of zero and a fluid density of 1,000 kg/m^3. The left and right boundaries are no flow. For the bottom layer, cells in columns 1 to 15 and 31 to 45 are inactive. Between these inactive cells, a constant-concentration boundary is specified with a concentration value of 280 kg/m^3.

A uniform and isotropic value of 0.8476 m/d was assigned for equivalent freshwater hydraulic conductivity in all layers, except for the bottom layer where the hydraulic conductivity was set at 8.475 x 10^{-4} m/d (three orders of magnitude lower than the rest of the model domain). This low value for hydraulic conductivity in the bottom layer limits salt from entering the model domain through advection–an important stipulation of the HYDROCOIN problem (Konikow and others, 1997). A value of 0.2 was uniformly assigned for porosity; the values of longitudinal and transverse dispersivity were set at 20 and 2 m, respectively; and molecular diffusion was set at zero.

For the HYDROCOIN problem, the standard version of MOCDENSE was modified to use a nonlinear equation of state to relate fluid density to solute concentration (Konikow and others, 1997). The SEAWAT code also was modified to use this slightly different equation of state. The equation of state used by the modified SEAWAT and MOCDENSE programs is represented by the following equation:

$$\frac{1}{\rho} = \frac{C}{\rho_s} + \left[\frac{1-C}{\rho_f}\right] \qquad (135)$$
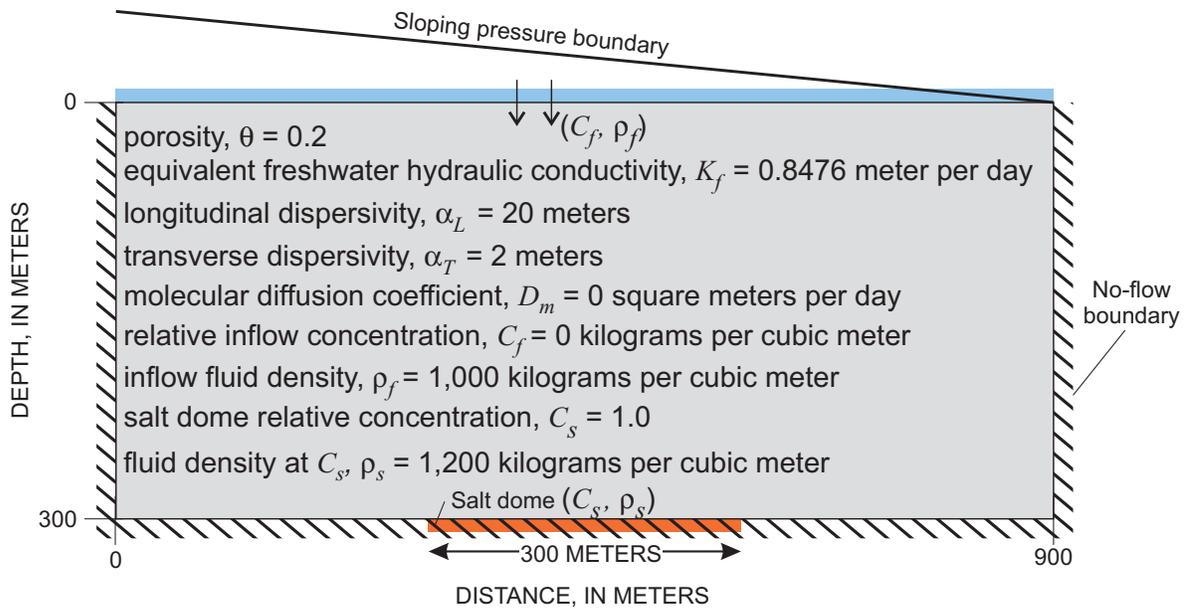
Figure 17. Boundary conditions and model parameters for the HYDROCOIN problem.

where ρ_s is the density of the brine (1,200 kg/m³) at a relative salinity concentration of 1.0 (Konikow and others, 1997). In the SEAWAT data sets, the salinity value for the salt dome is set at 280 kg/m³ - concentration that would result in a fluid density of 1,200 kg/m³ with the equation of state normally used by SEAWAT. Because equation 135 requires relative concentrations, the modified version of SEAWAT converts the concentrations to relative concentrations before applying equation 135.

The comparison of simulated results between SEAWAT and MOCDENSE is shown in figure 18. The relative salinity concentrations simulated by the two codes generally are consistent with one another; however, there is a discrepancy toward the upper right part of the model domain. While SEAWAT tends to produce slightly higher salinity concentrations in this region, the comparison between the two codes is considered acceptable.
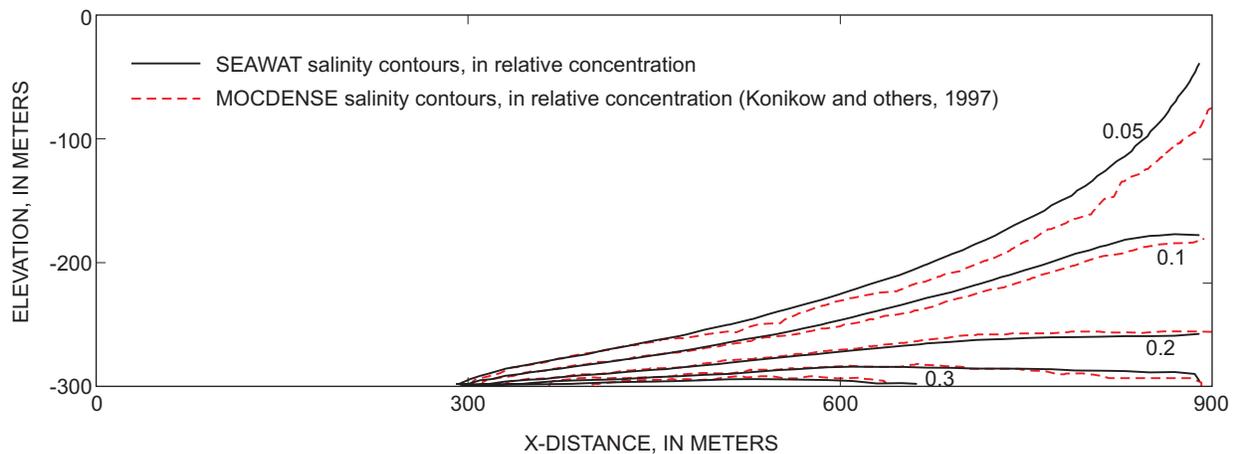

Figure 18. Comparison between SEAWAT and MOCDENSE for the HYDROCOIN problem.

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