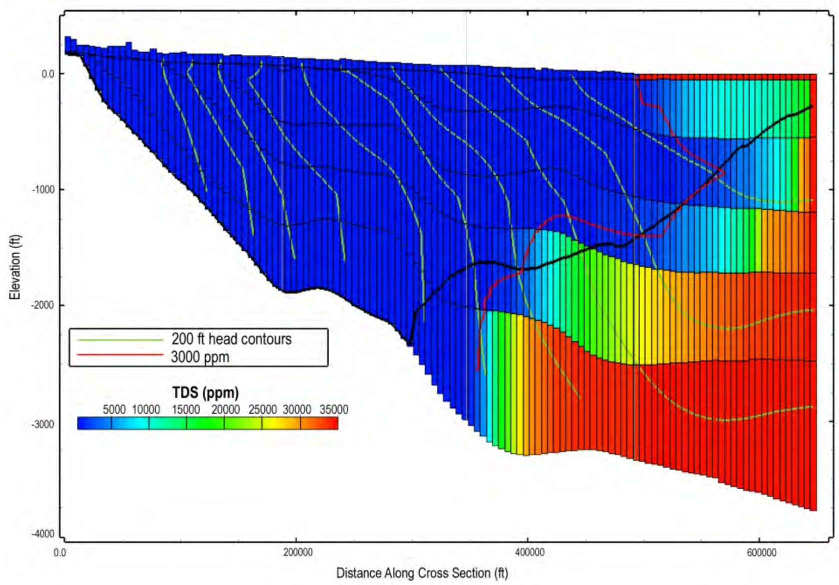
Assessment of Groundwater Modeling Approaches for Brackish Aquifers

Final Report

Prepared by

Neil E. Deeds, Ph.D., P.E.
Toya L. Jones, P.G.



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November 2011

Texas Water Development Board

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November 2011

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Executive Summary

The aquifers of Texas hold considerable brackish water resources. The characterization of these resources is an ongoing process, requiring consideration of both the basic hydrogeology of the underlying aquifer systems, and the potential complexities that high dissolved solids concentrations can add to resource analysis. One of these complexities is the potential for density gradients, caused by large variations in solids concentrations (or less likely, temperature or pressure), to affect both the occurrence (and natural flow conditions) and potential production of brackish water.

Under the Brackish Resources Aquifer Characterization System (BRACS) program, INTERA was contracted by the TWDB to help provide guidance for selecting appropriate groundwater codes for simulating brackish aquifers, including variable density effects.

We performed a literature review to assess typical brackish water applications, which are typically mixed-convection systems. In addition, the literature review included determining what groundwater codes are capable of simulating brackish water hydrogeology, and what the various characteristics of the codes are. We narrowed the list of codes to be reviewed by considering the quality of the documentation, how recently they were developed, and an indication of their userbase based on occurrence in the literature. The selected codes were CFEST, CODESA-3D, FEFLOW, FEMWATER, HydroGeoSphere, MODHMS, SEAWAT, SUTRA, SWI package for MODFLOW, SWIFT-2002, and TOUGH2. Both finite element and finite difference codes are represented in the list. The codes as a group are far more similar than different in terms of their characteristics.

We performed a high-level summary of the hydrogeologic features of the brackish water aquifers in Texas. This included a summary of the aquifers that serve as sources of desalination feeds in Texas.

We then provided analysis on how the characteristics of the various codes could affect the suitability of a code for each type of hydrogeologic feature. We developed a simple code selection procedure based on ASTM D6170-97 “Standard Guide for Selecting a Ground-Water Modeling Code,” which includes defining the purpose of the modeling, identifying needs not associated with physical processes, identifying important physical processes that need to be simulated, and developing a selection procedure.

A spreadsheet-based decision matrix was developed to inform the selection procedure. The user selects those code characteristics that are identified as needs, as well as those physical processes and hydrogeologic characteristics that are relevant to the modeling effort. The codes are then ranked by their summed scores for each of the characteristics and physical processes. A case study regarding selecting a code for modeling brackish water production in Matagorda County provides an example of using the code selection process.

With the background information provided in this work, and the straightforward code ranking approach, a modeler should be able to make an informed decision about choosing a code for brackish water resources problems.

1.0 Introduction

The aquifers of Texas hold considerable brackish water resources. The characterization of these resources is an ongoing process, requiring consideration of both the basic hydrogeology of the underlying aquifer systems, and the potential complexities that high dissolved solids concentrations can add to resource analysis. One of these complexities is the potential for density gradients, caused by large variations in solids concentrations (or less likely, temperature or pressure), to affect both the occurrence (and natural flow conditions) and potential production of brackish water.

Groundwater models have been used extensively in Texas to help in water resources evaluation and planning. A large contributor to groundwater modeling efforts in Texas is the Water Development Board (TWDB) Groundwater Availability Modeling (GAM) program. Models developed under the GAM program have routinely focused on fresh or slightly saline water resources. Brackish water has typically either not been included, or has not been a focus of the modeling efforts. Because of this, variable density effects have not been considered in any of the GAMs to date. The most popular code used for groundwater modeling, MODFLOW, will not simulate variable density flow.

INTERA was contracted by the TWDB, as one of the Brackish Resources Aquifer Characterization System (BRACS) projects, to help provide guidance for selecting appropriate groundwater codes for simulating brackish aquifers, including variable density effects. Overall, this includes three primary objectives:

1. Perform a literature review, assessing codes and conditions for brackish groundwater modeling (emphasizing variable density),
2. Recommend conditions where a specific code or codes might be most applicable, and
3. Provide a decision procedure for code selection.

In this report, we first describe results from the literature review, including a summary of selected codes and their capabilities, as well as an assessment of the types of hydrogeologic conditions under which brackish water occurs in Texas. The subsequent sections provide the approach for deciding which code might be most appropriate for a given brackish water modeling effort, and a case study where we put the decision approach to practical use.

2.0 Literature Review

2.1 Importance of Variable Density on Flow and Transport

2.1.1 Introduction to Mixed Convection Systems

In the current work, we emphasize the consideration of variable density when modeling flow in brackish aquifers. However, the buoyancy effects caused by density differences may not be important in all brackish aquifer modeling. In considering the relative importance of these effects, we provide a brief discussion of mixed convection systems.

When density differences are present in a flow system, solute transport may be dependent on three factors:

1. Hydraulic driven flow, called "forced convection" (or "advection"),
2. Buoyancy driven flow, called "free convection", and
3. Dispersion/diffusion.

A system in which flow is driven by both forced convection and free convection is called a "mixed convection" flow regime (e.g., Massmann and others, 2006). Many natural systems are mixed convection systems. We can see the potential importance of variable density flow by equating a typical hydraulic head gradient found in the field with a small density gradient (Simmons, 2005). For example, a typical natural aquifer gradient of 0.001 is equivalent to a density driving force resulting from a contrast of about 2,000 mg/L, which is well within the typical brackish water range (1,000 to 10,000 mg/L).

Under pumping conditions, the importance of variable density is less clear, since near-well gradients are much higher than typical natural gradients. Whether density driven flow has a significant impact is determined by a complex interplay among the properties of the mixed convection system, the properties of the porous media, and the occurrence of dispersion and diffusion (Simmons, 2005). Often, the only way to determine whether variable density is important for a given situation is to model it (or a simpler analogous system) both with and without density effects, and examine the difference.

2.1.2 Describing the Degree of Mixed Convection

There is no "rule of thumb" regarding when density effects are considered important enough that they must be considered in a modeling effort. However, there are dimensionless numbers associated with mixed convection that can be used to compare relative contribution among different scenarios. The Rayleigh number is described in Simmons and others (1999) in the reference list as the ratio between buoyancy-driven fluxes and those caused by diffusion and dispersion. This number is defined in the context of a salt lake system, which is typically characterized by a dense brine that overlies less dense groundwater. The value of the Rayleigh number (often symbolized as *Ra*) determines when the onset of instability occurs, and the denser fluid moves downward into the lake bed.

The second dimensionless number is the simply-named "mixed convection ratio", or the ratio of free to forced convection in a system. This number was introduced by Ward and others (2007) in the context of aquifer storage and recovery (ASR) in brackish aquifers. The higher the density contrast in the ASR system, the more "tilt" in the interface between the injected water and the denser ambient water, and the sooner the breakthrough of the ambient water during production.

2.1.3 Examples of Mixed Convection Systems

In this section, we discuss typical examples of mixed convection systems. These examples provide guidance as to when variable density is routinely considered in modeling applications.

Aquifer Storage and Recovery

As noted previously, when an ASR system is designed for injection of fresh water into a brackish water aquifer, variable density effects can be important at the leading edge of the fresh water "bubble" (Ward and others, 2007). The importance of variable density effects lies in the sensitivity of recovery performance to the mixed convection ratio.

Upconing

Upconing is typically described in the context of a stable density stratified system, where fresh (or lower TDS) water lies above brackish (or higher TDS) water. This hydrogeologic situation commonly occurs in coastal systems, and the Texas Gulf Coast is no exception. When the lower TDS water is pumped, the higher TDS water tends to migrate vertically towards the capture zone of the well, potentially increasing the TDS of the produced water.

Motz (1992) provides an analytical solution for estimating the degree of upconing based on a sharp interface approximation (where the fresh water abruptly transitions to brackish). This approximation is conservative (shows more impact) compared to numerical simulations with a smoothly varying density gradient (e.g., URS and INTERA, 2007).

Seawater Intrusion and Injection Barriers

Seawater intrusion, where denser seawater forms a "wedge" inland beneath the fresher aquifer, is a classic variable density problem. Shoemaker (2004) provides a good summary of the important parameters to consider for modeling seawater intrusion.

The installation of recharge wells to prevent or minimize intrusion is one of the strategies for protecting inland production. The Ghyben-Herzberg relation (e.g., Bear, 1972) describes an analytical relationship between the amount of inland freshwater head, and the relative intrusion of the seawater wedge. More recent work (Luyun and others, 2011) describes both laboratory scale experiments and supporting numerical modeling that explore the performance of injection wells in reducing intrusion.

Subsurface Desalination Feeds

The feed water for desalination may be taken from conventional inland brackish water aquifers, and simulating this production would carry the same characteristics as the upconing problem discussed previously. However, desalination plants may be built near the ocean, to allow for direct access to ocean water, as well as ocean brine disposal (e.g., Del Bene and others, 1994). One type of intake for the feed water consists of a well (may be horizontal or slanted) drilled from the inland side underneath the ocean bed. This configuration may leave the well screen in the "transition zone", where the water is being diluted by fresh groundwater from the inland side, where the density of the water is also transitioning.

Salt Disposal Pits

Saline surface water bodies overlying fresher groundwater can occur naturally, but also may occur in situations where brine is being disposed in surface pits. This has historically been common in the oil and gas industry, and also occurs at some desalination facilities, where evaporation ponds are used (e.g., Ahmed and others, 2000). Depending on the value of the Rayleigh number, the system may become unstable, and the denser fluid will migrate into the fresher water below (Simmons and Narayan, 1997, 1998).

Stream/Aquifer Interaction

Mixed-convection flow systems can exist when there is a significant density contrast between groundwater and a stream to which it discharges. Massmann and others (2006) used an analytic model to show that as mixed convection ratios increase (i.e., the groundwater becomes denser compared to the water in the stream), the amount of baseflow decreases.

2.2 Codes that Simulate Variable Density Flow and Transport

A literature review was conducted to identify groundwater modeling codes that simulate variable-density flow and transport. Bear and others (1999) provide a summary of concepts, methods and practices related to the investigation of seawater intrusion in coastal aquifers. That book includes a chapter that surveys computer codes used for the seawater intrusion problem along with case histories by Sorek and Pinder (1999) and a chapter on the code SUTRA (Voss, 1999). Those chapters were taken as the starting point for the literature review.

Bear and others (1999) is over 10 years old, so it includes many of the early variable-density codes but does not include the more recent codes. An additional search was conducted to identify recent variable-density flow and transport codes and/or recent modified versions of older codes. This search included contacting state agencies in Florida and California, where variable density codes are more routinely used for seawater intrusion and barrier modeling.

Table 2.2.1 provides a list of the 24 variable-density codes identified with the literature review. Note that this list is not exhaustive, as some of the codes encountered during the review were obviously "one-off" type academic codes, which did not have a user base beyond the original creator. The "one-off" codes were not considered in the review.

Table 2.2.1 Variable-Density Codes Identified in the Literature.

Code	Code	Code
3DFEMFAT/2DFEMFAT	HydroGeoSphere	SHARP
CFEST	MEL2DSLT	SUTRA
CODESA-3D	MLAEM/VD	SWIFT
DSTRAM	MOCDENSE	SWI package for MODFLOW
FAST-C(2D/3D)	MODHMS	SWIP
FEFLOW	SALTFRES	T3DVAP.F/MOR3D. F
FEMWATER	SALTHERM/3D	TOUGH2
HST3D	SEAWAT	TVD-2D/TVD-3D

Once codes were identified, a subset of the codes was selected based on a few high-level criteria, such as the availability of good documentation, whether development on the code was relatively recent, and some evidence of application in the general groundwater literature.

We did select one code that does not necessarily meet those latter criteria. The SWI package for MODFLOW, which was developed for modeling seawater intrusion with MODFLOW, was included because it provides a simplified methodology for simulating seawater intrusion and can be easily added to existing MODFLOW models. We felt that one code that was simple to apply should be considered in the overall selection process. Table 2.2.2 summarizes the 11 codes selected for final, detailed review.

Table 2.2.2 Variable-Density Codes Selected for Detailed Review.

Code	Theory/Reference Manual	User Guide/ Manual	Developer/Owner	Code Availability
CFEST	Freedman and others (2005)	Freedman and others (2006)	PNNL and CFEST, Inc.	proprietary
CODESA-3D	Lecca (2000)		CRS4 & the University of Padua (Italy)	proprietary
FEFLOW	Diersch (2009)	DHI-WASY GmbH (2010a,b)	DHI-WASY GmbH	proprietary
FEMWATER	Lin and others (1997)		US Army Corps of Engineers/ EPA(1)	public domain
HydroGeoSphere	Therrien and others (2010)			proprietary
MODHMS	proprietary	proprietary	HydroGeoLogic Inc.	proprietary
SEAWAT	Langevin and others (2008)	Guo and Langevin (2002)	USGS	public domain
SUTRA	Voss and Provost (2010)		USGS	public domain
SWI package for MODFLOW	Bakker and Schaars (2005)	Schaars and Bakker (2004)	Mark Bakker and Frans Schaars	public domain
SWIFT(2)	Reeves and others 1986	Benegar (2002); Earthward Consulting (2001)	(3)	proprietary
TOUGH2	Pruess and others (1999)		LBNL	proprietary

PNNL – Pacific Northwest National Laboratory
CFEST, Inc. – Consultants for Environmental System Technologies, Inc.
USGS – United States Geological Survey
LBNL – Lawrence Berkeley National Laboratory
(1) Developed by the U.S. Army Corps of Engineers and maintained by the EPA Center for Exposure Assessment Modeling
(2) Three versions of SWIFT were found: SWIFT-98, SWIFT for Windows, SWIFT-2002
(3) The developer/owner of the three versions of SWIFT found in the literature is unclear

The literature review for the selected codes focused on four main areas; general code characteristics, code graphical user interface (GUI) availability, code documentation and availability, and code applications. The following paragraphs discuss each of these areas individually. During the literature review, a website providing an overview of the code was found for many of the selected codes. These overviews varied in detail and content, with the sites for the publically available codes providing some specific detail and the sites for some of the commercially available codes providing more of a marketing document. The overviews found during the literature search are provided in Appendix A.

Code Characteristics

The code characteristics provide a means for comparing codes based on their physical and computational concepts. Code characteristics reviewed included:

- language
- coordinate systems
- numerical formulation
- solvers
- non-linear methods
- media types considered
- boundary conditions
- saturated/unsaturated
- aquifer type
- surface water/groundwater interaction
- treatment of water table
- initial density/concentration condition
- density inversions
- ability to incorporate structure features such as faults and karst
- MODFLOW compatible

A complete summary of the characteristics for the selected codes can be found in Table 2.2.3.

All of the codes are written in Fortran with the exception of FEFLOW, which is written in ANSI C/C++. The coordinate systems considered by the selected codes include Cartesian for all codes and radial, and/or axisymmetric for several codes. MODHMS also allows orthogonal curvilinear finite-difference grids for fitting irregular domain geometries.

In general, the selected codes fall into two numerical formulations; finite element or finite difference. Most of the codes include one choice for a direct solver and all of the codes have several choices in iterative solvers. The non-linear methods used by the codes include the Picard, Newton, and Newton-Raphson methods.

All of the codes can simulate porous media and several can also simulate fractured, double-porosity, or dual permeability media. Dirichlet and Neumann boundary conditions can be implemented with all of the codes and Cauchy boundary conditions with most of the codes. Several other boundary conditions such as infiltration of recharge, seepage faces, drains, and river leakage can be implemented in many of the codes. Many of the selected codes can simulate both the saturated and unsaturated zones while others consider only the saturated zone. Two of the selected codes can simulate fully integrated surface water and groundwater. With many of the codes, surface water can be implemented through a boundary condition. Two of the codes have no mechanism for incorporating surface water.

Two of the selected codes, CFEST and FEFLOW, are able to deform the numerical mesh to follow the location of the water table. For most of the codes, groundwater density is a function of concentration, which can be initialized independently for each grid cell. It appears, based on verification of the code against the Elder's free advection problem (Elder, 1966; 1967), that most of the codes can simulate density inversions. The exception is the SWI package for MODFLOW, which does not allow density inversions (Bakker and Schaars, 2005).

Structural features such as faults and karsts can be implemented indirectly using gridding and boundary conditions in several of the codes. The horizontal flow barrier package can be used to implement faults for the codes that are MODFLOW compatible. Only FEFLOW and HydroGeoSphere are capable of explicitly simulating conduit flow representative of karst features. The selected codes that are MODFLOW compatible are SEAWAT, MODHMS, and the SWI package for MODFLOW.

For some of the selected codes, the literature includes clear documentation of notable code capabilities and disadvantages, which are summarized in Table 2.2.4. Capabilities and disadvantages are left blank in this table in instances where no clear documentation was found in the literature.

Many of the code characteristics may be important for selecting a specific code for a specific application. For example, the gridding flexibility with a finite element code may be more appropriate for an aquifer with a complex geology and/or structure than the consistent gridding with a finite difference code. Some applications may require simulation of both the unsaturated and saturated zone. The type of media (i.e., single versus dual porosity) simulated by the code will be important when simulating fractured aquifers. In some instances, the boundary conditions that can be implemented with the code may be an important selection criteria. Selection of a code capable of simulating groundwater/surface water interaction will be important for some aquifers as will the ability to characterize karst features. For complex problems, the available iterative solvers may play a role in code selection.

Table 2.2.3 Characteristics of Selected Codes.

Characteristic	CFEST	CODESA-3D	FEFLOW	FEMWATER	HydroGeo-Sphere	MODHMS	SEAWAT	SUTRA	SWI package	SWIFT	TOUGH2
version	005		6	2.1		3	4	2.2	1.2	2002	2
last development	2005	2000	2003	1997			2011	2010	2005	2001	1999
dimensionality	3D	2D/3D	2D/3D	2D/3D	2D/3D	3D	2D/3D	2D/3D	3D	2D/3D	2D/3D
owner/developer	(1)	(2)	DHI-Wasy	(3)	(4)	HGL	USGS	USGS	(5)		LBNL
Code Language											
Fortran77	x			x		x	x			x	x
Fortran90		x						x			
Fortran 95					x						
Ansi C/C++			x								
Coordinate System(s)											
Cartesian	x	x	x	x	x	x	x	x	x	x	x
radial								x		x	
axisymmetric					x	x					
orthogonal curvelinear						x					
Numerical Formulation											
finite element, Galerkin scheme	x	x	x	x	x						
finite element, control volume					x						
finite difference						x	x		x	x	
hybridizations of finite-element & finite difference								x			
integral finite difference											x

Table 2.2.3, continued

Characteristic	CFEST	CODESA-3D	FEFLOW	FEMWATER	HydroGeo-Sphere	MODHMS	SEAWAT	SUTRA	SWI package	SWIFT	TOUGH2
Solver(s)											
Direct Solver(s)											
Gauss		x						x			
MA28											x
LUBAND											x
triangular-factorization											
not specified			x			x					
Iterative Solver(s)											
PCG	x	x	x	x		x	x	x			
Bi-CGSTAB		x	x		x						x
GRAMRB		x									
TFQMR		x									
SAMG			x								
SOR	x						x				
SSOR						x					
SIP						x	x				
ORTHOMIN					x	x		x			
GMRES	x				x			x			x
block iteration				x							
successive point iteration				x							
Jacobi iteration	x										
BiCGS											x
Lanczoes-type BiCGS											x
same as MODFLOW									x		

Table 2.2.3, continued

Characteristic	CFEST	CODESA-3D	FEFLOW	FEMWATER	HydroGeo-Sphere	MODHMS	SEAWAT	SUTRA	SWI package	SWIFT	TOUGH2
Non-Linear Method(s)											
Picard		x	x	x			x	x		x	
Newton		x	x								
Newton-Raphson				x	x	x					x
sequential iteration	x										
Media Type(s)											
porous	x	x	x	x	x	x	x	x	x	x	x
fracture			x		x	x		x		x	x
double porosity					x	x				x	x
dual continuum			x		x	x				x	x
Boundary Conditions											
Dirichlet BC	x	x	x	x	x	x	x	x	x	x	x
Neumann BC	x	x	x	x	x	x	x	x	x	x	x
Cauchy BC	x	x	x	x	x	x	x	x	x		
source/sink	x	x	x	x	x	x	x	x	x	x	x
free-water surface										x	
dynamic mesh for water table	x		x								
leakage (rivers)	x			x		x	x		x		
ET		x		x	x	x	x		x		
infiltration recharge		x		x	x	x	x		x		
seepage faces		x		x	x	x			x		
drain					x	x	x		x		
Carter-Tracy										x	
horizontal flow barriers						x	x		x		

Table 2.2.3, continued

<table>
<tr><th>Characteristic</th><th>CFEST</th><th>CODESA-3D</th><th>FEFLOW</th><th>FEMWATER</th><th>HydroGeo-Sphere</th><th>MODHMS</th><th>SEAWAT</th><th>SUTRA</th><th>SWI package</th><th>SWIFT</th><th>TOUGH2</th></tr>
<tr><td colspan="12">Saturation</td></tr>
<tr><td>saturated</td><td>x</td><td>x</td><td>x</td><td>x</td><td>x</td><td>x</td><td>x</td><td>x</td><td>x</td><td>x</td><td>x</td></tr>
<tr><td>unsaturated</td><td></td><td>x</td><td>x</td><td>x</td><td>x</td><td>x</td><td></td><td>x</td><td></td><td></td><td>x</td></tr>
<tr><td colspan="12">Aquifer Type</td></tr>
<tr><td>unconfined</td><td>x</td><td>x</td><td>x</td><td>x</td><td>x</td><td>x</td><td>x</td><td>x</td><td>x</td><td>x</td><td>x</td></tr>
<tr><td>confined</td><td>x</td><td>x</td><td>x</td><td>x</td><td>x</td><td>x</td><td>x</td><td>x</td><td>x</td><td>x</td><td>x</td></tr>
<tr><td>semi-confined</td><td>x</td><td>x</td><td>x</td><td>x</td><td>x</td><td>x</td><td></td><td>x</td><td></td><td></td><td>x</td></tr>
<tr><td colspan="12">Surface Water/Groundwater Interaction</td></tr>
<tr><td>fully integrated</td><td></td><td></td><td></td><td></td><td>x</td><td>x</td><td></td><td></td><td></td><td></td><td></td></tr>
<tr><td>through boundary conditions</td><td>x</td><td>x</td><td>x</td><td>x</td><td></td><td></td><td>x</td><td>x</td><td>x</td><td></td><td></td></tr>
<tr><td colspan="12">Variable Density</td></tr>
<tr><td>heterogeneous initial density</td><td>x</td><td>x</td><td>x</td><td>x</td><td>x</td><td>x</td><td>x</td><td>x</td><td></td><td>x</td><td>x</td></tr>
<tr><td>density inversion</td><td>(6)</td><td>x</td><td>x</td><td>x</td><td>x</td><td>(6)</td><td>x</td><td>x</td><td></td><td>(6)</td><td>x</td></tr>
<tr><td colspan="12">Structural Features</td></tr>
<tr><td>explicit faults</td><td></td><td></td><td></td><td></td><td></td><td>x</td><td>x</td><td></td><td>x</td><td></td><td></td></tr>
<tr><td>explicit karst</td><td></td><td></td><td>x</td><td></td><td>x</td><td></td><td></td><td></td><td></td><td></td><td></td></tr>
<tr><td colspan="12">Input/Output</td></tr>
<tr><td>pre-processor(s)</td><td></td><td></td><td>x</td><td></td><td>x</td><td>x</td><td>x</td><td>x</td><td></td><td></td><td>x</td></tr>
<tr><td>post-processor(s)</td><td></td><td></td><td>x</td><td></td><td>x</td><td>x</td><td>x</td><td>x</td><td></td><td></td><td>x</td></tr>
<tr><td>GUI(s)</td><td>x</td><td></td><td>x</td><td>x</td><td>x</td><td>x</td><td>x</td><td>x</td><td></td><td>x</td><td>x</td></tr>
<tr><td>MODFLOW compatible</td><td></td><td></td><td></td><td></td><td></td><td>x</td><td>x</td><td></td><td>x</td><td></td><td></td></tr>
<tr><td colspan="12">Documentation Publically Available</td></tr>
<tr><td>user manual</td><td>x</td><td rowspan="2">x</td><td>x</td><td rowspan="2">x</td><td rowspan="2">x</td><td rowspan="2">(7)</td><td>x</td><td rowspan="2">x</td><td>x</td><td>x</td><td rowspan="2">x</td></tr>
<tr><td>theory</td><td>x</td><td>x</td><td>x</td><td>x</td><td>x</td></tr>
</table>

Table 2.2.3, continued

Characteristic	CFEST	CODESA-3D	FEFLOW	FEMWATER	HydroGeo-Sphere	MODHMS	SEAWAT	SUTRA	SWI package	SWIFT	TOUGH2
Source Code											
available				x			x	x	x		x
not available	x	x	x		x	x				x	
Availability											
public domain							x	x	x		
commercial	x	x	x	x	x	x				x	x

PCG - preconditioned conjugate gradient
Bi-CGSTAB - biconjugate gradients stabilized
BiCGS - bi-conjugate gradient solver
TFQMR - transpose free quasi-minimal residuals
GRAMRB - minimum residuals
SAMG - algebraic multigrid
GMRES - general minimum residual
(1) Pacific Northwest National Laboratory and Consultants for Environmental System technologies, Inc.
(2) Jointly developed by CRS4 and the University of Padua (Italy)
(3) Developed by the US Army Corps of Engineers and maintained by the EPA Center for Exposure Assessment Modeling
(4) Jointly developed by Groundwater Simulations Group and Hydrogeologic, Inc.
(5) Mark Bakker and Frans Schaars with funding from the Georgia Coastal Incentive Grants Program and Amsterday Water Supply (WaterNet)
(6) Code likely simulations density inversions but that could not be verified
(7) Available only after purchasing the code

Table 2.2.4 Notable Capabilities and Disadvantages Documented in the Literature for the Selected Codes.

Code	Notable Capabilities[(1)]	Disadvantages[(1)]
CFEST	Allows the user to optionally specify parameters that control the logic used when convergences is not obtained; dynamic mesh at water table	Input is structured for several of the input files but unstructured, comma delimited for one of the input files; in some cases, the same input is given in more than one input file so care must be taken in creating the input files
CODESA-3D	Uses fully 3D tetrahedral elements defined automatically from a triangular 2D grid; employs several functional relationships to describe the saturated-unsaturated flow behavior	
FEFLOW	Incorporated and advanced interactive graphical working environment; capable of simulating large density contrasts and large temperature ranges; multi-layer pumping/injection wells accommodated in 3D; dynamic mesh at water table	Not very small and requires substantial computing capabilities, but not necessarily dependent on high-end or super-computing technology
FEMWATER		Has a small user base; variable density function was designed for salinity intrusion in coastal aquifers; “card style” input files
HydroGeoSphere		
MODHMS	In the MODFLOW family	
SEAWAT	Contains the same packages as available with MODFLOW; can control how often the flow field is updated; individuals familiar with MODFLOW and MT3DMS should be able to use SEAWAT with few difficulties; reads and writes standard MOFLOW and MT3DMS datasts, which are easily manipulated with commercially available pre- and post-processors	Does not check for consistency between the MODFLOW and MT3DMS input files; models designed with variable cell volumes are prone to numerical instabilities; transport calculations can only be transient; initial heads and concentrations must be at equilibrium with one another; problems with wetting and drying; problems with conversion from confined to unconfined; problems with drastically different aquifer properties in adjacent zones
SUTRA	Most widely used simulator in the world for seawater intrusion and other variable-density groundwater flow problems based on solute transport or heat transport per Voss (1999); can simulate either dispersed or relatively sharp transition zones between freshwater and saltwater	Coding stresses clarity and modularity rather than efficiency; manual construction and data preparation for meshes is labor intensive unless a GUI is used
SWI package for MODFLOW		
SWIFT-2002		Potentially long runtimes; lots of input
TOUGH2	Includes a tight and visible “version control” system for meeting stringent demands on reliability and referenceability of code applications	

(1) Blank cell indicates no clear documentation was found in the literature.

Code Graphical User Interface

Some users are more comfortable interacting with a code through a graphical user interface (GUI). A graphical user interface is available for all of the selected codes with the exception of CODESA-3D. Most graphical user interfaces and pre- and post-processors available for MODFLOW can be used for SEAWAT, MODHMS, and the SWI package of MODFLOW. FEFLOW and HydroGeoSphere were both developed within an advanced interactive graphical working environment. The Argus ONE graphical user interface is available for SUTRA and CFEST. FEMWATER is supported by the Department of Defense Groundwater Modeling System (GMS) and SWIFT-2002 is supported by Groundwater Vistas. PetraSim provides pre- and post-processing capabilities for the TOUGH2 family of codes.

Code Documentation and Availability

Documentation and availability of the selected codes is summarized in Table 2.2.2. With the exception of MODHMS, the literature search yielded a theory/reference manual and/or user manual/guide for all of the selected codes, even those that are proprietary. MODHMS is proprietary to HydroGeoLogic, Inc., who states on its website that code documentation is provided upon purchase of the code. In general, documentation for the selected codes was thorough. The only exceptions are instances where the selected code is an add-on to another codes, such as the SWI package for MODFLOW, or developed from another code and only the additional capabilities are addressed in the documentation. In these cases, it is necessary to look at the documentation for the original code as well as the specific documentation for the additional or enhanced features. Several versions of SWIFT were found during the literature review. The original theory and implementation manual by Reeves and others (1986) applies to all versions of the code. A copy of that manual was found during the literature search. A user guide was found for SWIFT for Windows (Benegar, 2000) during the literature review as was an online user guide for SWIFT-2002 (Earthward Consulting, 2001).

Four of the codes, FEMWATER, SEAWAT, SUTRA, and the SWI package for MODFLOW, are available to the public at no cost. All of the other selected codes are proprietary and available for purchase. Although FEMWATER and SUTRA are publically available, and the

GMS graphical user interface for FEMWATER and the Argus One graphical user interface for SUTRA must be purchased.

Code Applications

The selection of a code for a specific use will not only consider characteristics of the code but also historical use of the code for similar types of applications. Therefore, the literature review included a search of applications of the selected codes to various simulation scenarios. The search focused on, but was not restricted to, the following applications:

- Seawater intrusion
- Regional brine/solute migration
- Submarine groundwater discharge
- Aquifer storage and recovery
- Simulation of karstic aquifers
- Simulations including faults
- Regional groundwater flow
- Simulations of fractured media

Because of their broad definitions, the use of a code for some applications types may exist but are not explicitly recognized here. For example, it is likely that all of the codes have been applied to a regional groundwater flow scenario and a solute/brine migration scenario although one was not found for every code. Table 2.2.5 summarizes the types of applications found for the selected codes. In the table, a "direct" application is one where a specific code characteristic, such as a conduit flow package for karst, was implemented.

Table 2.2.5 Applications Found for Selected Codes.

Application	CFEST	CODASA-3D	FEFLOW	FEMWATER	HydroGeoSphere	MODHMS	SEAWAT	SUTRA	SWI package	SWIFT	TOUGH2
Seawater Intrusion	x	x	x	x	x	x	x	x	x	x	x
Regional Groundwater Flow	x	x	x		x	x	x	x		x	x
Integrated Surface Water/Groundwater Interaction					x	x					o
Karst Geology	o		x		x			o			
Faulted Geology	o		x		x	x	o			o	x
Fractured Geology			o		x			x		x	x
Submarine Groundwater Discharge			x				x	x		x	
Brine/Solute Migration	x	x	x	x	x	x	x	x		x	x
Aquifer Storage and Recovery	x		x				x	x	x	x	

x = direct application
o = indirect application

During the literature review, a fairly extensive citations list was found for several of the selected codes. Those lists are provided in Appendix B. The list for MODHMS includes references for MODHMS and for MODFLOW-SURFACT, which was the predecessor code for MODHMS.

2.3 Brackish Water Hydrogeology

A review was conducted to gain an understanding of the hydrogeology for brackish water in the state of Texas. This review focused on the brackish groundwater manual for the Texas Regional Water Planning Groups by LBG-Guyton Associates (2003). This manual provides an overview of brackish groundwater in each of the major and minor aquifers in Texas as well as available brackish resources in formations not identified as a major or minor aquifer. The overall purpose of the review was to develop an understanding of the hydrogeology of the brackish water resources in the context of the characteristics a code would need to simulate those resources.

The review focused on the following aquifer characteristics.

- Regional setting
- Primary aquifer material
- Hydrologic units
- Strata geometry
- Structural continuity
- Media type
- Significant structure features
- Heterogeneity
- Cross-formational flow
- Surface water interaction
- Density distribution

The results of the review are briefly described below and summarized in Table 2.3.1.

Regional Setting

The regional setting found for the brackish water resources include basin fill deposits, plain deposits, mountainous, reef complex, Gulf-ward dipping, radially dipping, and flood plain deposits. The aquifers located along the Texas Gulf coast are Gulf-ward dipping while those around the Llano Uplift are radially dipping. The basin fill aquifers are located predominately in west Texas and the floodplain aquifers are located adjacent to major Texas rivers. The flat plain aquifers are located in the Texas panhandle and north-central Texas. Both the mountainous aquifer and the reef complex aquifer are located in far west Texas.

Primary Aquifer Material

The primary aquifer material found for the brackish water resources include alluvial sediments, sandstone, limestone/dolomite, evaporates, and volcanic. The major aquifers in Texas consist predominately of alluvial sediments and limestone.

Hydrologic Units

Aquifers in Texas can consist of either a single hydrologic unit or multiple units. For example, the Ogallala Aquifer consists of a single hydrologic unit while the Trinity Aquifer consists of up to nine units in south central Texas and only one unit in west Texas.

Strata Geometry

The geometry types of strata found for the aquifers includes flat, wedge, bowl, linearly dipping, and radially dipping. In general, the strata is flat for aquifers consisting of plain deposits, bowl shaped for aquifers consisting of basin fill deposits, linearly dipping for aquifers along the Gulf coast and the mountainous aquifers, and radially dipping for aquifers around the Llano Uplift. Only one aquifer, the Hueco-Mesilla Bolson Aquifer, has wedge-shaped strata.

Structural Continuity

Most of the aquifers in Texas are structurally continuous; that is, they are continuously connected both laterally and vertically. Several of the Texas aquifers, however, are laterally discontinuous because they are separated by a structural high or consist of discontinuous individual deposits. Other aquifers are vertically discontinuous in that they consist of multiple subaquifers separated by aquitards or are completely displaced vertically by faults.

Media Type and Structural Features

The media for the majority of Texas aquifers is porous. However, the media in several of the limestone aquifers and the volcanic aquifer is fractured. Solution channels and/or cavities have been identified in most of the aquifers containing limestone and/or evaporate sediments and many of the aquifers are faulted. The sediments in all of the Texas aquifers are heterogeneous to some degree.

Cross-formational Flow

Cross-formational flow within the aquifer and/or vertically or laterally from adjacent aquifers is a significant component of overall groundwater flow for many of the aquifers. Surface water interaction is also significant for most of the aquifers.

Density Distribution

Two of the minor aquifers in Texas are not a source of brackish groundwater. These are the Igneous and Rita Blanca aquifers. Data are insufficient to determine whether the Marathon Aquifer is a significant source of brackish groundwater. The remaining major and minor aquifers in Texas contain brackish groundwater. For these aquifers, the density of the groundwater increases as the salinity increases. The groundwater salinity varies laterally in all of the aquifers containing brackish groundwater. In addition, the groundwater salinity also increases with depth for most of the aquifers. For all of the aquifers that dip toward the Gulf coast, the groundwater salinity also increases downdip. Salinity inversion, that is higher salinity groundwater overlying groundwater with a lower salinity, is found in eight of the Texas aquifers. For several of these aquifers, the inversion is slight and occurs in localized areas. For others, however, the inversion is significant and widespread.

All of the selected codes discussed in Section 2.2 should be able to incorporate the different regional settings, primary aquifer material, hydrostratigraphy, strata geometry, structural continuity, heterogeneity, and cross-formational flow found for the major and minor aquifers in Texas. All of the selected codes will work for the aquifers with porous media and will work if the aquifers with fractured media are modeled as an equivalent porous media. Of the selected codes, only FEFLOW, HydroGeoSphere, SWIFT, and TOUGH2 can explicitly model fractured media.

Surface water can be directly incorporated with MODHMS and HydroGeoSphere, both of which are integrated surface water/groundwater codes. In addition, it is possible to indirectly incorporate surface water through boundary conditions with most of the other selected codes.

Two of the selected codes, FEFLOW and HydroGeoSphere, can explicitly incorporate karst conduits. Faults can be incorporated with MODHMS, SEAWAT, and the SWI package using the MODFLOW horizontal flow barrier package. All of the other selected codes can likely be configured such that faults can be incorporated through gridding and boundary conditions. For heavily faulted aquifers, the grid flexibility available with the finite-element codes may be desirable.

For the majority of the selected codes, density is a function of solute concentration and the initial concentration can be assigned independently for each model grid cell allowing for a heterogeneous initial concentration distribution. The exception is the SWI package for MODFLOW, which models each aquifer, or zone, with a single model layer. With that package, two density distributions are available. The first is the stratified flow option where the density is constant both laterally and vertically in each zone and discontinuous from zone to zone. The second is the variable density flow option where the density varies linearly in the vertical direction in each zone and is continuous from zone to zone.

Density inversion is not allowed with the SWI package for MODFLOW. Examples of the application of the other selected codes to the free convection Elder's problem was found for all of the codes, with the exception of CFEST, MODHMS, and SWIFT. Although an application to a problem with density inversions was not found for CFEST, MODHMS or SWIFT, neither was specific information stating that these codes cannot simulate density inversions.

Table 2.3.1 Summary of Brackish Groundwater Hydrogeology for Texas Major and Minor Aquifers.

Aquifer	Reg. Set.[1]	Prim. Sed. Type[2]	Hydrologic Units		Strata Geometry					Strata Continuity[3]			Media Type		Structure Features[4]		Cross Flow[5]	SW/ GW[6]	Density Distribution[7]			
			single	multiple	flat	wedge	bowl	dipping	radially dipping	cont	dis vert	dis hor	porous	fracture	solution	fault(s)			lateral	depth	downdip	inversion
Major Aquifers																						
Hueco Bolson	BF	ALL	x			x				x			x						x	x		
Mesilla Bolson	BF	ALL	x			x				x			x						x	x		x
Pecos Alluvium	BF	ALL	x				x					x	x				x	x	x	x		x
Ogallala	P	ALL	x		x					x			x				x	x	x			
Seymour	P	ALL	x		x							x	x					x	x			
Edwards-Trinity (Plateau)	FL	LS		x	x					x					x			x	x			x
Edwards (Balcones Fault Zone)	D	LS	x					x		x					x	x		x	x		x	
Trinity	D	S/LS		x				x		x	x					x		x	x	x	x	x
Carrizo-Wilcox	G	S		x				x		x			x				x		x	x	x	x
Gulf Coast	G	S		x				x			x		x				x	x	x	x	x	x
Minor Aquifers																						
Bone Spring-Victorio Peak	BF	LS		x	x					x				x	x			x	x	x		
Igneous	M	VOL		x				x			x			x				x	not source[8]			
West Texas Bolsons	BF	ALL		x	x							x	x				x	x	x			
Rustler	BF	E	x				x					x	x		x	x	x	x	x	x		
Marathon	BF	LS		x						x				x	x		x	x	unknown[9]			
Capitan Reef	R	LS	x							x					x		x		x	x		
Dockum	BF	ALL	x				x			x			x				x	x	x		x	
Rita Blanca	P	LS		x	x						x		x						not sign. source[10]			
Edwards-Trinity (High Plains)	P	SS/LS		x	x						x		x				x		x	x		x

Table 2.3.1, continued

Aquifer	Reg. Set.[1]	Prim. Sed. Type[2]	Hydrologic Units		Strata Geometry					Strata Continuity[3]			Media Type		Structure Features[4]		Cross Flow[5]	SW/ GW[6]	Density Distribution[7]			
			single	multiple	flat	wedge	bowl	dipping	radially dipping	cont	dis vert	dis hor	porous	fracture	solution	fault(s)			lateral	depth	downdip	inversion
Blaine	P	ALL/E	x		x					x					x		x	x	x		x	
Whitehorse-Artesia	P	S/DO	x		x					x			x					x	x		x	
Lipan	P	ALL	x		x					x			x					x	x			
Hickory	RD	SS	x						x			x	x			x	x		x		x	
Ellenburger-San Saba	RD	LS/DO	x						x			x		x	x	x	x		x		x	
Marble Falls	RD	LS	x						x			x		x	x	x	x	x	x		x	
Woodbine	D	SS	x					x		x			x						x	x	x	x
Blossom	D	SS	x					x		x			x						x		x	
Nacatoch	D	S		x				x			x		x			x			x		x	
Queen City-Sparta	G	SS		x				x			x		x						x		x	
Yegua-Jackson	G	S		x				x		x			x						x	x	x	
River Alluviums	F	ALL	x		x					x			x					x	x			

[1] Regional Setting: BF - basin fill, P - plain, FL - flat, D - dipping, G - Gulfward dipping, M - mountainous, R - reef complex, RD - radially dipping, F - floodplain

[2] Primary Sediment Type: ALL - alluvium, E - evaporite, DO - dolomite, LS - limestone, S - sand, SS - sandstone, VOL – volcanic

[3] cont - continuous, dis vert - discontinuous vertically, dis hor - discontinuous horizontally

[4] solution - solution channels/cavities

[5] cross-formational flow

[6] surface water/groundwater interaction

[7] lateral - density varies laterally, depth - density increases with depth, downdip - density increases downdip, inversion - density inversions in aquifer

[8] not a source of brackish water

[9] brackish water resource unknown due to insufficient data

[10] not a significant source of brackish water

2.4 Brackish Water Desalination Feeds

The high total dissolved solids concentration of brackish groundwater may limit its direct use for public supply, irrigation, and manufacturing. The process of desalination, which removes salts, converts brackish groundwater into usable freshwater. Desalination of both surface water and groundwater is a current practice in the State of Texas. A review of the desalination database maintained by the TWDB was conducted in order to identify feed aquifers for desalination facilities that process groundwater. A discussion of the TWDB desalination database can be found in Nicot and others (2006) and Shirazi and Arroyo (2011). Also conducted was a cross reference of the information in that database with data in the TCEQ Public Water Supply database (TCEQ, 2011).

With the exception of the northern Panhandle area, desalination facilities are found throughout the State. The TWDB desalination database identifies 36 desalination facilities in the State that treat groundwater. A cross reference of those facilities with the TCEQ Public Water Supply database identified 24 active facilities that treat groundwater. The TWDB desalination database appears to include all well sources (fresh and brackish) for each public water supply system operating a desalination facility. Therefore, the TCEQ Public Water Supply database was checked to identify which of those well sources are treated via desalination.

Considering both the data in the TWDB desalination database and the data in the TCEQ Public Water Supply database, six major aquifers and two minor aquifers were found to feed desalination facilities. The major aquifers are the Gulf Coast, Carrizo-Wilcox, Trinity, Edwards-Trinity (Plateau), Ogallala, and Hueco-Mesilla Bolsons aquifers and the minor aquifers are the Woodbine and Bone Spring-Victorio aquifers. Three formations located in the Big Bend area of Texas not classified as an aquifer also provide water to desalination facilities. Using the TCEQ Public Water Supply database, approximately 100 wells were identified as sources for the desalination facilities and the number of wells per facility ranged from 1 to about 20. The average range in total dissolved solids concentration found for the wells supplying water to the desalination facilities was about 1,000 to 5,000 mg/L. Table 2.4.1 summarizes the number of desalination facilities and brackish feed wells by aquifer. The data in this table were obtained from the TCEQ Public Water Supply database since that database explicitly identifies well sources treated via desalination.

Table 2.4.1 Aquifer Feeds for Desalination Facilities.

Aquifer	Number of Desalination Facilities	Number of Feed Wells
Major Aquifer		
Gulf Coast	7	34
Carrizo-Wilcox	4	9
Trinity	3	5
Edwards-Trinity (Plateau)	1	4
Ogallala	1	1
Hueco-Mesilla Bolson	3	34
Minor Aquifer		
Woodbine	1	1
Bone Spring-Victorio	1	1
Formations Not Classified as an Aquifer		
Boquillas Formation	1	5
Cretaceous System	1	1
Santa Elena Limestone	1	2

We can see from the table that the Gulf Coast aquifer has the largest number of desalination facilities tapping its brackish water. In Section 5, we provide a modeling approach case study for brackish water production in the Gulf Coast Aquifer.

3.0 Linking Brackish Hydrogeology with Code Characteristics

In the previous section, we discussed the basic characteristics of 11 codes that are capable of simulating the variable density flow that can be important in modeling water resource applications in brackish aquifers. In addition, we summarized the basic hydrogeology of the aquifers that contain the majority of the brackish water resources in Texas.

Providing guidance on code selection requires that those code characteristics that are particularly suitable for given hydrogeologic scenarios be identified. During the literature review, we looked for specific articles that described why codes may have been used for particular modeling problems. Unfortunately, we did not find many examples where authors described the characteristics of codes that drove the code selection process beyond the most general requirements (i.e., the code was capable of simulating a physical process that was inherent in the conceptualization). There are many examples in the variable density literature of codes being validated against test problems, and other codes, but none that we could find that compared the performance of more low-level options, such as solvers.

Given this paucity of directly relevant literature, the general guidance we provide as to what code characteristics will generally work best for particular hydrogeologic scenarios are sometimes based on the experience of the current authors, as well as general modeling guidelines. The structure of this section follows the headings in Table 2.3.1.

Regional Setting and Primary Sedimentation Type

These are not directly relevant to code selection.

Hydrologic Units

All of the considered codes will simulate multiple hydrogeologic units. However, in the context of single layer, unconfined aquifer models, the treatment of the water table (and perhaps unsaturated flow) can be important. For example, SEAWAT suffers from the same poorly executed strategy for dealing with thin saturated thickness and dry cells as MODFLOW. Codes that handle variably saturated flow and those that can dynamically adjust the grid to match the elevation of the water table will perform better under these conditions.

Strata Geometry

The strata geometry is mostly relevant in the choice between finite element and finite difference codes. This is because a finite element grid offers far more flexibility for complex geometries than does the typical block centered finite difference grid. So for some complex geometries, such as bowl or radially dipping geometries, a finite element code may be a better choice if a highly realistic representation is necessary (and the data is available to support it).

Strata Continuity

Horizontal discontinuities are sometimes difficult to model with finite difference codes, such as SEAWAT or MODHMS. The reason for this is because flow is conceptualizated as either horizontal (within a layer) or vertical (between) layers. When a hydrogeologic unit that is represented by a particular layer pinches out horizontally, the layer cannot just be terminated in the middle of the active area, since horizontal communication with the abutting unit (represented by a new layer) would be considered by the model as vertical.

In a typical finite element grid, even when the grid is built using the concept of hydrogeologic layers, communication is element-to-element, without a conceptualization of horizontal or vertical flow. So when horizontal discontinuities are numerous, a finite element approach may prove to be simpler.

Vertical discontinuities typically exist due to the presence of aquitards. All of the codes considered can represent aquitards, either through physical representation or through leakance terms.

Media Type

All of the codes considered in this study simulate porous media flow. Some of the codes can also simulate dual porosity flow, which is represented for fracture/matrix networks where there is no advective flow in the matrix. In addition, some codes simulate dual continuum flow, where both the fracture and matrix continuums can have advective flow.

For brackish water applications, dual porosity can be important when the matrix comprises a significant portion of the storage, especially when the saline concentration in the fracture is different than that in the matrix due to displacement by a either a fresher or more saline fluid (as might happen during production).

In Texas, the potential for dual continuum flow exists in the karst aquifers, such as the Edwards (Balcones Fault Zone). They have historically been modeled as single porosity, equivalent porous media systems, but future applications may consider a different conceptualization.

Structural Features

In general, if the realistic geometry of complex structure features, such as faults or salt domes, needs to be represented in a model, finite element codes will allow a more accurate representation. However, faults as simple conduits or flow barriers can be represented in both finite difference and finite element codes using a permeability contrast.

Solution channels that can make up the primary flow paths in karst systems are best represented discretely using non-darcian flow equations. Some of the codes (e.g., FEFLOW and HydroGeoSphere) allow this representation, and score the highest with respect to these features.

Cross Formational Flow

All of the considered codes will simulate cross-formational flow.

Surface water/Groundwater Interaction

Surface water and groundwater interaction is represented in the codes either rigorously, where surface water flow is simulated, or through boundary conditions, where the surface water system is a head dependent source or sink. Because fully integrating surface water flow adds significant complexity to the modeling task, it would not be recommended as a routine approach for many groundwater modeling problems.

Density Distribution

With only a few exceptions, all of the codes handle density distributions that vary both laterally and vertically. Only the SWI package for MODFLOW will not allow inverted density distributions where the denser fluid lies above the lighter fluid.

4.0 Approach to Code Selection

In the current section, we recommend a general approach for selecting a code based on the basic code characteristics, the hydrogeology of the aquifer that is to be modeled, and a few other factors relevant to the application that might be important. As noted in ASTM D6170-97, "Standard Guide for Selecting a Ground-Water Modeling Code," there are two basic steps in a systematic code-selection process. One step involves defining the requirements for the particular modeling application. The other step involves ranking the various codes according to their ability to meet these requirements.

The systematic decision process is briefly described below in the context of these two basic steps. A more detailed discussion of these descriptions follows in separate subsections.

1. **Define the purpose of the modeling—**In defining requirements for a given modeling project, the modeler must first consider the overall purpose of the modeling exercise. For example, the modeling may be for design, planning, or some combination of both. The purpose is important in defining how accurate a result is required, and thus how potentially complex the model will be. Unnecessary complexity will add effort and cost to a project.

2. **Define essential needs not related to physical processes—**Some essential needs might be specific to the viability of the modeling project but may not be specific physical processes. For example, perhaps integration with an existing model is necessary given project resources. If an existing model is built using MODFLOW, then it might be essential that the variable-density codes be mostly compatible in terms of grid structure or other characteristics. Another potential need is that the code be in the public domain or that it be low-cost for stakeholders.

3. **Define the physical processes that must be simulated—**For the purposes discussed here, we assume that brackish water flow must be simulated. Perhaps the interaction between surface water and groundwater is important, and must be simulated. Change in water quality may also be important, and simulating this process could be a requirement. The modeler must review the hydrogeologic characteristics of the site, develop a site conceptual model, and determine what physical processes are essential for adequate simulation.

4. **Create a decision matrix for ranking the codes by their applicability—**A decision matrix provides a summary of the needs and how well each code meets these needs. A code must meet all of the essential needs in order to be considered. The relative importance of the non-essential needs can be characterized by assigning weighting factors to each. This is a subjective process, but the sum score of the weights allows a straightforward ranking of the codes.

As part of the current work, we developed a simple spreadsheet-based matrix tool that helps the user rank the codes according to essential needs, physical processes, hydrogeologic features, and known applications. The essential needs and physical processes draw primarily from

Table 2.2.3. The ranking by hydrogeologic features, for those not directly linked to physical processes, are based on the guidance in Section 3.0. Finally, the known applications (called “Simulation Scenarios” in the matrix) draw from Table 2.2.5.

Once the selections have been made by the user, the codes are ranked based on a summed weighting scheme. Individual weights for each category for each code are kept in a simple flat database worksheet in the same workbook. We discuss this matrix tool in more detail as we discuss the code selection steps in the following sections.

4.1 Purpose of the Modeling

Defining the purpose of the modeling is the critical first step in not only the code selection process, but also in the overall modeling approach. The modeler must consider the necessary model scale, (i.e., a regional, subregional, or local model). If the model is to be used for planning purposes, it is typically at the regional or subregional scale. If the model is to be used for design purposes, it is typically a local scale model.

The scale of regional models may allow some of the code characteristics that are associated with discrete (e.g., fracture flow) or smaller scale structural features (e.g., salt domes) to be considered non-essential. For local scale models, assumptions such as fractures as equivalent porous media may break down. So the scale of the model can be important in considering code characteristics.

In general, models should be only as complex as they need to be for their purpose. If a 2-D model (slice or radial) will fill the need, then the model will be much easier to build and less computationally intensive. Codes such as SWIFT, with the option for 2-D radial flow, may serve this niche in some cases.

If the purpose of the modeling includes quantitative impacts on specific discharge features, such as springs or streams, code selection should consider both the availability of these features as boundary conditions, and how realistically they are represented, so they can be considered as essential physical processes (see Section 4.3).

4.2 Essential Needs Not Related to Physical Processes

The reality of selecting a code for a particular groundwater model is that many needs are unrelated to the actual physical processes that are to be simulated. Most of the codes that are discussed in this work share the same basic characteristics, and will do an adequate job in simulating most of the hydrogeologic systems that are present in Texas.

One of the needs that has become more important as the field of groundwater modeling has matured is the graphical user interface (GUI). Some modelers are not comfortable working directly with the ASCII files that comprise the typical model inputs. Also, the comfort level of a given modeler with a particular GUI can influence the code selection process.

The cost and licensing of a code can drive selection as well. Although single instances of the proprietary codes are typically not too costly for most users, in cluster environments the number of licenses can multiply quickly, adding tens of thousands of dollars to the cost. A code such as SEAWAT, which is both free to use and to distribute with a finished modeling project, has an advantage in this area.

Often models are built in areas where existing models can be leveraged for update or improvement. In this case, whether the chosen code is directly or somewhat compatible with the code used for the existing model can be important. For example, if a current model has been built with MODFLOW, and a new variable-density model is being developed, then SEAWAT is a natural choice, since its grid and inputs are directly compatible with MODFLOW inputs. Similarly, if the current model is built using a finite element code, then choosing another finite element code for the new model would simplify the conversion, since the grid structure would be more similar.

These essential needs not related to physical processes are selected in the first part of the spreadsheet matrix interface. Some of the needs are very specific as to the code characteristic, such as the direct solver or non-linear method. These are included in case the user has a specific need such as a solver comparison.

4.3 Physical Processes

The physical processes that need to be included in a code are defined during the model conceptualization. Note that all of the codes that are described in this work will simulate variable density (mixed convection) flow, so that choice is inherent in the decision matrix.

Most of the physical processes that would be defined in the conceptualization can be explicitly identified as part of the code characteristic selection process. However, some knowledge of how particular discharge or other boundary features are typically represented in groundwater models is required. For example, none of the codes have an explicit boundary condition for springs. Springs are typically represented with a "drain" boundary condition, which is a head dependent flux boundary that only allows discharge, not recharge.

In the decision matrix tool, the "Physical Processes Related" group contains the hydrogeologic characteristics as well as explicit physical processes that can be simulated with the codes. In addition, it contains a choice of "Simulation Scenarios", examples that have been previously documented in the literature for particular codes. With the decision matrix tool, we included an additional spreadsheet workbook that contains all of the sources on which the physical process related code scores were based (when a source was available). This allows the user to go to that spreadsheet to determine why a particular weight was chosen (or if there is a particular literature source associated with it).

4.4 Decision Matrix Tool

Once the user has selected the essential needs for the modeling effort, in terms of both those related to physical processes and those that are unrelated, activating the "Rank Codes" button produces a ranked matrix of codes in the "Code Ranking" worksheet. The selection code then performs a lookup of scores, based on the combinations of codes/characteristics and codes/physical processes. The scores for individual categories are kept in flat lists in worksheets in the same workbook. The scores vary from -2 to 2, where -2 indicates that a characteristic or physical process is not applicable in a particular code, and 2 indicates that the characteristic is applicable or the physical process is explicitly modeled. A score of zero indicates that the relationship is unknown. A 1 is assigned when a characteristic is partially applicable, or a physical process is simulated, but not as explicitly as with other codes. As noted in the previous section, a separate workbook is provided that shows the weights that are assigned for each code and physical process (or hydrogeologic characteristic), as well as a reference, when available.

A simple sum of the weights for each of the codes decides their rank. The highest ranked code is not necessarily the absolute best code for the application, since the weighting scheme is not customized for each application. However, the top few codes should provide the user with a short list for their selection. A re-analysis of what weights were given for the various characteristics or hydrogeologic scenarios may help the user to refine their final selection.

In the next section, we describe a case study for a particular modeling application, where the modeling approach is described, and the code selection is based on the decision matrix tool.

5.0 Case Study: Brackish Production in Matagorda County

A case study is presented here to illustrate the decision processes involved in selecting the appropriate code or codes for modeling a specific problem related to brackish groundwater. Development of this illustration assumes that the need to construct a numerical model has been established. The discussion is divided into (1) a description of the problem, (2) the brackish groundwater resources, (3) the modeling needs, and (4) the code selection process.

5.1 Problem Description

Two major groups, rice farmers and industry, share limited groundwater resources in Matagorda County, Texas. An assessment of brackish water resources in this county is being conducted for the Coastal Plains Groundwater Conservation District with the purpose of estimating brackish groundwater resources in the county for potential future production. A concern related to the production of brackish groundwater is the potential for contaminating overlying freshwater. The purpose of this case study evaluation is to identify the important modeling needs related to assessing the impact of freshwater contamination due to brackish groundwater production and select the codes that best fit those needs.

Matagorda County is underlain by the Gulf Coast Aquifer system, which consists of, from shallowest to deepest, the Chicot Aquifer, Evangeline Aquifer, Burkeville confining unit, and Jasper Aquifer. Table 5.1.1 summarizes the mean thickness, total formation volume, an assumed porosity, and estimated total groundwater volume of each of these formations. The Gulf Coast Aquifer system dips towards the Texas coast as shown in Figure 5.1.1. Only the Chicot and Evangeline aquifers and the upper portion of the Burkeville confining unit are shown in this figure because they are the only units of the Gulf Coast Aquifer system with relevance to the brackish water resources in the county.

Table 5.1.1 Thickness and Volume for the Aquifers of the Gulf Coast Aquifer System in Matagorda County.

	Formation			
	Chicot	**Evangeline**	**Burkeville**	**Jasper**
Mean Thickness (feet)	1,166	2,795	822	2,136
Aquifer Volume (million AF)	801	1,921	565	1,468
Assumed Porosity	0.25	0.25	0.25	0.25
Estimated Total Groundwater Volume (million AF)	200	480	141	367

AF = acre-feet

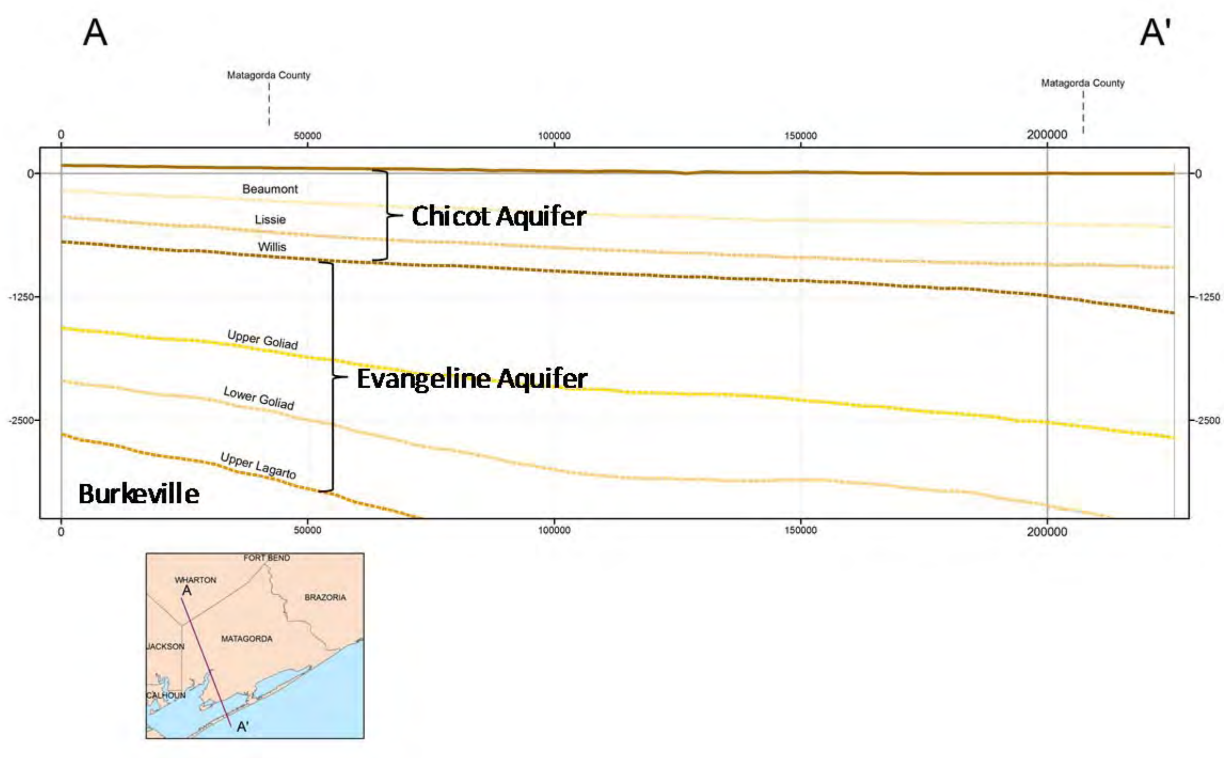


Figure 5.1.1 Northwest to southeast cross-section of the Chicot and Evangeline aquifers and Burkeville confining unit in Matagorda County.

5.2 Brackish Groundwater Resources

Considerations in evaluating the production of brackish groundwater include volume available, the total dissolved solids concentration of the available water, the hydraulic properties of the production zone, the depth to the production zone, and the proximity to existing wells and boundary conditions. The classification of water quality relative to salinity used in developing the distribution of fresh and saline groundwater and calculating the volume of brackish groundwater is shown in Table 5.2.1. The distribution of fresh and brackish water in the Gulf Coast Aquifer system was estimated using total dissolved solids concentration data collected by the Texas Water Development Board and resistivity geophysical log data. That distribution was then used to estimate the available brackish groundwater.

Vertical profiles of water quality were developed at locations with groundwater samples and/or geophysical log data to construct elevation surfaces for the 1,000, 3,000 and 10,000 parts per million total dissolved solid concentration. From those surfaces, the depth to the brackish groundwater zone and the thickness of the brackish groundwater zone were obtained. The depth to the top of the brackish groundwater zone ranges from about 90 to 1,400 feet. The shallower depths are located along the eastern county boundary, in the central portion of the county along the coast, and the southwestern corner of the county. The deepest depths to brackish groundwater are located in the north-central portion and northeast corner of the county. The thickness of the brackish groundwater zone ranges from about 6 to 1,750 feet in the county with the thickness less than 1,000 feet over most of the county.

Table 5.2.1 Salinity Classification.

Classification	Total Dissolved Solids Concentration (ppm)
Freshwater	< 1,000 ppm
Slightly Saline Water	1,000 to 3,000 ppm
Moderately Saline Water	3,000 to 10,000 ppm
Very Saline Water	> 10,000 ppm

ppm = parts per million

Figure 5.2.1 illustrates the formation structure and water quality along the same northwest to southeast cross-section as shown in Figure 5.1.1. This figures shows that the depth of the formations increases toward the Gulf coast while, in general, the depth of the saline water boundaries decreases toward the Gulf coast. Also illustrated is the fact that the thickness of the brackish groundwater zone is less than the thickness of the freshwater and brine groundwater zones over portions of the county.

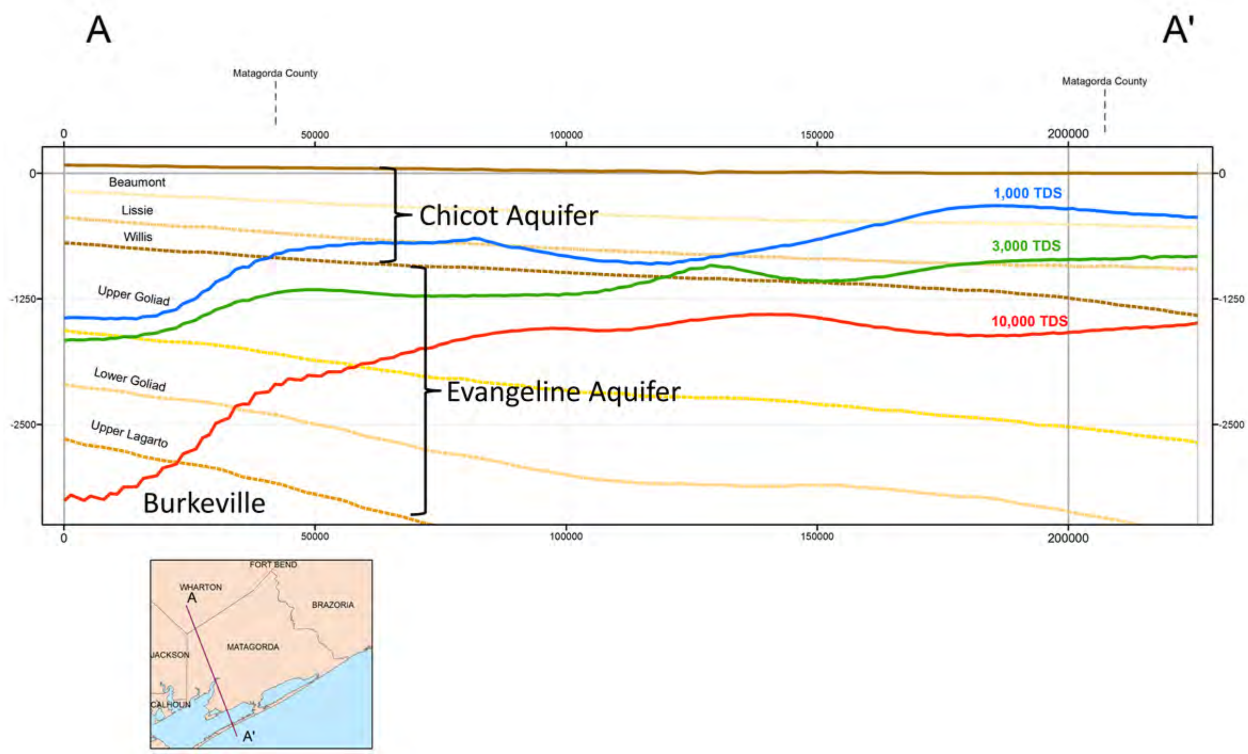


Figure 5.2.1 Northwest to southeast cross-section showing formation structure and water quality zones.

In general, the transmissivity in the portion of the Gulf Coast Aquifer system containing freshwater is higher than the transmissivity in the portion of the aquifer system containing brackish water (Figure 5.2.2). In general, the transmissivity ranges from about 1,500 to 10,000 feet squared per day in the freshwater portion of the aquifer system and ranges from about 500 to 5,000 feet squared per day in the brackish groundwater portion. Therefore, pumping from the upper portion of the less transmissive brackish groundwater zone will likely result in capture from the overlying more transmissive freshwater zone.

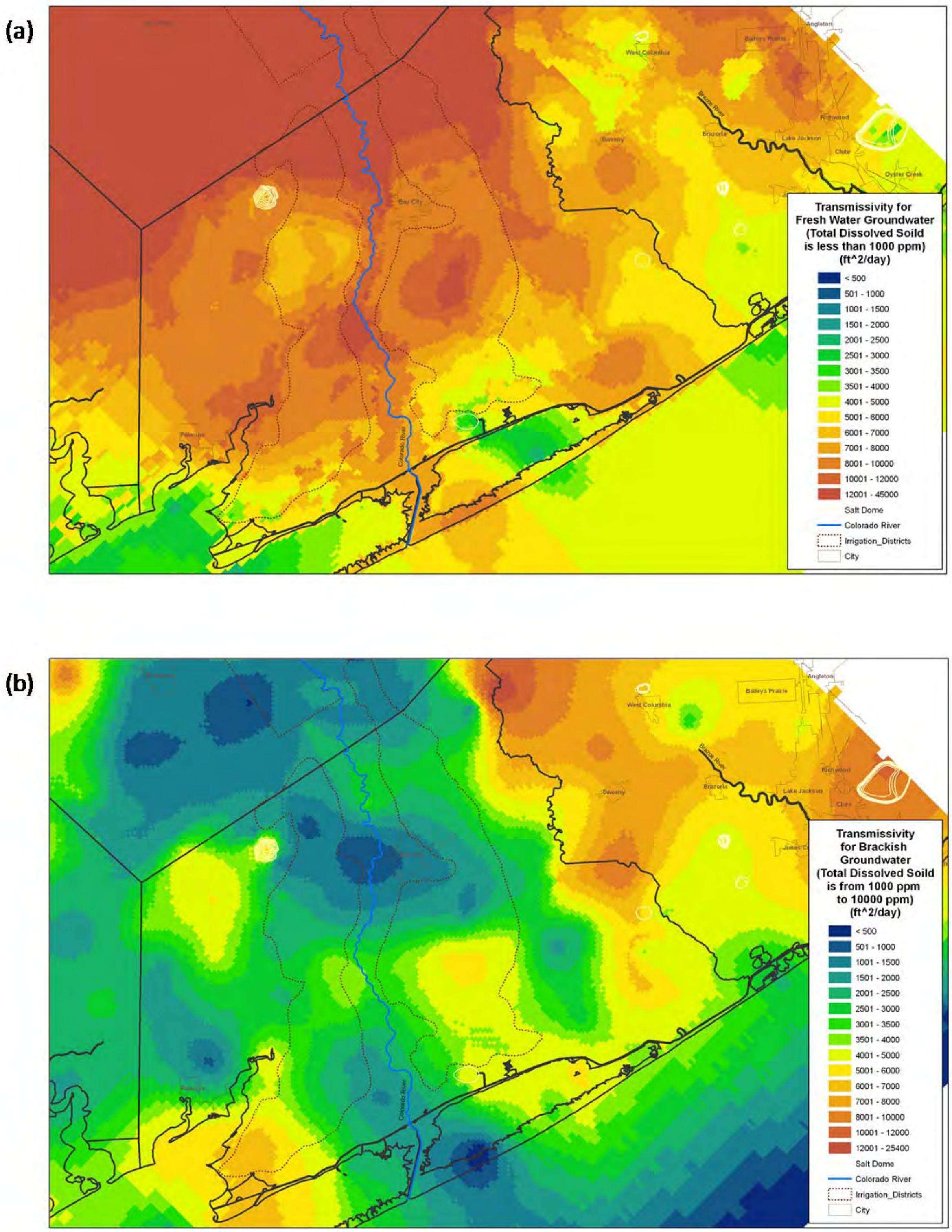


Figure 5.2.2 Transmissivity of the Gulf Coast Aquifer system in the (a) freshwater portion and (b) brackish groundwater portion.

5.3 Modeling Needs

Matagorda County has limited fresh groundwater resources and two large groundwater user groups; rice farmers and industry. An evaluation of total dissolved solids concentrations indicates that the amount of available brackish groundwater is about the same as the amount of available fresh groundwater in the county. Therefore, considering the potential for producing brackish groundwater almost doubles the available groundwater in the county. A major concern with the production of brackish groundwater is the potential for contaminating (i.e., increasing the total dissolved solids concentration) the freshwater portion of the aquifer system. A second consideration is the efficiency of producing brackish groundwater from large depths and from a less transmissive portion of the aquifer system. Numerical modeling is a method for estimating the potential impact of brackish groundwater production and assessing the capability of effectively producing brackish groundwater.

5.3.1 Purpose of the Modeling

This model is considered to be a design model at the scoping level; that is, we are not trying to reach an optimal production rate or set of well characteristics, but rather test the viability of a typical production well in the brackish section under different conditions.

For this test case, a sub-regional rather than a regional groundwater model is recommended since future brackish groundwater production will likely occur in more localized areas within the county. Although Matagorda County is located along the Texas coast, the effects of seawater intrusion are not of concern for this case study because vertical mixing between the overlying freshwater portion of the aquifer system and the underlying brackish portion is the focus of the evaluation rather than horizontal mixing.

Because this is a scoping level modeling effort, we should consider what model simplifications can be made in terms of dimensionality and geometry. A 2-dimensional model could be constructed, either as a vertical slice along dip (e.g., following Figure 5.2.1.), or as a radial model. One drawback to the radial model is that it restricts the code selection considerably, to either SUTRA or SWIFT, and it does not allow any change in structural or concentration elevations along strike or dip.

Whether changes in concentrations and structure should be considered is dependent on the radius of influence of the well, since we would prefer that the extent of the model exceed this radius of influence. Consider a well in a confined section, producing 500 gpm with a transmissivity of 2000 ft^2/d (a middle range value, based on Figure 5.2.2b), and a storativity of $1x10^{-4}$. Using the Cooper-Jacobs equation, we can estimate the drawdown after one year of pumping (this neglects vertical pressure support and so the radius of influence will be overestimated somewhat).

At the well (1 ft radius), the drawdown is about 90 ft. If we take the radius of influence to be the point at which the drawdown is 10% of the drawdown at the well then the distance is about 40,000 ft. Because this is a significant distance relative to the size of Matagorda County, we recommend that structure and concentration change would need to be considered in the model. Therefore, a 2-D radial model is not recommended.

A 2-D dip section model could include the spatial variation in structural elevations and concentration along the major structural axis. However, a production well is difficult to conceptualize in a 2-D vertical section. The no-flow boundaries that are inherent to the 2-D section on either side of the well along strike force a conceptualization of either an infinite series of image wells on either side of the production well, or a line sink (i.e., an infinite horizontal well along strike). Neither of these conceptualizations is realistic. For this case, a 3-D model with an extent that is larger than the approximate radius of influence of the well is recommended.

5.3.2 Essential Needs Not Related to Physical Processes

We are comfortable with or without GUIs for this case. Cost and licensing are not a concern for this case, since the model will not likely be run in a cluster environment. We do not need to recompile the code, so the source code need not be available.

There is an existing MODFLOW model in the region, from which some structure and/or physical properties may be assigned, so a code with a finite difference formulation is preferred. We do not have a preference for a particular solver approach.

5.3.3 Needs Related to Physical Processes and Hydrogeology

Because this is a classic mixed-convection system, with significant concentration changes over short vertical distances, we recommend that variable density be considered in the modeling effort. Once the model is constructed, the impacts of variable density can be assessed in a series of initial sensitivity runs. If buoyancy effects are small, then variable density can be ignored for the remainder of the simulations, likely improving run times.

The structural setting of the model consists of geologic units that dip toward the Gulf of Mexico. There are no structural features (e.g., faults or salt domes) that need to be incorporated in the model. Pumping of brackish water is assumed to occur at or near the top of the brackish groundwater zone. Because pumpage will be the only stress in the model and the brackish groundwater lies at depth, detailed representation of the water table is not required.

Hydraulic conductivity varies both laterally and vertically. The transmissivity of the freshwater portion of the aquifer system is two to three times higher than that of the brackish portion. The density distribution as a function of total dissolved solids concentration varies both laterally and vertically with no density inversions. Because the concentration of the produced water is of interest, we need the code to do full solute transport. Interaction with surface water is not a concern for this case study nor is flow through the unsaturated zone. The portion of the aquifer system considered by the model is confined and the media type is porous. Boundary conditions for the model will be Dirichlet (constant head) at the lateral boundaries and Neumann (fixed flux) representing pumpage. The primary model needs are summarized in Table 5.3.1.

Table 5.3.1 Primary Model Needs for the Case Study.

Parameter	Type
Numerical Formulation	Finite Difference
Coordinate System	Cartesian (3-D)
Solver Type	No Preference
Aquifer Type	Confined
Media Type	Porous
Saturation	Saturated
Solute Transport	Yes
Structural Features	No Preference
Boundary Conditions	Dirichlet (fixed head), Neumann (fixed flux)
Hydraulic Properties	Heterogeneous
Surface water/groundwater interaction	No Preference
Density Distribution	Variable both laterally and vertically

5.4 Code Selection

Having defined the needs for the code selection process, we can use the decision matrix tool to help guide our code selection. Figures 5.4.1 and 5.4.2 show the characteristic selection worksheets and the code rankings from the selection process.

Based on the selected characteristics, the three codes with the highest ranking are MODHMS, SEAWAT, and SWIFT-2002. Of these three, MODHMS and SEAWAT are preferred over SWIFT-2002, just based on the familiarity of the modelers with those two codes. MODHMS has a reputation for having better solvers than SEAWAT for flow problems, but we are not familiar with the solver differences for variable density transport problems. We would recommend starting with a SEAWAT-based model, with the option of trying MODHMS if there are convergence or stability problems.

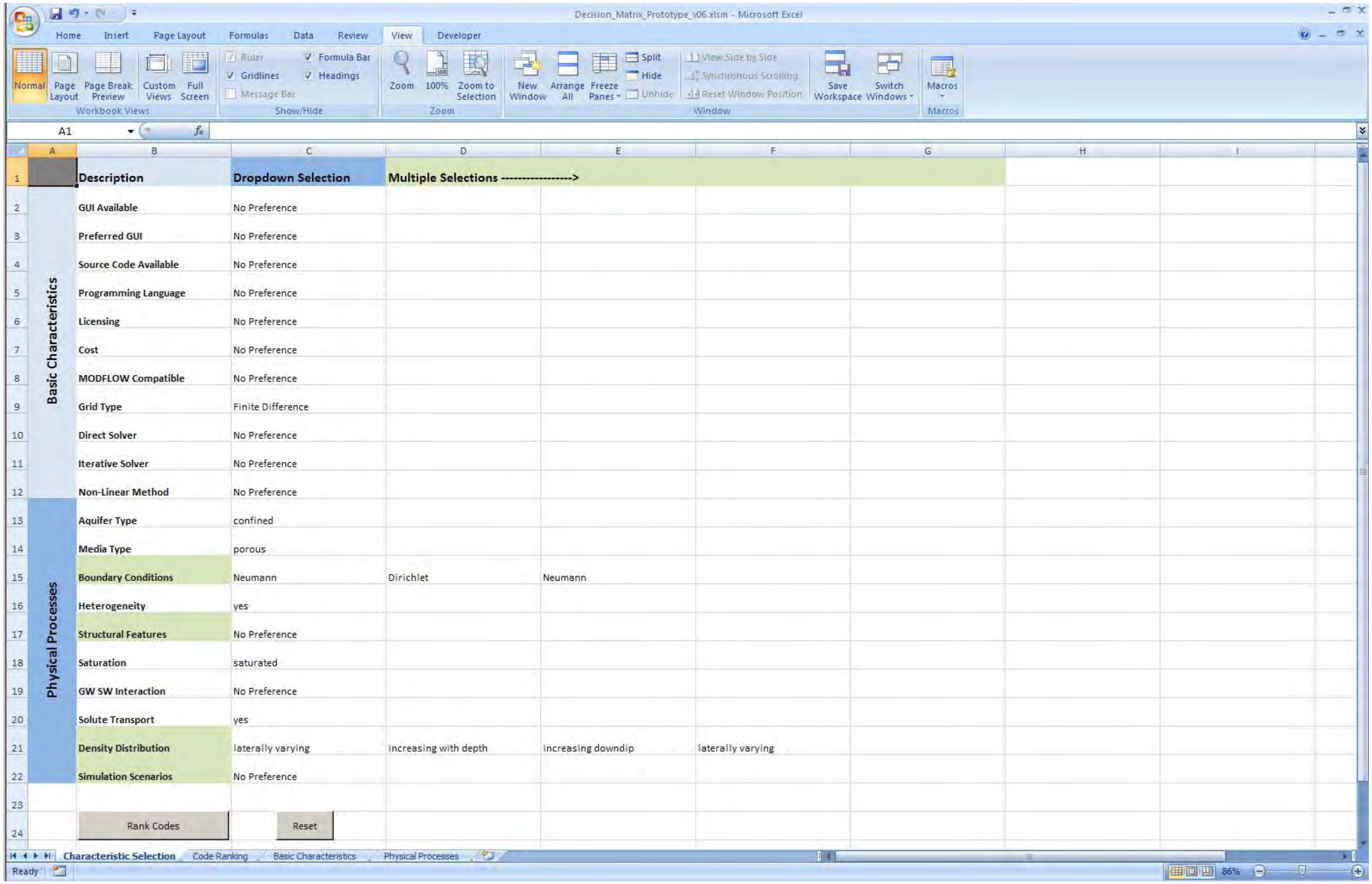
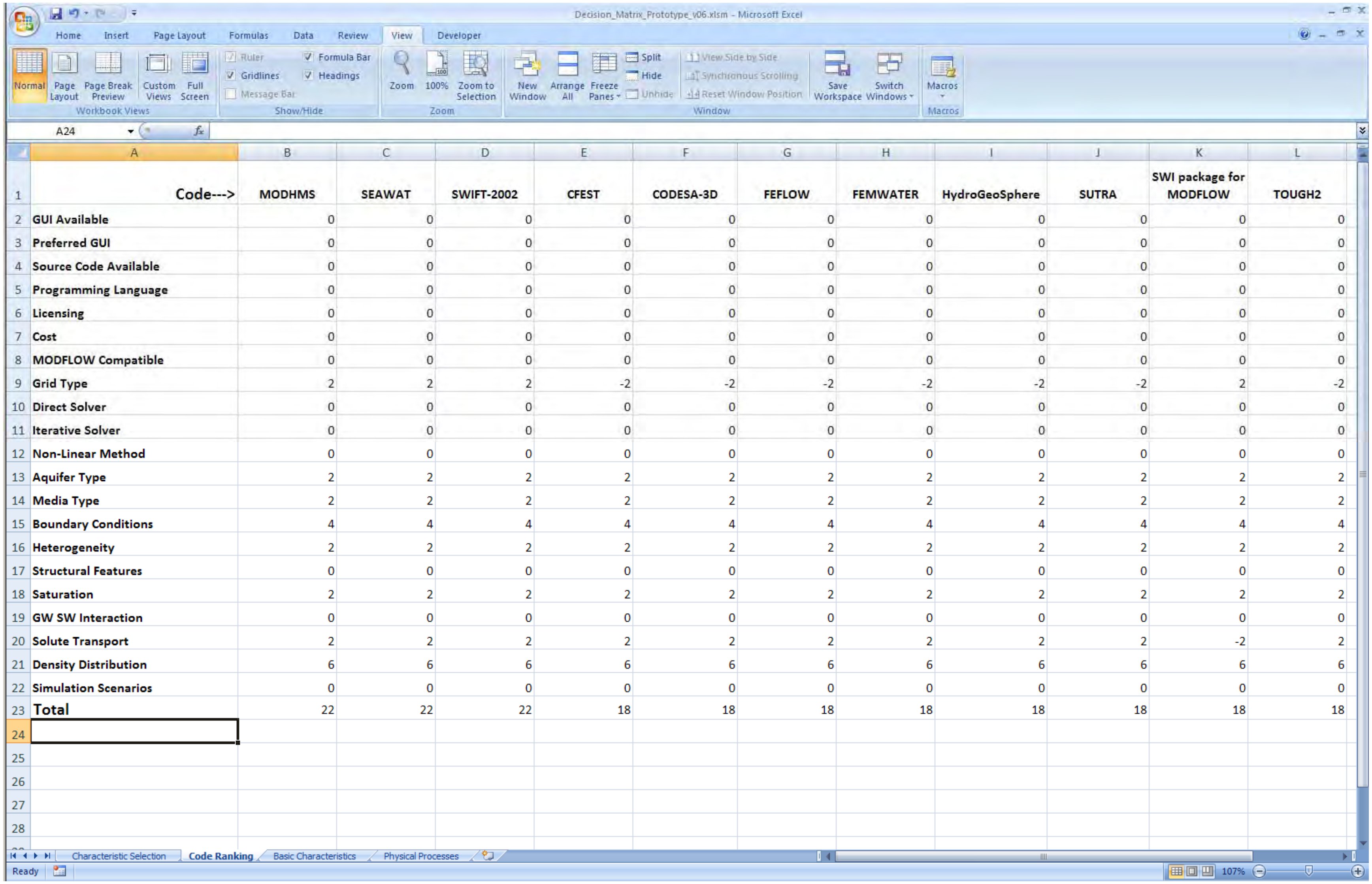


Figure 5.4.1 Characteristic selection worksheet for the case study.



Code--->	MODHMS	SEAWAT	SWIFT-2002	CFEST	CODESA-3D	FEFLOW	FEMWATER	HydroGeoSphere	SUTRA	SWI package for MODFLOW	TOUGH2
GUI Available	0	0	0	0	0	0	0	0	0	0	0
Preferred GUI	0	0	0	0	0	0	0	0	0	0	0
Source Code Available	0	0	0	0	0	0	0	0	0	0	0
Programming Language	0	0	0	0	0	0	0	0	0	0	0
Licensing	0	0	0	0	0	0	0	0	0	0	0
Cost	0	0	0	0	0	0	0	0	0	0	0
MODFLOW Compatible	0	0	0	0	0	0	0	0	0	0	0
Grid Type	2	2	2	-2	-2	-2	-2	-2	-2	2	-2
Direct Solver	0	0	0	0	0	0	0	0	0	0	0
Iterative Solver	0	0	0	0	0	0	0	0	0	0	0
Non-Linear Method	0	0	0	0	0	0	0	0	0	0	0
Aquifer Type	2	2	2	2	2	2	2	2	2	2	2
Media Type	2	2	2	2	2	2	2	2	2	2	2
Boundary Conditions	4	4	4	4	4	4	4	4	4	4	4
Heterogeneity	2	2	2	2	2	2	2	2	2	2	2
Structural Features	0	0	0	0	0	0	0	0	0	0	0
Saturation	2	2	2	2	2	2	2	2	2	2	2
GW SW Interaction	0	0	0	0	0	0	0	0	0	0	0
Solute Transport	2	2	2	2	2	2	2	2	2	-2	2
Density Distribution	6	6	6	6	6	6	6	6	6	6	6
Simulation Scenarios	0	0	0	0	0	0	0	0	0	0	0
Total	22	22	22	18	18	18	18	18	18	18	18

Figure 5.4.2 Code ranking worksheet for the case study.

6.0 Summary and Conclusions

Under the Brackish Resources Aquifer Characterization System (BRACS) program, INTERA was contracted by the TWDB to help provide guidance for selecting appropriate groundwater codes for simulating brackish aquifers, including variable density effects.

We performed a literature review to assess typical brackish water applications, which are typically mixed-convection systems. In addition, the literature review included determining what groundwater codes are capable of simulating brackish water hydrogeology, and what the various characteristics of the codes are. We narrowed the list of codes to be reviewed by considering the quality of the documentation, how recently they were developed, and an indication of their userbase based on occurrence in the literature. The selected codes were CFEST, CODESA-3D, FEFLOW, FEMWATER, HydroGeoSphere, MODHMS, SEAWAT, SUTRA, SWI package for MODFLOW, SWIFT-2002, and TOUGH2. Both finite element and finite difference codes are represented in the list. The codes as a group are far more similar than different in terms of their characteristics.

We performed a high-level summary of the hydrogeologic features of the brackish water aquifers in Texas. This included a summary of the aquifers that serve as sources of desalination feeds in Texas.

We then provided analysis on how the characteristics of the various codes could affect the suitability of a code for each type of hydrogeologic feature. We developed a simple code selection procedure based on ASTM D6170-97, which includes defining the purpose of the modeling, identifying needs not associated with physical processes, identifying important physical processes that need to be simulated, and developing a selection procedure.

A spreadsheet-based decision matrix was developed to inform the selection procedure. The user selects those code characteristics that are identified as needs, as well as those physical processes and hydrogeologic characteristics that are relevant to the modeling effort. The codes are then ranked by their summed scores for each of the characteristics and physical processes. A case study regarding selecting a code for modeling brackish water production in Matagorda County provides an example of using the code selection process.

With the background information provided in this work, and the straightforward code ranking approach, a modeler should be able to make an informed decision about choosing a code for brackish water resources problems.

7.0 Acknowledgements

The authors acknowledge Mr. John Meyer as the TWDB technical lead and the contributions made by two groundwater conservations districts. The Coastal Plains Groundwater Conservation District provided financial support and the information used in the case study. The Post Oak Savannah Groundwater Conservation District contributed financial support. Both groundwater conservation districts supported this study to help develop reliable methods for predicting the impacts of pumping brackish water on the supply of fresh water and of pumping freshwater on the location of the interface zone between freshwater and brackish water.

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APPENDIX A

Code Overviews

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APPENDIX A
CODE OVERVIEWS

During the literature review, a website providing an overview of the code was found for all of the selected codes. Those overviews vary in detail and content, with the sites for the publically available codes typically providing some specific detial and the sites for some of the commercially available codes typically providing more of a marketing document. Several versions of SWIFT are available. An overview was found for SWIFT-2002, SWIFT for Windows, and SWIFT-98. This appendix contains a copy of the code overviews found during the literature review.

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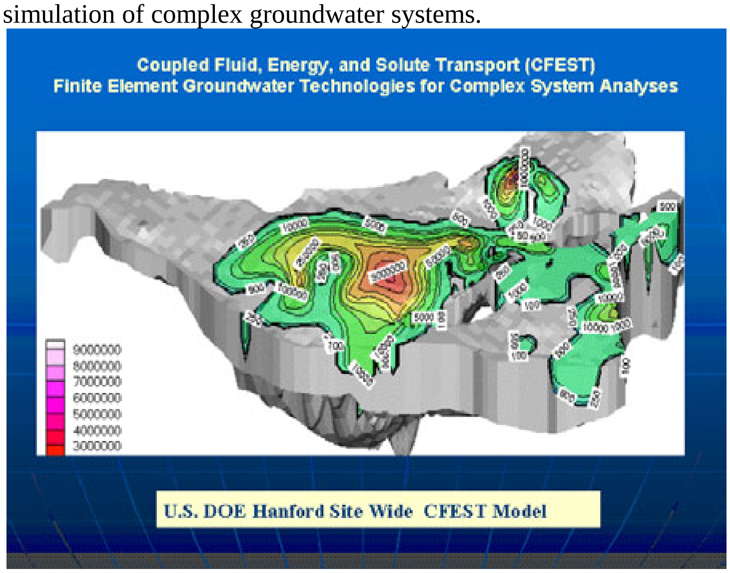
Coupled Fluid, Energy, and Solute Transport (CFEST)

CFEST groundwater flow and transport code is a 3D finite element technology for simulation of complex groundwater systems.

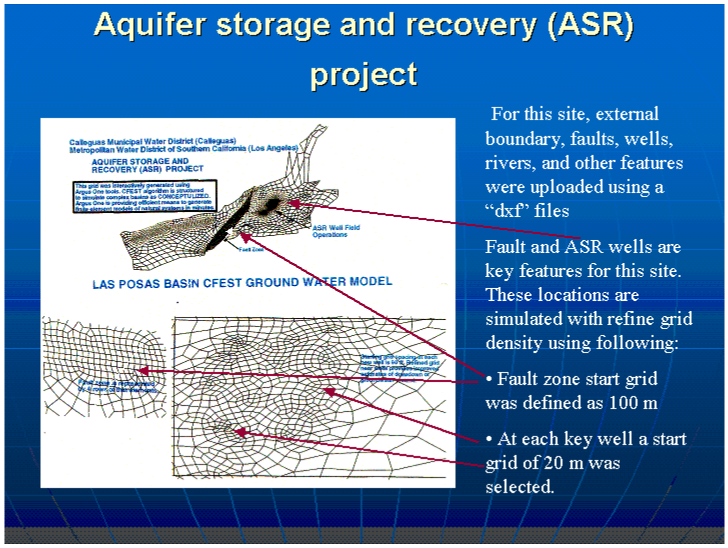


CFEST code applications include complex federal projects (DOE, EPA, DOD) and other projects.

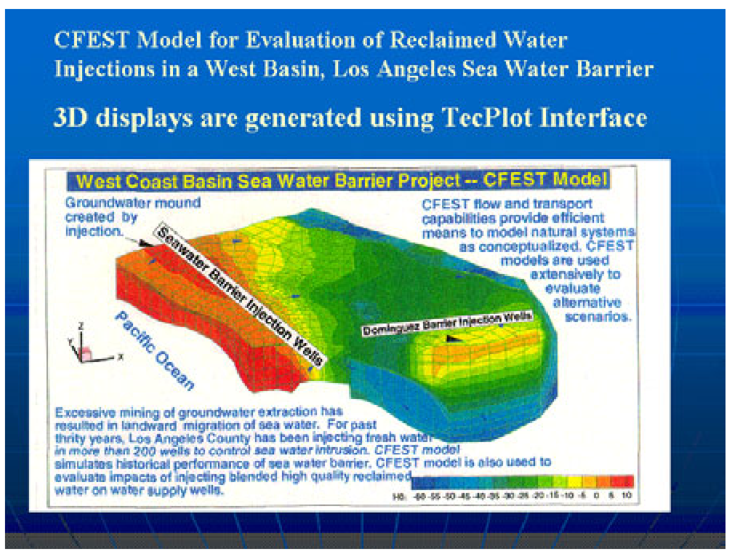
PARTIAL LIST OF FIELD APPLICATIONS OF CFEST TOOLS

DOE -Hanford Site Richland, WA	EPA Aerojet Superfund Site, Sacramento, CA
DOE -Lawrence Livermore Laboratory, CA	EPA -Long Island Reservoir, New York, NY
DOD- El Toro Marine Base, CA	Regional effluent disposal facilities, Florida
EPA -170 square mile San Gabriel Basin, CA	West Basin Sea-Water Intrusion Evaluation, CA
EPA –Sixty million gallon acid disposal pit, CA	50 million gallon/day effluent disposal site, CA
EPA –Abandoned Iron Mountain Mine ,CA	DOE- Nuclear waste repository assessments, TX

CFEST is interfaced with Argus One (http://www.argusint.com/). Complex system grids are generated interactively in hours. User can define external boundaries, wells, faults, rivers, recharge basins, and other features interactively or by importing ESRI shape files or Autocad "dxf" files. Starting size of grid at wells, faults, rivers, and other key features are inserted by clicking the given feature.

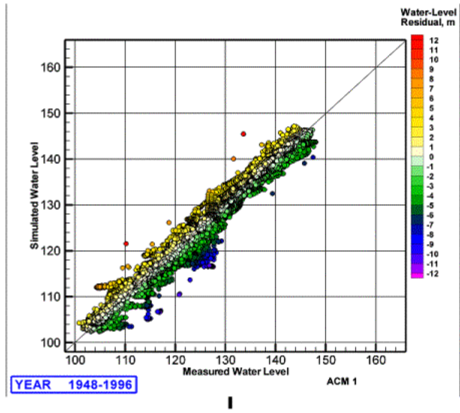


CFEST tools are also interfaced with state of the art plotting programs like TecPlot (http://www.amtec.com/ and EVS (Environmental Visualization System) (http://www.ctech.com//).



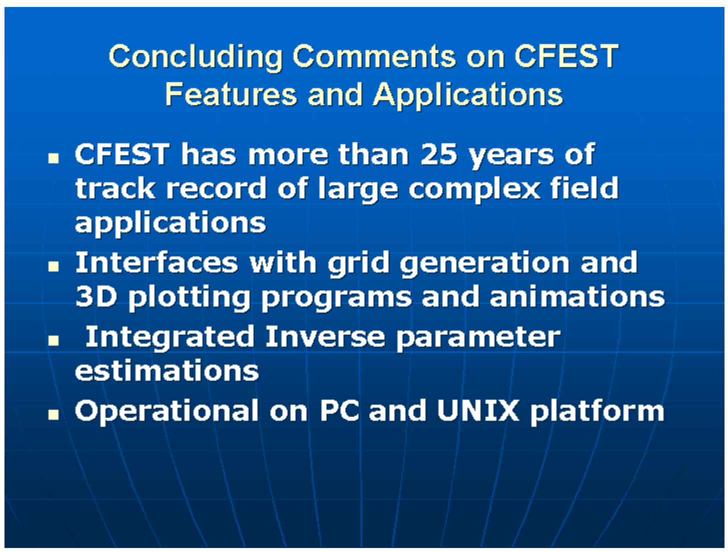
CFEST-UCODE tool provide inverse parameter estimation.

U.S. DOE Hanford WA CFEST-UCODE Inverse Parameter Estimation



Approximately 450,000 water level measurements were used to for inverse hydrologic parameters (e.g. K, Ss, surface recharge, boundary recharge and more) estimations.

Figure in left frame represent match between field measurement and simulated results.



A quick browsing of 3-D models and field application slides provides additional information CFEST groundwater flow and transport technologies.

Phone: (949) 724 1696 Fax: (949) 724 1695 Email: skg@cfest.com

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ACTIVITY:CODESA-3D

CODESA-3D hydrogeological model

CODESA-3D is the hydrogeological computational service of the AQUAGRID application of the GRIDA3 problem solving platform. References to the other GRIDA3 services either to be put upstream in a computational pipeline (e.g. EIAGRID-geophysical imaging) or downstram (e.g. BONGRID-remediation technologies) or both (AGISGRID-distribited GIS) to the AQUAGRID application are also provided here as a means to create a *chain of GRID services* by workflow composition.

Introduction

CODESA-3D is a fully-distributed physically-based hydrogeological model. CODESA-3D acronym stands for COupled DEnsity-dependent variably SAturated flow and miscible transport 3D model [G. Gambolati et al., 1999; G. Lecca, 2000]. The flow module considers the case of variably saturated porous medium, applicable both to the unsaturated (soil) and the saturated (groundwater) zone. The transport module assumes the complete mixing between freshwater and saltwater bodies giving rise to a variably dense filtrating fluid with a non-reacting solute (salt). CODESA-3D is a three-dimensional finite element simulator for groundwater flow and solute transport in variably saturated porous media on unstructured domains. The flow and solute transport processes are coupled through the variable density of the filtrating mixture made of water and dissolved matter (salt, pollutants). The flow module simulates the water movement in the porous medium, taking into account different forcing inputs: infiltration/evaporation, recharge/discharge, withdrawal/injection, etc., while the transport module computes the migration of the salty plume due to advection and diffusion processes. Model parameters and system excitations are assumed variable in space and/or time.

Typical applications of the model are so-called **density-dependent problems** in subsurface hydrology; in particular the model has been applied to the saltwater intrusion problem of coastal aquifer. Denser-than-water non-aqueous phase liquids (DNAPLs), such as chlorinated organic contaminants, are other examples of density-dependent contaminants, which can be modeled with CODESA-3D.

Recently the code has been coupled with a genetic algorithm to compute optimal pumping volumes for an hypothetical aquifer under constraints by SWIMED project partners [Qahman et al., 2005].

CODESA-3D computer code can be obtained from CRS4 (Italy) through a license agreement for research purposes only.

CODESA-3D highlights

- Short course on CODESA-3D hydrogeological model delivered at the Summer School on Advanced Numerical Modeling of Flow and Transport in Soils and Aquifers of the University of Siena (Italy).
- CODESA-3D manual, catalogued as CRS4-Technical-Report, 2000.

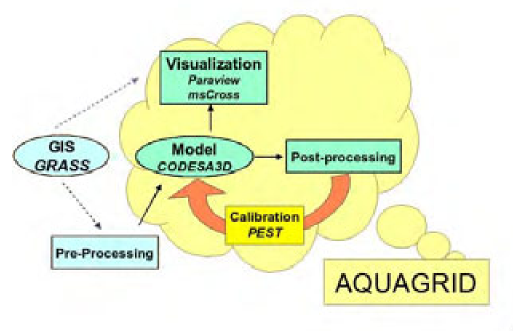
- CODESA-3D model output featuring as the image of the week (21 March, 2007) of the US NSF magazine “International Science Grid This Week”;
- CODESA-3D is one of the Grid services, based on gLite Grid middleware, of the Grid Infn Laboratory for Dissemination Activities (GILDA) testbed.
- CODESA-3D is one of the Grid application services, based on gLite Grid middleware, of the CyberSAR compute portal.

Software Usage Mode

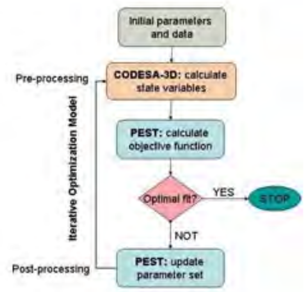
A general description of CODESA-3D input and output dataset is provided here to present a typical user application.

CODESA-3D automatic calibration using PEST

Generally speaking, calibration of a model requires that a suitable method of spatial parameter characterization be defined in order to adjust model parameters until model outputs correspond well to specific laboratory and/or field measurements of the system which is simulated. In particular, for groundwater models the adjustable parameters are usually given by main hydrogeological properties (e.g. hydraulic permeability) and/or system excitations (e.g. abstraction volumes) while control data are represented by piezometric heads and/or salt concentrations measured in the field. Model calibration is a complex task. To perform it for a 3D fully-distributed physically-based hydrological model we need to build up an iterative chain of interdependent software tools and data (**application workflow**, see Figure 4) through the interdisciplinary expertise of GIS experts, modelers and hydrogeologists.



PEST is a nonlinear model-independent parameter estimation package that can be used to estimate parameters for any existing model even if the user do not have the model source code. PEST is currently being used in many field of science and engineering and it has become a groundwater industry standard. Indeed some of the most popular computer codes like SWAT, MODFLOW, MT3D, GMS, etc, use it to implement automatic calibration modules. PEST adjust model parameters in order to reduce to a minimum the discrepancy between model-generated outputs and the corresponding field measurements. The computer code does it taking the control of the embedded model and running it as many times as is necessary in order to determine the optimal set of model parameters in a weighted least square sense. For linear models the algorithm can give the optimal parameter set just in one iteration while for nonlinear models (CODESA-3D falls under this category) parameter estimation is an iterative process. At each iteration step the relationship between selected model parameters (inputs) and model-generated observations (outputs) is linearized by means of the Taylor expansion about the actual best parameter set, hence the derivatives of all outputs with respect to all parameters are calculated. Then the linearized problem is solved for a better parameter set and this set is tested by a new model run. The iterative procedure is stopped when the objective function, generally speaking the sum of squared deviations between model outputs and field measures, reduces to a minimum corresponding to a user-defined threshold.

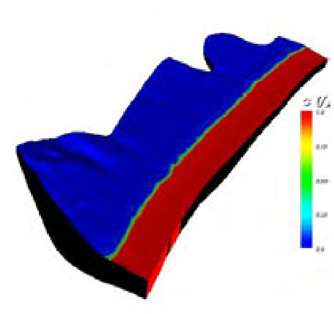


As the calibration process proceeds, PEST continuously records the sensitivity of each adjustable parameter to the observation dataset which is available for user inspection. Trough this information the modeler can discover those parameters that influence mostly the calibration and those that are practically not relevant to it. In addition at the end of the process, PEST writes a large amount of useful auxiliary data (parameter correlation coefficient matrix, parameter covariance matrix etc.). All this information helps a lot the modeler to refine the conceptual model of the system under study, to exploit available data and to efficiently plan future campaign of data acquisition. Besides the traditional way of using PEST in performing parameter estimation (model calibration), predictive analysis mode determines the maximum/minimum model predictions while still maintaining the model calibrated below a user-defined threshold. This mode allows the user to assess upper and lower bounds of the uncertainty interval associated with model predictions, which is definitely the true added value of any modeling analysis.

The optimization model is represented by the **integrated system, shown in Figure 5**, between executables (models and tools) and datasets performing an iterative calibration process. In particular, CODESA-3D outputs feed a post-processor that extracts pertinent data from large model files and put them into smaller text files for easier PEST access. Hence PEST computes the objective function and, if required, calculates the next optimal parameter set. PEST outputs are written in a small file which in turn is pre-processed to generate appropriate CODESA-3D input files. This process results in a single batch job made of a chain of 3 executables in succession ("composite model").

Visualization

Visualization of CODESA-3D model output is based on *open source* computer programs. Today it is currently performed (**see Figure 6** showing the salt relative concentration map plotted on top of the 3D aquifer geometry) by means of the parallel visualization application ParaView using batch scripts. Further developments will be based on Web-GIS technologies by means of the:



- MapServer development environment,
- GRASS open source GIS,
- mscross library, developed at CRS4.

The visualization of the CODESA-3D input and output dataset has common activities with the related GRIDA3 GIS application service AGISGRID.

References

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- Qahman K. et al. Optimal and sustainable extraction of groundwater in coastal aquifers Stochastic Environmental Research and Risk Assessment © Springer-Verlag 2005, doi 10.1007/s00477-004-0218-0

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Editorial

FEFLOW in a Generational Change

Prof. Hans-Jörg G. Diersch
Director of GMC

This issue of DHI-WASY Aktuell exclusively focuses on FEFLOW, our finite-element simulation system for 3D and 2D flow, mass and heat transport in porous and fractured media. We are announcing the beginning of a new generation of FEFLOW, called ***FEFLOW 6****. It delivers a compelling advancement in what modelers in the field of groundwater and porous media have, until now, only envisioned – best-in-class simulation capabilities assembled into a comprehensive and flexible simulation environment. FEFLOW 6 is a notable milestone in FEFLOW's 30-year history. FEFLOW was born in 1979 as a fragile and modest child, made its first steps in an academic well-sheltered kindergarten, grew continuously and became autonomous and successful in business. It was a development that required many hands and contributions. However, the advancements of FEFLOW notwithstanding, the journey is not (perhaps will never be) complete. To address the modeling challenges on the horizon, DHI-WASY will continue to reinvest in development and research and to explore new technologies for FEFLOW. In providing FEFLOW 6, we feel suitably prepared to cope with the future challenges in subsurface and porous media modeling. The future begins now.*

Content

FEFLOW 6

A New Working Environment

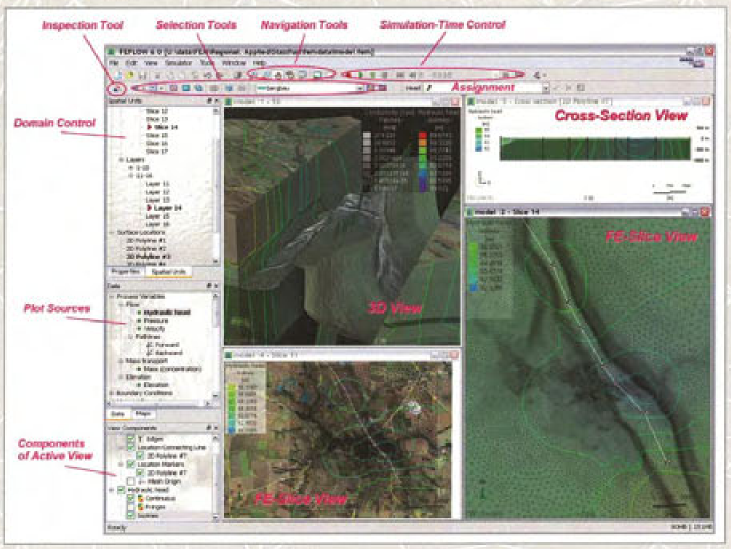


Fig. 1: The FEFLOW 6 user interface with multiple simultaneous views of the model

Volker Clausnitzer

One, perhaps the essential, motivation for the development of FEFLOW has been to facilitate efficient iterations of the modeling cycle from model set-up to simulation to visual and quantitative output of the results. It is probably fair to say that, in the process, FEFLOW pioneered the fully integrated graphical user interface for subsurface modeling software. Over the course of three decades, its computation capabilities have evolved to allow successful application to an increasing variety of problems. This is true in terms of physical processes as well as concerning the spatial and temporal scales, now spanning a range from millimeters to several hundred kilometers, and from fractions of a second to thousands of years, respectively.

Along the way, a persisting tenet has been to "keep the simulation honest" between input and output: Given a particular discretization, an oscillating solution may just be a mathematical consequence and will in such a case indeed be shown, foregoing any hidden internal fudging (really, changing) of user-specified input or intermediate results aimed at "nice-looking" results. While well-defined smoothing methods are available in FEFLOW, they are subject to user control and never invoked by default. This still applies fully to the most recent release, FEFLOW 6. Utilizing current GUI toolkit and graphics technology, FEFLOW 6 does however represent a break with the FEFLOW appearance that has become familiar to many users over the years. The likely most striking contrast in the user interface reflects the change away from a strictly hierarchical menu structure implying a serial workflow with a comparatively fixed sequence of operations. Instead, the new design keeps all functionality accessible whenever possible to ensure maximum flexibility and efficiency for the user.

Essentially, FEFLOW 6 gives the modeler more degrees of freedom together with the accompanying means of control. Figure 1 shows an example layout of the user interface with the basic toolbars (labeled on top), the key control panels (labeled on the left), and a set of views showing different aspects of the current state of the model. The docking feature of toolbars and panels makes the user interface truly customizable.

Another, less apparent yet fundamental change with respect to all previous FEFLOW versions is found in the workflow philosophy itself: the selection process has been completely separated from any assignment (or other model-modifying) operation. Specifically, element or node selections can be created by using any one, or a combination, of the available selection tools, including various mouse tools and intersection of map polygons. At any time, the current (volatile) selection can be made persistent (internally stored) for later use. All assignments or modifications are automatically directed at the current selection of nodes or elements. Changes in the model state due to user input or simulation progress are immediately reflected by all open views in which the respective parameter has been activated for plotting.

Besides a **Supermesh view** for supermesh design, there are three types of view window for finite-element problems:

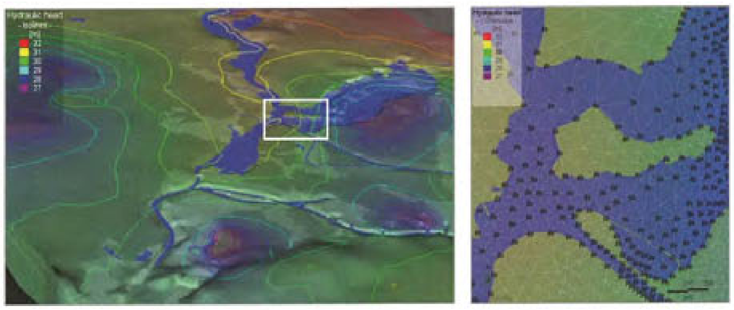


Fig. 2: Surface-water bodies and their representation as map and boundary conditions

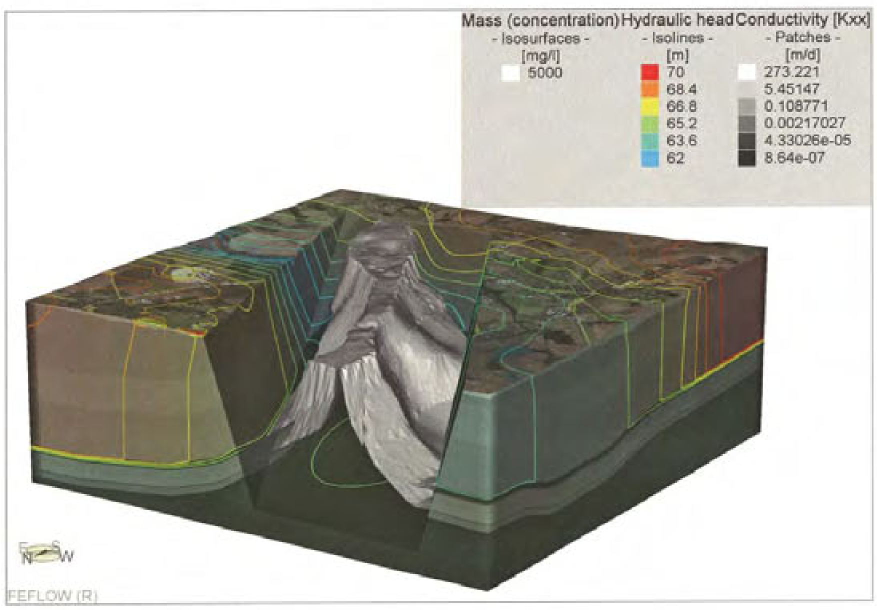


Fig. 3: A combination of data plots on a partially carved-out model domain (salt diapir in a sedimentary basin, 5x vertical exaggeration)

- **FE-slice view**, showing a 2D representation of a particular slice of the FE-mesh (a more flexible version of the main working area known from previous versions)
- **Cross-section view** for vertical, multi-segmented cross-sections of three-dimensional FE-problems
- **3D view** for three-dimensional FE-problems

The new capability of multiple simultaneous views of the same problem will benefit both model set-up and visualization of results. For example, several views of the vicinity of a cross-sectional line are shown in Figure 1, together with a view of the corresponding vertical cross section itself. Figure 2 presents plots of surface water bodies as surface maps in 3D and 2D views, the latter also showing a representation of the associated boundary conditions. While view-related memory is dynamically released whenever appropriate, a practical limit on the number of simultaneous views possible will be imposed by the available RAM on a given workstation.

Full mouse- and panel-controlled navigation is available in all view-window types, including zooming in or out at a particular point (all view types), panning (all view types), and rotation (2D in FE-slice views, 3D in 3D-views). Notably, the view windows remain interactive and their settings accessible even during simulation computations. The **mesh inspector**, trusted companion through many FEFLOW releases, has been augmented by a sensitivity to element- and node-assigned data in 3D views.

As the plots of hydraulic conductivity, head isolines and a solute-concentration isosurface in Figure 3 illustrate, multiple parameters can be represented in the same view by choosing contrasting color sequences and different plotting styles. Element-based (material) parameters are always shown as noninterpolated patches while nodal scalar data can be plotted either in a continuously interpolated manner or at user-specified levels as fringes or as isolines/isosurfaces.

Velocity fields (nodal vector data) require representation of both direction and magnitude. Magnitude alone can be plotted similar to any other scalar parameter. The standard 2D and 3D arrow plots use arrow length to express magnitude (Figure 4). In addition, FEFLOW 6 provides a vector plot style that avoids arrow heads and instead indicates direction by increasing opacity, and a bullets style that represents magnitude by color rather than size and is thus especially useful for the visualization of low-velocity regions (Figure 5). As an alternative to vector plotting, pathlines provide spatial and travel-time information for virtual particles released at user-specified locations (Figure 6).

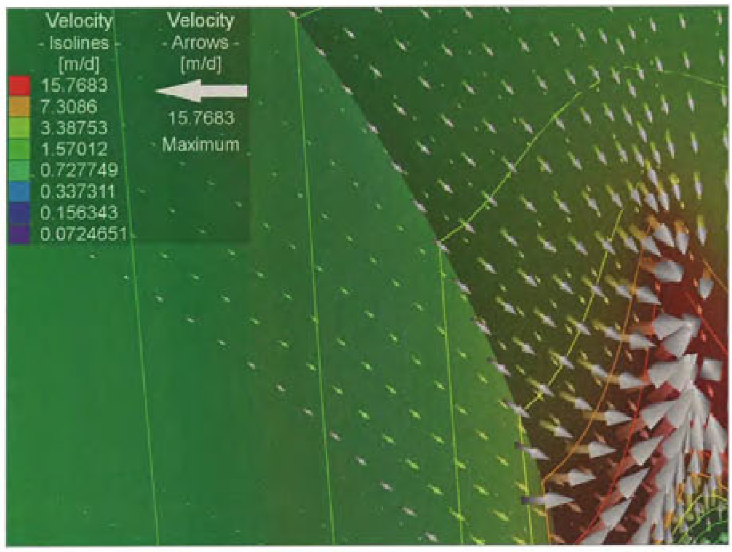
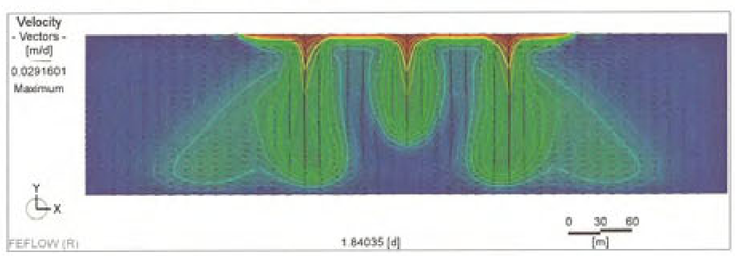


Fig. 4: Three-dimensional velocity-field visualization via arrows and translucent color plots



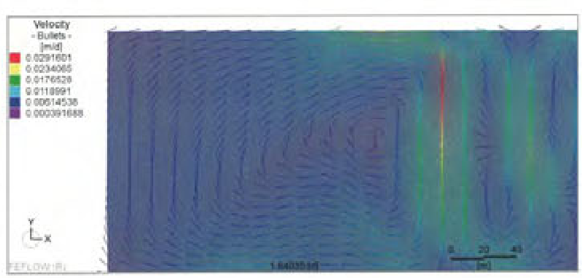
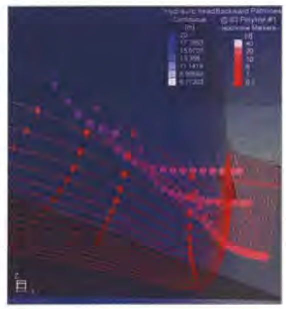


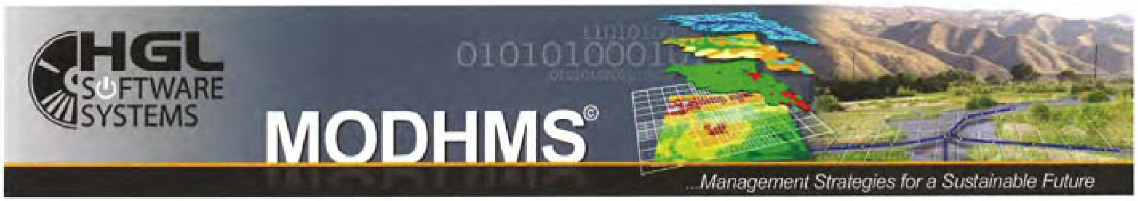
Fig. 5: Velocity-field visualization for the two-dimensional Elder problem via vector lines (top) and bullets (bottom)

Flexible and powerful means of visualization require effective control of the various view components, especially in a 3D view where any individual slice and layer can potentially be shown together with cross sections, isosurface plots and the possibly clipped or carved model domain. A dedicated tree control makes all individual components of a view window accessible. Individual properties such as colors, opacity, plot ranges and isolevels are controlled via property panels. Since all settings of each open view are stored together with the finite-element problem, identical views will be restored the next time the respective problem file is opened.



While individual data plots can be exported as scalable vector graphics for use in external plotting software, there is also the possibility to obtain "snapshots" of a complete view window where all view components are rendered at a user-specified resolution up to pixel numbers that are suitable for poster printing.

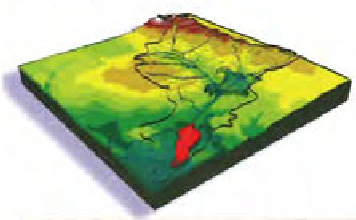
Fig. 6: Pathlines and isochrone markers



MODHMS Overview

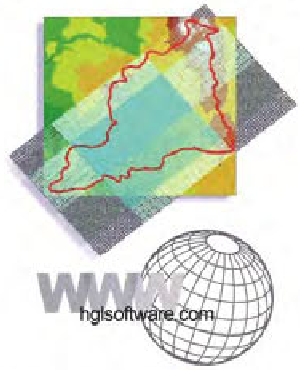
MODHMS®, HGL's latest and most advanced software code, interfaces seamlessly with the popular MODFLOW code to provide a physically based, spatially distributed, conjunctive surface/subsurface modeling framework hydrologic system. Developed to meet the growing demand for quantifying available water within a hydrologic system and for numerical simulation of complex hydrological processes, MODHMS® extends our MODFLOW-SURFACT™ subsurface modeling code to include overland and channel flow and transport. We use these tools to give water resources managers unsurpassed capability to simulate the complete hydrological cycle and address complex water resources management issues including…

- Integrated water resource assessment
- Groundwater availability & safe-yield analysis
- Conjunctive surface water-groundwater use
- Stream flow restoration
- Flood prediction and mitigation
- Agricultural irrigation management
- Cleanup of industrial contaminants
- Watershed-scale analysis of point source and nonpoint source pollution
- Fluvial hydraulic analysis



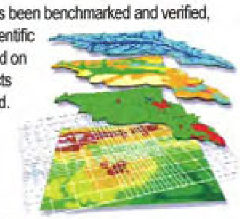
Advanced Features

- Fully implicit coupling of all regimes for mass-conserved and robust solutiosn to systems with strong interactions between regimes
- Curvilinear grid option to conform model to geometric or topographic features
- Friction formulas for surface flow and retention formulas for unsaturated flow including pseudo-soil functions representing unconfined flow
- Adaptive time-stepping for speed and accuracy
- Picard and Newton-Raphson schemes for efficiency and robustness of non-linear flow solutions
- Implicit TVD transport schemes for highly accurate, physically consistent transport solutions
- Advanced PCG and ORTHOMIN solvers
- Combination of steady-state and transient simulation options during any stress period
- Zone budget calculations
- Any or all of the hydraulic regimes (overland, channel, and subsurface) may be simulated individually, or in combination
- Restart option to restart a simulation from any point in between time periods without modifying input files



Why Choose HGL's Code?

- The project scope requires a code that is capable of simulating overland, subsurface, and stream channel flow domains interacting with each other, and the associated solute transport therein in a temporally varying, spatially distributed manner.
- MODHMS® treats the flow of water and transport solutes in a hydrologic system in a rigorous, mechanistic manner by mathematically representing surface and subsurface domains as a holistic system that is solved simultaneously. Thus, key processes that control groundwater/surface water interactions are inherently simulated as part of the numerical solution.
- MODHMS® has been benchmarked and verified, subjected to scientific review, and used on modeling projects around the world.



Benefits

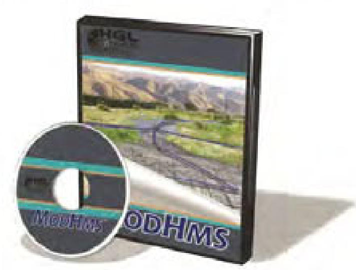
FAST AND EFFICIENT — ***Get results sooner! Computational efficiencies enable MODHMS® to run up to 75 percent faster than competing systems.***

COMPATIBILITY — ***Seamless interface with the USGS's MODFLOW code. Compatible with ICPR pond-routing model, XPSWMM for dense stormwater drainage networks, and many others...***

TESTED — ***Benchmarked, verified, and subjected to scientific review.***

ACCEPTED — ***By federal and state agencies across the United States and used on modeling projects around the world.***

As a leader in modeling and water resources technologies, we leverage our experience, knowledge, and innovative techniques to resolve the most complex issues. MODHMS®, our most powerful modeling code yet, represents the latest addition to our consulting toolbox of innovative, sustainable, and cost-effective water resources solutions. For more information, please contact Jan Kool, Ph.D. at (703) 478-5186.



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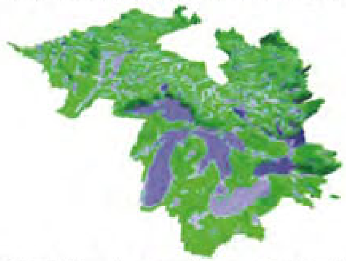
HydroGeoSphere

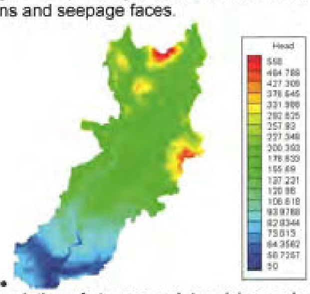
A Three-dimensional Numerical Model for Fully-integrated Subsurface and Surface Flow and Solute Transport



HydroGeoSphere is a powerful numerical simulator for supporting water resource and engineering projects pertaining to hydrologic systems with surface and subsurface flow and mass transport components. It is an upgraded version of the **FRAC3DVS** discrete fracture model where surface water simulation capabilities have been added and where all features of **FRAC3DVS** are retained. **HydroGeoSphere** has the following attributes:

Fluid Flow

- Complete hydrologic cycle modeling using detailed physics of surface and subsurface flow in one integrated code.
  - Surface domain represented as 2-D areal flow for the entire surface or as 2-D runoff into 1-D channels.
  - Subsurface domain consists of 3-D unsaturated and/or saturated flow.
  - Both domains naturally interact through physically-based fluid exchange terms.
- Physically-based accounting of all components of the hydrologic cycle water budget.
  - Temporally and spatially varying evapotranspiration based on land use/land class and seasons.
  - Impact of snowmelt on hydrologic regime.
- Accurate delineation and tracking of the water table position.
- Handling of non-ponding or prescribed ponding recharge conditions and seepage faces.



- Accommodation of storage, solute mixing and variable flow distribution along wellbores.
- Representation of fractured geologic materials with arbitrary combinations of porous, discretely-fractured, dual-porosity and dual-permeability media for the subsurface.
- Density-dependent flow and transport.

Mass and Heat Transport

- Simulation of non-reactive and reactive chemical species transport, and heat transport in the associated surface and subsurface flow fields.
- Accurate handling of fluid and mass exchanges between fractures and matrix including matrix diffusion effects and solute advection in the matrix.
- Chain-reactions of radionuclide components.
- Calculation of water age and solute transit time probabilities.

Numerical Methods

- Fully-implicit coupling approach for all domains provides for a robust mass conserved solution scheme.
- Advanced computational algorithms that allow the code to perform unprecedented, fully-integrated, 3-D simulation/animation on a personal computer.
  - Adaptive time-stepping schemes with automatic generation and control of time steps.
  - Efficient ILU-preconditioned iterative sparse-matrix solver.
  - Efficient Newton-Raphson linearization option.
- Fluid and solute mass balance tracking.
- Unstructured finite-element grids.
  - Advanced meshing of irregular discrete fractures.
  - Axi-symmetric grid option.
  - 8-node block or 6-node prism elements, 3- and 4-node plate elements for fractures and surface water, and 2-node line elements for wells and tile drains.
- Finite difference option (7-point template).

Pre- and Post-processing

- User-friendly pre-processor with **GridBuilder** and **GMS** compatibility for mesh generation and problem setup.
- Import options for **GIS** formatted data.
- Export options for **Tecplot** visualizations.

Applications and Research Investigations

HydroGeoSphere can perform event-based and continuous simulations on widely varying spatial and temporal scales. Examples of field applications include:

- Integrated water resource assessment and watershed hydrologic analysis.
- Land-use or climate-change impacts on both surface and subsurface water.
- Contaminant fate in surface and subsurface water.
- Fractured rock hydrogeology.

Developers and Contact Information

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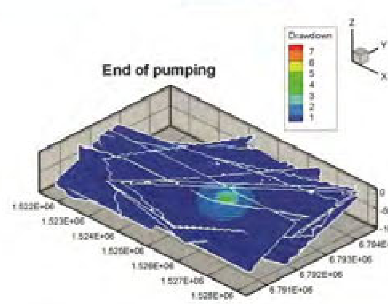

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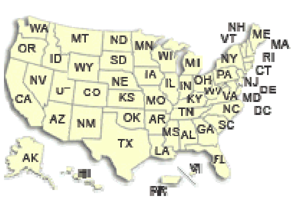

SEAWAT > Summary of SEAWAT v.4

SEAWAT Version 4: A computer program for simulation of multi-species solute and heat transport

By Christian D. Langevin (U.S. Geological Survey, Fort Lauderdale, Florida),
Daniel T. Thorne, Jr. (Georgetown College, Georgetown, Kentucky),
Alyssa M. Dausman (U.S. Geological Survey, Fort Lauderdale, Florida),
Michael C. Sukop (Florida International University, Miami, Florida), and
Weixing Guo (Schlumberger Water Services, Fort Myers, Florida)

Summary of SEAWAT Version 4

Abstract

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

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

The report contains revised input instructions for the MT3DMS Dispersion (DSP) Package, Variable-Density Flow (VDF) Package, Viscosity (VSC) Package, and CHD

Package. The report concludes with seven cases of an example problem designed to highlight many of the new features.

Method

The variable-density ground-water flow equation is solved using a finite- difference approximation similar to the one solved by MODFLOW-2000. The solute- transport equation is solved using one of the approaches available with MT3DMS.

History

SEAWAT Version 4.00.04 2011/02/07 - This version of SEAWAT contains fixes for a problem in the Drain Observation Package and in the Transport Observation Package. In some instances, the Drain Observation Package would report a non-zero drain flux for a drain that was not receiving water from the aquifer. The error was in the Observation Process and not in the head solution or reported water budgets. There was also a name conflict in the common statement for the Transport Observation Package. It is unclear if this error had any effect on simulation results. The 32 and 64-bit executables released with this distribution were compiled using Intel Visual Fortran Composer, which allows the programs to run on the Windows 7 operating system.

SEAWAT Version 4.00.03 2009/09/21 - This version of SEAWAT contains fixes for a variety of issues encountered since version 4.00.02: (1) the GMG solver had problems converging for problems with rewetting (thanks to Kim Gordon for helping identify this problem); (2) the program was updated with MODFLOW Version 1.18.01; (3) there was an error in a conditional statement in the DRT package that may have affected calculated DRT fluxes; (4) the MNW fluxes passed to MT3DMS were offset by one transport time step; (5) the BCF package had problems with rewetting, which was caused by the use of HDRY in a calculation (thanks to Vincent Post for finding this error); (6) an error was corrected in the HUF2 package; (7) if fluid density was specified as a function of pressure, densities were incorrectly updated for cells that had rewet; (8) all tabs were removed from the SEAWAT source code. An additional feature was added to SEAWAT to improve runtimes for variable-density flow and solute transport models with many rivers, wells, and/or general-head boundaries. Density is stored with the package array by specifying an AUXILIARY variable in the respective flow package using the name WELSSMDENSE, RIVSSMDENSE, or GHBSSMDENSE. With this feature, the boundary density is calculated only once for each MODFLOW time step and stored in the package array. This storage occurs right after the SSM routine reads the boundary concentrations.

SEAWAT Version 4.00.02 2008/09/19 - This version of SEAWAT contains fixes for two memory conflicts. The first was with the MNW Package. The second was between the OBS Process and the Integrated MT3DMS Process.

SEAWAT Version 4.00.01 2008/04/29 - This version of SEAWAT contains a fix for a minor programming error that may have caused the dcdt term of the flow equation to be too large.

SEAWAT Version 4.00.00 2008/03/28 - First release of SEAWAT Version 4. SEAWAT now contains capability to simulate simultaneous solute and heat transport. This SEAWAT version contains MODFLOW Version 1.18.00 and MT3DMS Version 5.2. This SEAWAT version also contains fixes for several bugs found in previous SEAWAT versions: (1) groundwater fluxes for perched water table conditions with strong density variations were not calculated properly; (2) in the budget calculations, there was an error in the flux calculated for the front face of constant head cells;

(3) for mixed steady state and transient simulations, if the first stress period was specified as steady state, all remaining stress periods were simulated as steady state.

SEAWAT-2000 Version 3.13.00 2006/04/21 - This version of SEAWAT was updated with MODFLOW Version 1.16.00. Additionally, ETS and DRT are now compatible with the VDF proces

SEAWAT-2000 Version 3.12.00 2006/03/14 - This version of SEAWAT was updated with MT3DMS Version 5.10, which includes a new zero-order growth/decay option within the reactions package. This option may be useful for simulating groundwater age as a separate species.

SEAWAT-2000 Version 3.11.02 2005/09/23 - This version of SEAWAT contains a fix for a minor bug that may have caused some transport timesteps to be too short.

SEAWAT-2000 Version 3.11.01 2005/07/25 - This version of SEAWAT contains a bug fix for head-dependent flux calculations for some boundary types.

SEAWAT-2000 Version 3.11.00 2005/04/29 - Added MODFLOW-2000 Version 1.15.00 and MT3DMS Version 5.00. Also added compatability between MNW wells and the VDF Process for freshwater parts of a model domain.

SEAWAT-2000 Version 3.10.01 2004/03/30 - This version of SEAWAT contains bug fixes for three coding errors: (1) In the previous version, the value for HDRY was not always written to the output head file if a cell went dry during the simulation. (2) A runtime error was encountered in certain instances when the IMT Process was used with the GWF Process (instead of the VDF Process). (3) If MODFLOW timesteps were shorter than the calculated transport timestep, the density array was not updated properly.

SEAWAT-2000 Version 3.10 2004/02/13 - This version of SEAWAT contains substantial improvements over previous releases. The program is now based on MODFLOW-2000 (Version 1.12.01) and MT3DMS (Version 4.500), and uses the concept of a process. Details of SEAWAT-2000 are described in U.S. Geological Survey Open-File Report 03-426.

SEAWAT Version 2.12 2002/09/13 - Fixed problem with calculation of EVT fluid density. Thanks to Adam Taylor and Barclay Shoemaker. Also fixed bug in calculation of default riverbed thickness. Thanks to Lou Motz and Nebiyu Tiruneh from the University of Florida for locating this problem.

SEAWAT Version 2.11 2002/08/09 - Fixed bug that caused program to bomb for certain problems involving wetting and drying. Thanks to Trayle Kulshan and Steve Gorelick from Stanford University for help in locating this problem.

SEAWAT Version 2.10 2002/02/07 - Code consists of MODFLOW-88 and MT3DMS Version 3.50.A. Upgraded the CFACE subroutine with the improved CFACE subroutine from MT3DMS Version 4.00. Reformulated flow equation to conserve fluid mass. Redesigned boundary conditions to represent variable-density flow. Added an iterative method for coupling flow and transport. Program redesigned as double precision.

SEAWAT Version 1.1 1998/05/01 - Initially released by Weixing Guo (Missimer

International, Inc.) and Gordon D. Bennett (S.S. Papadopulos & Associates, Inc.)

Data Requirements

In order to use SEAWAT, initial conditions, hydraulic properties, and stresses must be specified for every model cell in the finite-difference grid.

Output Options

Primary output is head and concentration, which can be written to the listing file or to separate binary files. Other output includes the complete listing of all input data, drawdown, flow budget, and transport budget data. Flow budget data are printed as a summary in the listing file, and detailed budget data for all model cells can be written into a separate file. All binary output is written to files that are opened with the FORM='BINARY' option. This means that some pre- and post-processors may not be able to read the output unless the open statements are modified, the program is recompiled, and the model is rerun.

System Requirements

SEAWAT is written in Fortran 77 with the following extensions: use of variable names longer than 6 characters, Fortran 90 statements for dynamic memory allocation, a call to SUBROUTINE GETARG to retrieve command-line arguments, and two calls to DATE_AND_TIME, which is a Fortran 90 intrinsic subroutine. Generally, the program is easily installed on most computer systems. The code has been used on DOS-based 386 or greater computers having a math coprocessor and 4 mb of memory.

Processes

GLO1 -- Global Process
GWF1 -- Ground-Water Flow Process
VDF1 -- Variable-Density Flow Process
OBS1 -- Observation Process
SEN1 -- Sensitivity Process
PES1 -- Parameter-Estimation Process
IMT1 -- Integrated MT3DMS Process

Process compatibility issues are described in the user's manual. In general, the VDF and IMT Processes are not compatible with SEN and PES, and are only slightly compatible with OBS. VDF is an alternative to GWF, and thus the two cannot be used concurrently in a simulation.

Packages Compatible with the Variable-Density Flow (VDF) Process

BAS6 -- Basic
BCF6 -- Block-Centered Flow
LPF -- Layer Property Flow
HUF2 -- Hydrogeologic Unit Flow. Note that VDF is not yet compatible with the Layer Variable-Direction Horizontal Anisotropy (LVDA) capability. The LVDA capability should not be used with the VDF process. The VDF process is compatible with the three features described in Open-File Report 03-347.
HFB6 -- Hydraulic Flow Barrier
DRN -- Drain
RIV -- River
GHB -- General-Head Boundary

EVT -- Evapotranspiration
WEL -- Well
RCH -- Recharge
CHD -- Time-Variant Constant Head
FHB -- Flow and Head Boundary
MNW -- Multi-Node Well
DRT -- Drains with Return Flow
ETS -- Evapotranspiration with a Segmented Function
SIP -- Strongly Implicit Procedure
SOR -- Slice-Successive Overrelaxation
PCG -- Preconditioned Conjugate Gradient Solver (also called PCG2)
DE4 -- Direct Solver
GMG -- Geometric Multi-Grid Solver
OC -- Output Control Option
LMT6 -- Linkage with MT3DMS
BTN -- Basic Transport
ADV -- Advection
DSP -- Dispersion
SSM -- Source/Sink Mixing
RCT -- Reaction
GCG -- Generalized Conjugate Gradient Solver
TOB -- Transport Observations
OBS -- Observation
HOB -- Hydraulic-Head Observation
GHOB -- General-Head Boundary Observation
DROB -- Drain Observation
DTOB -- Drain with Return Flow Observation
RVOB -- River Observation
CHOB -- Constant-Head Flow Observation

Other packages (distributed with MODFLOW-2000) are included in SEAWAT, however, these additional packages may not be compatible with the VDF Process.

Documentation

The basic documentation is contained in the following three reports:

Langevin, C.D., Thorne, D.T., Jr., Dausman, A.M., Sukop, M.C., and Guo, W., 2007, SEAWAT Version 4: A Computer Program for Simulation of Multi-Species Solute and Heat Transport: U.S. Geological Survey Techniques and Methods. Book 6, Chapter A22, 39 p.

Langevin, C.D., Shoemaker, W.B., and Guo, W., 2003, MODFLOW-2000, the U.S. Geological Survey Modular Ground-Water Model--Documentation of the SEAWAT-2000 Version with the Variable-Density Flow Process (VDF) and the Integrated MT3DMS Transport Process (IMT): U.S. Geological Survey Open-File Report 03-426, 43 p.

Guo, W., and Langevin, C.D., 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, 77 p.

Users will also need documentation for MODFLOW-2000 and MT3DMS, and possibly the references cited in those reports.

Point of Contact

Support is provided for correcting bugs and clarification of how SEAWAT is intended to work. Only limited assistance can be provided for applying SEAWAT to specific problems by contacting the point of contact listed below:

Christian Langevin
U.S. Geological Survey (USGS) Office of Groundwater
411 National Center
12201 Sunrise Valley Drive
Reston, VA 20192

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SUTRA *Version 2.2*

A model for 2D or 3D saturated-unsaturated, variable-density ground-water flow with solute or energy transport

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Information

SUTRA is a model for saturated-unsaturated, variable-density ground-water flow with solute or energy transport. **SUTRA** *Version 2.2* allows specification of time-dependent boundary conditions without programming FORTRAN code, and offers optional output files that summarize specifications and computed results at boundary condition nodes.

A Release Notes file containing installation instructions is included with the software. It can also be downloaded separately using the link below.

SUTRA 2.2 Release Notes, Portable Document Format (PDF) (149 KB)

The SutraSuite Online User Reference web site provides a convenient, interactive source of information about theoretical and practical aspects of **SUTRA** simulation. It includes news, advice on how to get started using **SutraSuite**, an overview of the software, a gallery of **SUTRA** simulation results, answers to frequently asked questions, a glossary, in-depth discussions of selected topics, and technical support information, including a troubleshooting guide.

Software (*Version 2.2*, Sept 2010)

To download the installation files, click on the links below. (Some web browsers will automatically run the installation program after downloading it. If your browser does not automatically run the installation program, save the installation file on your computer and run it by double-clicking on its icon.) To install the software, follow the instructions provided by the installation program. It is recommended that you accept the default settings during installation.

NOTE: The installation files may be updated from time to time to fix bugs or make other improvements. A "critical" update is one that is required for the proper functioning of some aspect of a code or example problem. If a critical update to an installation file has been issued since you last downloaded that file, it is highly recommended that you check the list of updates on the "SutraSuite Installation File Updates" page to determine whether the update affects your **SutraSuite** applications. If so, uninstall your current installation (if one exists), then download and install the latest revision of the installation file using the corresponding link below. Minor updates are of lesser importance and may be considered entirely optional. For details on how to install an update, or to view a complete listing of updates to the installation files for **SUTRA** and the **SUTRA** examples, see the "SutraSuite Installation File Updates" page.

Source code, documentation, and executable for Microsoft Windows 9x, NT, ME, 2000, or XP (Self-extracting file, 8.1 MB) *[No critical updates]*

Examples (Self-extracting file, 40.9 MB) *[No critical updates]*

Documentation

The following documentation for **SUTRA** *2.2* is included with the software. It can also be downloaded separately using the link below.

Voss, C. I., and Provost, A.M., 2002 (Version of September 22, 2010), SUTRA, A model for saturated-unsaturated variable-density ground-water flow with solute or energy transport, U.S. Geological Survey Water-Resources Investigations Report 02-4231, 291 p.

SUTRA Documentation, Portable Document Format (PDF) (3.7 MB)

The SutraSuite Online User Reference web site provides additional information in a convenient, online format.

Related Programs

- SutraPrep
- SutraGUI
- SutraPlot
- Model Viewer
- GW_Chart
- CheckMatchBC

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Sea Water Intrusion Package

The Sea Water Intrusion (SWI) package for MODFLOW

The Sea Water Intrusion (SWI) package is intended for the modeling of regional seawater intrusion with MODFLOW. The SWI package simulates the evolution of the three-dimensional density distribution through time; effects of the density distribution on the flow are taken into account explicitly. The main advantage of the SWI package is that each aquifer can be modeled with a single layer of cells. An existing MODFLOW model of a coastal aquifer can be modified to simulate seawater intrusion through the addition of one input file. The SWI package can simulate interface flow, stratified flow, and continuously-varying density flow. The SWI package is free and open-source software and is released under the Eiffel Forum License, version 1; for more information see the manual.

Applications of the SWI package

This section contains applications and comparisons of the SWI package. You are invited to submit a description of your SWI model, an abstract of your findings, a report, or any other information you deem interesting. If you want your SWI model added here, please email it to Mark Bakker.

- A little movie of the evolution of the brackish zone.
- A little movie of the three-dimensional development of a fresh water lens below a square island with constant infiltration.

Developers

The SWI package was developed by Mark Bakker and Frans Schaars. For the development of new features for SWI, or for the development of seawater intrusion models, or assistance with modeling projects, contact Mark Bakker or Frans Schaars

Funding

Development of the SWI package was funded by

- Georgia Coastal Incentive Grants Program, administered by the Georgia Department of Natural Resources
- Amsterdam Water Supply (WaterNet), Vogelenzang, The Netherlands

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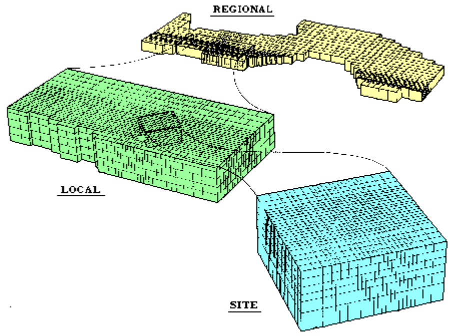
SWIFT FOR WINDOWS®

SWIFT for Windows

Overview

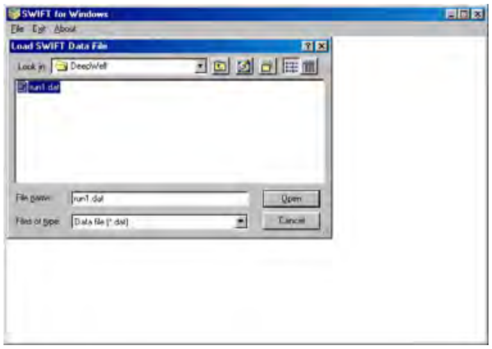
- Three-Dimensional Groundwater Flow and Transport Model
- Equations for Pressure, Temperature, Brine, Radionuclides
- Windows® Interface
- Dual Porosity and Fractured Media

SWIFT for Windows is a fully transient, three-dimensional model which simulates the flow and transport of fluid, heat (energy), brine, and radionuclide chains in porous and fractured geologic media. The primary equations for fluid, heat, and brine are coupled with fluid density, fluid viscosity, and porosity. Steady-state options are available for the fluid and brine equations, and both Cartesian and cylindrical coordinate systems may be used. However, the latter system is restricted to two-dimensional, r-z simulations. Both dual-porosity and discrete-fracture conceptualizations may be considered for the fractured zone. Migration within the rock matrix is characterized as a one-dimensional process.



Features

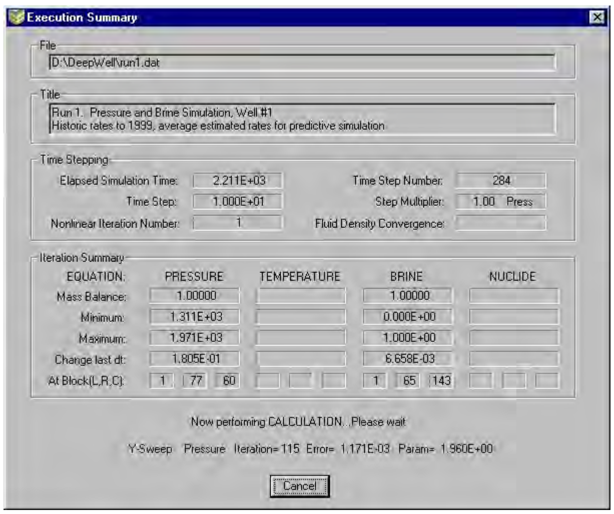
Windows® Interface SWIFT for Windows is a 32-bit application intended for use on all currently supported Microsoft Windows desktop operating systems, with a Pentium or better processor. Running SWIFT for Windows is easy with the interface which prompts the user for the data set to simulate, tracks the progress of the simulation, and lists the output files created.



Postprocessor Interface (UNSWIFT) Contour maps of pressure, temperature, brine, or concentration in any window in any plane can be quickly processed directly into uniformly-spaced grid files for the Surfer® contouring software.

STLINE Particle Tracking Allows transient flowpath evaluation of streamlines and export to Surfer® as lines or posted symbols.

Windows Runtime Monitor The Windows Runtime Monitor displays essential simulation data while the simulation is running. The Windows Runtime Monitor tracks the simulation progress, highlighting the current program activity at the base of the screen. The time step, interval and other data are updated on the screen through the course of the simulation. Below the frame, system RAM requirements, matrix convergence (L2SOR only), creation of map file, and error messages are displayed. Auxiliary files for restart or binary input are also prompted.



Equations SWIFT for Windows is comprised of the four transport processes: fluid, heat, brine, and radionuclide chains. For porous media, only the global (three-dimensional) process simulator is used. For fractured media, the global process simulator is used for the fractured media, and the local (one-dimensional) process simulator is used for the rock matrix.

Basic Assumptions and Characteristics

- Single-phase fluid flow governed by Darcy's law
- Three-dimensional transport in the global system, and one-dimensional transport in the local rock-matrix subsystem
- Local rock matrix may be characterized by either prisms or spheres
- Linear variations in porosity and fluid density with respect to the dependent variables
- Viscosity is dependent on temperature and brine concentrations only
- Nonlinear isothermal equilibrium adsorption (Freundlich or linear)
- Injection wastes are miscible with the resident fluids
- Confined or unconfined aquifer (transient or steady-state free water surface)
- Hydraulic and thermal conductivities may be heterogeneous and/or anisotropic
- Longitudinal and transverse dispersivities may vary throughout the domain
- Variable rock compressibility (storativity)
- Dual or simulataneous discretization

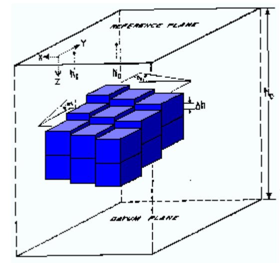
Method of Solution Discretization is performed by the finite-difference method using centered or backward weighting in the time and space domains. Matrix solution is performed either by Gaussian elimination or by two-line successive overrelaxation.

Boundary Conditions A variety of boundary conditions and source terms may be invoked for both the porous and fractured media. These include:

- Prescribed pressure (head), temperature, and brine concentration
- Prescribed flux of fluid (water), heat, brine, or nuclide mass
- Wellbore injection/production submodel subject to pumping constraints
- Aquifer influence function (i.e., Carter-Tracy infinite reservoir)
- Dual porosity domain extension
- Waste-leach radionuclide submodel for waste repository nuclides and heat
- Freewater surface with recharge

Typical Application

SWIFT can be applied to a variety of groundwater problems, ranging from simple well flow to complex transport analysis.



- Deep-well injection of hazardous waste; isothermal/nonisothermal, constant/variable density
- Seawater intrusion
- Optimization of well fields to reduce intrusion and upconing
- Prediction of hazardous waste migration
- Well performance and pumping test analysis
- Complex variable-block elevation and thickness data (input via a separate binary file)

Summary

With sufficient memory resources, SWIFT can be used to model complex field applications at a reasonable price. There is optional training available, and the package includes over 70 verification and sample problems.

Distribution, Requirements and Pricing

Licensing A single-node license is defined as a single PC or workstation installation. Additional licenses may be purchased, and each additional license includes a User's Guide.

Distribution and Installation The SWIFT for Windows package includes a User's Guide, Source Code, and data sets. All documentation is electronic using Adobe™ format and are distributed on CD. Executables for the FORTRAN are included. Installation of source code and data files is straightforward.

Basic Package:

- SWIFT for Windows Data Input Guide
- All FORTRAN source code and 70 verification problem input and output data sets on CD-ROM

Platform SWIFT for Windows is available on PC's only. It is compatible with the Windows® 95/98, and WindowsNT® v4.0 operating systems.

Other Required Software Modifications to SWIFT for Windows may require recompilations using Lahey® LF95 Fortran compiler. Postprocessing of two-dimensional maps can be contoured using UNSWIFT to create grid files for Surfer®, or the new SWIFT Output Data Reader, an ArcView product.

Installation Requirements:

- Pentium® with 32+ MB RAM
- Lahey® LF95
- Surfer® for postprocessing

Ordering and Shipment Payment options include: check, Master Card, VISA, and pre-approved purchase orders (call first). The code will be delivered within 10 business days of full payment. For orders shipped within Virginia, sales tax of 4.5 percent must be added. Overseas deliveries are an additional $30.

Price - The SWIFT for Windows code includes installation support only.

- Single-license: $395
- Additional or corporate support is available on a contract basis.

Download Order Form

Technical Support

Technical support is limited to installation and initial use. Tetra Tech GEO will provide advice, analysis, and suggestions for improvement of model application and use only under separate contract. Client confidentiality is maintained.

Download User's Guide
The entire SWIFT for Windows User's Guide is available in Adobe™ (.pdf) format. The file is 1.07 MB

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The entire SWIFT for Windows Theory and Implementation is available in Adobe (.pdf) format. The file is 1.35 MB

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SWIFT-2002

1 INTRODUCTION

The input data of the SWIFT-2002 (Sandia Waste-Isolation Flow and Transport Model) model provides an important compliment to two other reports. Reeves et al. [1986a] gives the theory and formulation of the model whereas Reeves et al. [1986b] provides instruction problem sets, complete with listings of the data input and output. In addition, Finley and Reeves [1981] provides illustrative problems which, although designed for SWIFT, may be used for an initial orientation to SWIFT-2002. Verification and validation tests of the SWIFT code are presented by Ward et al. [1984].

1.1 THE SWIFT MODELS

The SWIFT model was originally developed, maintained and applied by Sandia National Laboratories. The Nuclear Regulatory Commission has sponsored this work under its high-level nuclear-waste program. Between 1982 and 1985 the capability of SWIFT has been enlarged to include fractured media, a free-water surface and extended boundary conditions. Since 1985, GeoTrans has modified the code funded through internal research and development. Revisions include a conversion to Fortran 77, extended options for matrix solutions, contour mapping and boundary conditions and postprocessing options. This code is designated as SWIFT III. In 1990, a PC version of SWIFT (SWIFT/386) was developed in which a run-time monitor was added to improve user friendliness. Since then the code has been further enhanced to include multiple values of rock compressibility. A utility program, UNSWIFT, provides an interface between the map output and the contouring program SURFER7. The five models, SWIFT, SWIFT II, SWIFT III SWIFT/386, SWIFT/486, SWIFT-98 and SWIFT-2002 are fully transient (with steady-state options), three-dimensional, finite-difference codes, which solve the coupled equations for flow and transport in geologic media. The five models may be used for evaluation of repository site performance and repository design performance.

The processes considered are:

- fluid flow,
- heat transport,
- brine migration,
- radionuclide-chain transport.

Flow, heat and brine transport are coupled via fluid density, fluid viscosity and porosity. Together they provide the velocity field on which the radionuclide transport depends.

The media considered are:

- porous media (SWIFT, SWIFT II, SWIFT III, SWIFT/386, SWIFT/486, SWIFT-98 and SWIFT-2002),

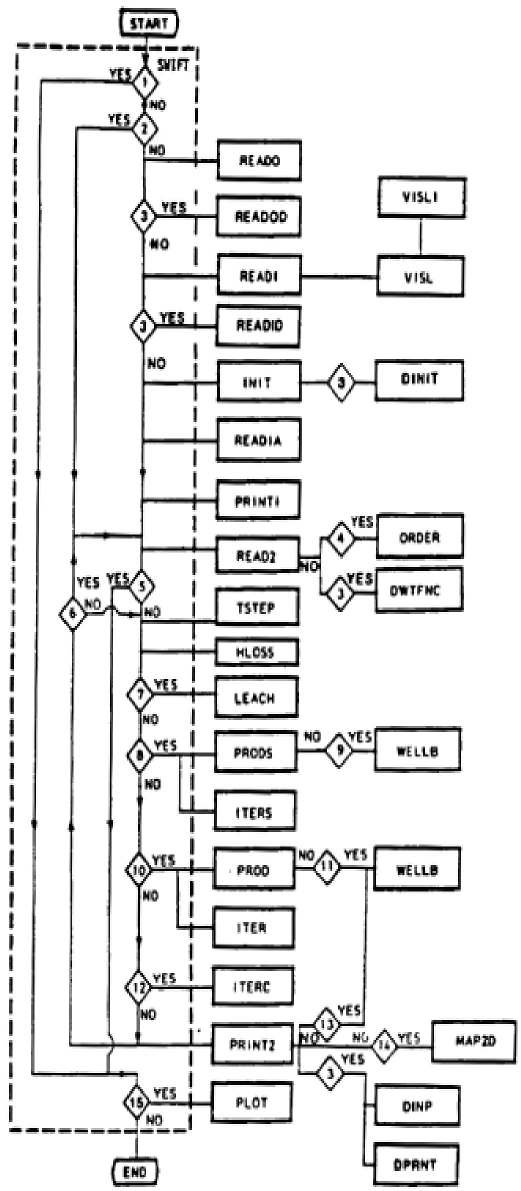
- fractured media (SWIFT II, SWIFT III, SWIFT/386, SWIFT/486, SWIFT-98 and SWIFT-2002).

As discussed in Reeves et al. [1986a], the SWIFT-2002 model permits local one-dimensional subsystems to be attached, as desired, to the grid blocks comprising the global system. The local units may be used either to characterize the second porosity of a fractured media or to extend the boundaries of the system in a computationally inexpensive manner.

1.2 PROGRAM STRUCTURE

The SWIFT-2002 program consists of a main routine and approximately 90 supporting subroutines. Its general structure is illustrated by Figure 1-1, a flow chart of the main routine. The basic organization is focused upon the three global integration modules ITER, ITERS and ITERC. Subroutine ITER solves the coupled partial differential equations for fluid flow, heat transport and brine transport under transient conditions, ITERS integrates the flow and brine equations under steady-state conditions and ITERC solves the coupled partial differential equations for transport of a radionuclide chain. All other routines provide support functions for the integration. The support function of interest in this report is that of data input.

Figure 1-1. General Structure of SWIFT-2002.



Conditions for Figure 1-1 (numbered diamonds) are as follows:

(1) Are plots desired for a previous run?
(2) Is this a restart run?
(3) Is dual porosity to be included?

(4) Is the reduced-bandwidth direct method of solution used? (multi-dimensional problems only)
(5) Is the run to be terminated at this time step?
(6) Are the recurrent data to be read at this time step?
(7) Is the waste-leach submodel employed?
(8) Is the steady-state pressure solution sought?
(9) Are steady-state wellbore calculations to be performed?
(10) Is the transient pressure solution sought?
(11) Are the transient wellbore calculations to be solved?
(12) Are the radionuclide transport calculations to be performed?
(13) In the transient wellbore calculations, are the well rates to be calculated semi-implicitly?
(14) Are any two-dimensional contour maps desired?
(15) Are any plots desired for this run?

1.3 DATA

Data input occurs in eight of the subroutines shown in Figure 1-1, which may be viewed in several different ways. Seven of the routines are positioned outside the recurrent time-step loop extending from READ2 to PRINT2. These routines read time-independent data. The other routine, READ2, is positioned inside the recurrent time-step loop. Therefore, it reads time-dependent data. Regarding the storage allocation function, the three routines SWIFT, READ0 and READ0D provide data which optimally partition the common-block arrays. Here SWIFT reads such information for the global-system arrays, READ0 for the radionuclide arrays and READ0D for the local-subsystem arrays. In regard to the dual-porosity function, routines READ0D and READ1D provide input pertaining specifically to the local porosity, whereas the other routines provide input pertaining to the global porosity. Finally, the data input records divide naturally into groups depending upon the program unit in which they are read. Table 1-1 gives the "shorthand" notation used by each group and a brief description of the function of each group.

To facilitate data input, the use of record type identifiers is strongly encouraged. These identifiers, i.e., M-1, R1-1, R2-7-1 may be entered in columns 71-80 on the input data sets. Blank records are typically blank in columns 1-70 and the field identifier placed in columns 71-80, i.e., R1-26-BLK. This scheme has been used in the verification data sets and has been maintained for upward compatibility with previous versions of SWIFT, SWIFT II, and SWIFT III. In maintaining this compatibility, an exception arises in record type R2-12 (section 8.8) where columns 1-80 are all reserved for data input.

Chapters 2 through 9 define, in detail, the data entered within each data group. Other useful items, such as auxiliary disk files, units of measurement and a variable index are treated in the remaining chapters and in the first three appendices. However, for easy reference, the final appendix is reserved for the input-error diagnostics which are printed by the code.

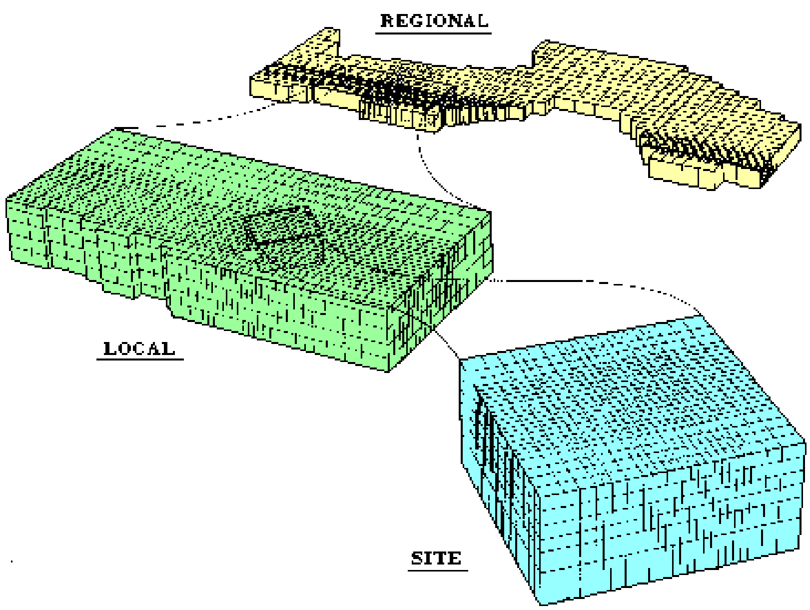
Table 1-1. Data Input Groups.

Routine	Notation	Data Function
SWIFT	M*	General problem setup
	P	Plotting data
READ0	R0	Radionuclide-chain information
READ0D	R0D	Dimensioning data of the local arrays
READ1	R1*	Properties of the global system
READ1D	R1D	Properties of the local subsystems
INIT	I*	Initialization data
READ1A	R1A	Specification of waste-leach submodel
NMONINP	N	Nuclide monitor block
READ2	R2*	Time-dependent data

*Indicates mandatory input. All others are optional.

SWIFT-98 DESCRIPTION

SWIFT-98



- Three-Dimensional Groundwater Flow and Transport
- Pressure, Temperature, Brine, Radionuclides
- PC Interface
- Dual Porosity and Fractured Media

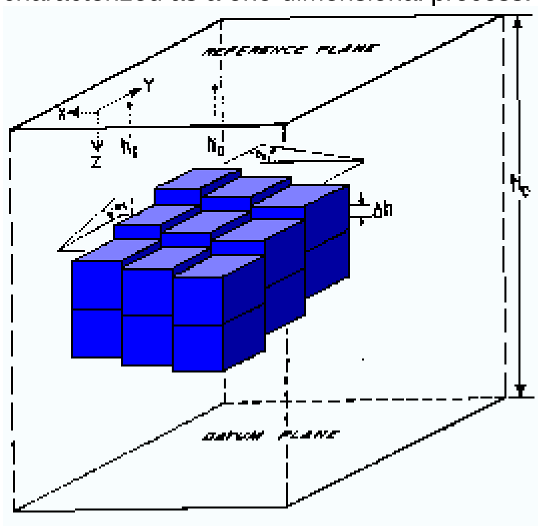
Introduction to SWIFT
SWIFT Features
SWIFT Basic Assumptions
SWIFT Method of Solution
SWIFT Equations
SWIFT Boundary Conditions
SWIFT Typical Applications
SWIFT Postprocessing
SWIFT STLINE Particle Tracking
SWIFT Runtime Monitor
SWIFT Basic Package
SWIFT Requirements

- Three-dimensional groundwater flow and transport
- Pressure, temperature, brine, radionuclides
- PC Interface

- Dual porosity and fractured media

INTRODUCTION TO SWIFT

SWIFT - 98 is a fully transient, three-dimensional model which simulates the flow and transport of fluid, heat (energy), brine, and radio nuclide chains in porous and fractured geologic media. The primary equations for fluid, heat, and brine are coupled with fluid density, fluid viscosity, and porosity. Steady-state options are available for the fluid and brine equations, and both Cartesian and cylindrical coordinate systems may be used. However, the latter system is restricted to two-dimensional, r-z simulations. Both dual-porosity and discrete-fracture conceptualizations may be considered for the fractured zone. Migration within the rock matrix is characterized as a one-dimensional process.



SWIFT FEATURES

- A run-time monitor displays the simulation progress, convergence, mass balance, and dialog.
- Versatile interface to SURFER for contouring pressure, temperature and concentration.
- Extensive error checking.
- Auxiliary files for variable structure grid, restart, mapping, mass balance, well summary and concentration discharge.
- STLINE code for particle tracking.
- Easy installation, 70 verification QA/QC data sets.

SWIFT BASIC ASSUMPTIONS AND CHARACTERISTICS

- Single-phase fluid flow governed by Darcy's law
- Three-dimensional transport in the global system, and one-dimensional transport in the local rock matrix subsystem
- Local rock matrix may be characterized by either prisms or spheres
- Linear variations in porosity and fluid density with respect to the dependent variables
- Viscosity is dependent on temperature and brine concentrations only
- Nonlinear isothermal equilibrium adsorption (Freundlich or linear)

- Injection wastes are miscible with the resident fluids
- Confined or unconfined aquifer (transient or steady-state free water surface)
- Hydraulic and thermal conductivities may be heterogeneous and/or anisotropic
- Longitudinal and transverse dispersivities may vary throughout the domain
- Variable rock compressibility (storativity)
- Dual or simultaneous discretization

SWIFT METHOD OF SOLUTION

Discretization is performed by the finite-difference method using centered or backward weighting in the time and space domains. Matrix solution is performed either by Gaussian elimination or by two-line successive overrelaxation.

SWIFT EQUATIONS

SWIFT comprises the four transport processes: fluid, heat, brine and radionuclide chains. For porous media, only the global (three-dimensional) process simulator is used. For fractured media, the global process simulator is used for the fractured media, and the local (one-dimensional) process simulator is used for the rock matrix.

SWIFT BOUNDARY CONDITIONS

A variety of boundary conditions and source terms may be invoked for both the porous and fractured media. These include:

- Prescribed pressure (head), temperature, and brine concentration
- Prescribed flux of fluid (water), heat, brine, or nuclide mass
- Wellbore injection/production submodel subject to pumping constraints
- Aquifer influence function (i.e., Carter-Tracy infinite reservoir)
- Dual porosity domain extension
- Waste-leach radionuclide submodel for waste repository nuclides and heat
- Freewater surface with recharge

SWIFT TYPICAL APPLICATIONS

SWIFT can be applied to a variety of groundwater problems ranging from simple well flow to complex transport analysis.

- Deep well injection of hazardous waste, isothermal/nonisothermal, constant/variable density
- Hazardous waste site characterization and remediation (RI/FS)
- Pump-and-treat, hydraulic containment and other waste remediation
- Saltwater intrusion, upconing
- Aquifer thermal energy storage
- High-level radioactive waste performance assessment

- Fractured media, dual porosity

SWIFT POSTPROCESSING

Postprocessor Interface (UNSWIFT) - Contour maps of pressure, temperature, brine, or concentration in any window in any plane can be quickly processed directly into uniformly-spaced grid files for the SURFER contouring software.

SWIFT STLINE PARTICLE TRACKING

Allows transient flowpath evaluation of streamlines and export to SURFER as lines or posted symbols.

SWIFT RUNTIME MONITOR

The runtime monitor displays essential simulation data on a conventional PC monitor using standard ANSI characters. The monitor tracks the simulation progress, highlighting the current program activity at the base of the screen. The time step, interval and other data are updated on the screen through the course of the simulation. Below the frame, system RAM requirements, matrix convergence (L2SOR only), creation of map file, and error messages are displayed. Auxiliary files for restart or binary input are also prompted.

SWIFT BASIC PACKAGE

- SWIFT Data Input Guide
- SWIFT and SWIFT II documents (4 publicly available NTIS reports)
- All FORTRAN source code and 70 verification problem input and output data sets on diskettes

With sufficient memory resources, SWIFT can be used to model complex field applications at a reasonable price. SWIFT users can choose either support or nonsupported. Optional training is available.

SWIFT Requirements: Pentium with 32 MB RAM and Lahey LF90 Version 4.5 compiler, and Surfer for postprocessing graphics.

TOUGH2 Software

Summary

TOUGH2 offers the flexibility to handle different fluid mixtures, the properties of which are described in separate Equation-of-State (**EOS**) modules. **TOUGH2** uses an integral finite difference method for space discretization, and first-order fully implicit time differencing. A choice of a sparse direct solver or various preconditioned conjugate gradient algorithms is available for linear equation solution. Thermophysical properties of water are represented, within experimental accuracy, by steam table equations. The program provides options for specifying injection or withdrawal of heat and fluids. Double-porosity, dual-permeability, and multiple interacting continua (MINC) methods are available for modeling flow in fractured porous media.

Although primarily designed for geothermal reservoir studies and high-level nuclear waste isolation, **TOUGH2** can be applied to a wider range of problems in heat and moisture transfer, and in the drying of porous materials. The **TOUGH2** simulator was developed for problems involving strongly heat-driven flow. To describe these phenomena a multi-phase approach to fluid and heat flow is used, which fully accounts for the movement of gaseous and liquid phases, their transport of latent and sensible heat, and phase transitions between liquid and vapor. **TOUGH2** takes account of fluid flow in both liquid and gaseous phases occurring under pressure, viscous, and gravity forces according to Darcy's law. Interference between the phases is represented by means of relative permeability functions. The code includes Klinkenberg effects and binary diffusion in the gas phase, and capillary and phase adsorption effects for the liquid phase. Heat transport occurs by means of conduction (with thermal conductivity dependent on water saturation), convection, and binary diffusion, which includes both sensible and latent heat.

Equation-of-State Modules

TOUGH2 provides multiple equation-of-state (EOS) modules, which define the components and phases and related thermophysical propeties (such as density, viscosity, enthalpy) of the fluid mixture being considered. The chosen EOS module is linked to the TOUGH2 core, which sets up the mass and energy balance equations, and solves the resulting strongly couples, nonlinear algebraic equations using Newton-Raphson iterations for each time step, which involves the calculation of a Jacobian matrix and the solution of a set of linear equations.

The following table lists the currently available EOS modules and the components and phases they handle.

TOUGH2 – http://esd.lbl.gov/research/projects/tough/software/tough2.html

Module	Components	Phases	Manual	Sample Problems	Comments
EOS1	water, water with tracer, heat	aqueous, gas	TOUGH2 User's Guide	r1q, rfp, rvf	Basic module for geothermal applications; see also EOS7 and EWASG
EOS2	water, CO_2, heat	aqueous, gas	TOUGH2 User's Guide	rfp	Basic module for near-surface, gaseous CO_2 applications; see also ECO2N, ECO2M, EOS7C, EWASG and TMVOC
EOS3	water, air, heat	aqueous, gas	TOUGH2 User's Guide	rhp, sam1	Basic module for vadose zone applications
EOS4	water, air, heat	aqueous, gas	TOUGH2 User's Guide	rhp	Same as EOS3, including vapor pressure lowering effects
EOS5	water, hydrogen, heat	aqueous, gas	TOUGH2 User's Guide	n/a	Applicable to corrosion-gas producing waste repositories
EOS7	water, brine, air, heat	aqueous, gas	TOUGH2 User's Guide	rf1	For multiphase, density-driven flows where salinity does not reach saturation levels; see also EOS7R, EWASG, ECO2N, and ECO2M
EOS7R	water, brine , air, radionuclide $_1$, radionuclide $_2$, heat	aqueous, gas	TOUGH2 User's Guide	rdica, rdif7	Same as EOS7, with parent-daughter radionuclides
EOS7C	water, brine, NCG (CO_2 or N_2), tracer, CH_4, heat	aqueous, gas	EOS7C User's Guide	sam7c 1-3	Applicable to CO_2 or N_2 in natural gas (CH_4) reservoirs; CO_2 is gaseous or supercritical; real gas law; tracer
EOS8	water, air, oil, heat	aqueous, gas, NAPL	TOUGH2 User's Guide	rcol8	Oil component is not volatile nor soluble, i.e., it is present only in the NAPL phase (“dead oil”)

EOS9	water	aqueous	TOUGH2 User's Guide	reos9a, rpm	Richards equation; saturated-unsaturated flow
EOS9nT	water, tracer, colloids	aqueous	EOS9nT User's Guide	Test 1-6	Richards equation; saturated-unsaturated flow; transport of multiple, non-volatile solutes/colloids; radioactive decay (including ingrowth), adsorption, advection/diffusion/dispersion, filtration, colloid-assited tracer transport, first-order chemical reaction
EWASG	water, NaCl, NCG (CO_2, air, CH_4, H_2, N_2), heat	aqueous, gas, solid	TOUGH2 User's Guide	rhbc	Applicable to geothermal reservoirs with saline fluids and a noncondensible gas; temperature-dependent NaCl solubility; includes sal precipitation and dissolution
ECO2N	water, brine, CO_2	aqueous, CO_2-rich phase	ECO2N User's Guide	r1dv, rcc3, rtab, rtp7	Applicable for simulation of geologic CO_2 sequestration in saline aquifers; CO_2 in gaseous, liquid and supercritical phases; no crossing of saturation line; salt precipitation and dissolution; see also EOS2 and ECO2M
ECO2M	water, brine, CO_2	aqueous, gaseous/liquid/ supercritical CO_2	ECO2M User's Guide	r1d, rcc3, rtab, rwaf	Multiphase version of ECO2N; includes transition between super and sub-critical conditions, and phase change between liquid and gaseous CO_2
T2VOC	water, air, VOC, heat	aqueous, gas, NAPL	T2VOC User's Guide	r3d, rblev, rfs, rgdif, rtce	Three-phase module for environmental applications; see also TMVOC and the T2VOC page
TMVOC	water, VOCs, NCGs	aqueous, gas, NAPL	TMVOC User's Guide	r2dl, r7c, rad, rblm, rbt, rdif2, rh2l, rtcem, rz2d	Three-phase module for simulating flow of multicomponent mixtures of VOC and one or multiple NCGs; see also T2VOC and the TMVOC page
NAPL: nonaqueous phase liquid NCG: noncondensible gas VOC: volatile organic compound					

Features & Capabilities

TOUGH2 is a general-purpose numerical simulation program for multi-dimensional fluid and heat flows of multiphase, multicomponent fluid mixtures in porous and fractured media. TOUGH2 solves mass and energy balance equations that describe fluid and heat flow in general multiphase, multicomponent systems. Fluid advection is described with a multiphase extension of Darcy's law; in addition there is diffusive mass transport in all phases. Heat flow occurs by conduction and convection, the latter including sensible as well as latent heat effects. The description of thermodynamic conditions is based on the assumption of local equilibrium of all phases. Fluid and formation parameters can be arbitrary nonlinear functions of the primary thermodynamic variables.

For numerical simulation the continuous space and time variables must be discretized. Space discretization is made directly from the integral form of the basic conservation equations, without converting them into partial differential equations. This "integral finite difference" method (IFDM) avoids any reference to a global system of coordinates, and thus offers the advantage of being applicable to regular or irregular discretizations in one, two, and three dimensions. The IFDM also makes it possible, by means of simple preprocessing of geometric data, to implement double- and multiple-porosity methods for fractured media. Time is discretized fully implicitly as a first-order backward finite difference. This together with upstream weighting of flux terms at interfaces is necessary to avoid impractical time step limitations in flow problems involving phase (dis-)appearances, and to achieve unconditional stability.

Applications

See TOUGH2 User's Guide and bibliography.

Licensing & Download

- See price list of available TOUGH2 modules.
- See price list for special TOUGH2 modules (e.g., EOS7C, EOS9nT).

Documentation

- TOUGH2 User's Guide
- ECO2N User's Guide
- ECO2M User's Guide
- T2VOC User's Guide
- TMVOC User's Guide
- EOS7R User's Guide
- EOS7C User's Guide
- EOS9nT User's Guide
- T2SOLV User's Guide
- T2DM User's Guide
- T2WELL User's Guide
- Hysteresis Module User's Guide

APPENDIX B

Publications Lists Found During the Literature Review

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APPENDIX B

Publications Lists Found During the Literature Review

During the literature review, a publication/citations list was found for several of the selected codes. This appendix contains those lists. The list for MODHMS includes references for MODHMS and for MODFLOW-SURFACE, which is the predecessor code for MODHMS. The list for TOUGH2 is extensive and includes applications for all modules of the code. Some of the lists are several years old, so do not include recent publications.

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FEFLOW Publications List Available in the Literature

FEFLOW Publications

The following list contains a number of publications about FEFLOW and about projects where FEFLOW has been used. This list is not complete, of course. If you know about any additional publications that should be listed here, please send the reference(s) to our support team!

We use JabRef (http://jabref.sourceforge.net/) for editing the BibTex database.

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Download this list as BibTeX file.

Order by: Author Year Journal Bibtex Type of Publication

2010

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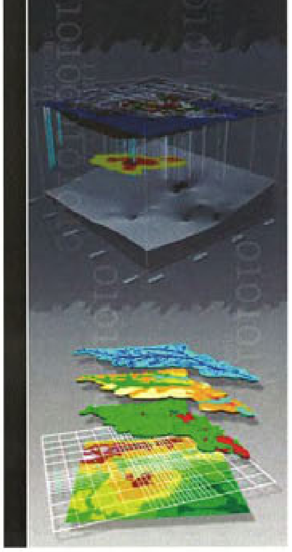

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