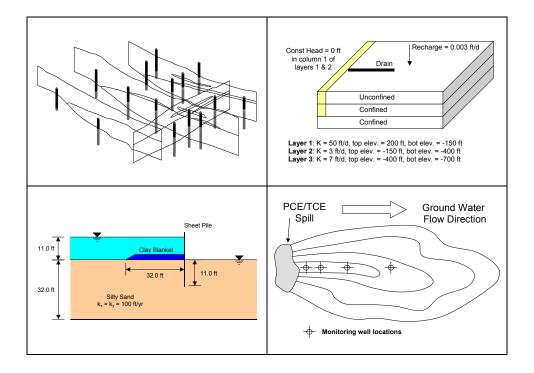
Groundwater Modeling System

TUTORIALS



Volume III

- FEMWATER
- SEEP2D
- UTCHEM
- GIS Module



GMS version 5.0

GMS 5.0 Tutorials

Copyright © 2004 Brigham Young University – Environmental Modeling Research Laboratory

All Rights Reserved

Unauthorized duplication of the GMS software or user's manual is strictly prohibited.

THE BRIGHAM YOUNG UNIVERSITY ENVIRONMENTAL MODELING RESEARCH LABORATORY MAKES NO WARRANTIES EITHER EXPRESS OR IMPLIED REGARDING THE PROGRAM GMS AND ITS FITNESS FOR ANY PARTICULAR PURPOSE OR THE VALIDITY OF THE INFORMATION CONTAINED IN THIS TUTORIAL DOCUMENT.

The software GMS is a product of the Environmental Modeling Research Laboratory (EMRL) of Brigham Young University.

emrl.byu.edu

Last Revision: July 19, 2004

TABLE OF CONTENTS

1	INT	RODUCTION	1-1
	1.1	SUGGESTED ORDER OF COMPLETION	
	1.2	DEMO VS. NORMAL MODE	
	1.3	FORMAT	
2	FEN	IWATER – FLOW MODEL	2-1
	2.1	DESCRIPTION OF PROBLEM	
	2.2	GETTING STARTED	
	2.3	REQUIRED MODULES/INTERFACES	
	2.4	BUILDING THE CONCEPTUAL MODEL.	
	2.4.1	1 0 0 0	
	2.4.2	5 0	
	2.4.3	0 0	
	2.4.4		
	2.4.5	8	
	2.4.6	5 8 5	
	2.4.7	8 - 78	
	2.4.8		
	2.4.9	0	
	2.5	BUILDING THE 3D MESH.	
	2.5.1	J 8	
	2.5.2	8	
	2.5.3 2.5.4	0	
	2.5.4		
	2.5.0		
	2.5.0	Hiding Objects	
	2.0	CONVERTING THE CONCEPTUAL MODEL	
	2.8	SELECTING THE ANALYSIS OPTIONS	
	2.8.1		
	2.8.2	5 I	
	2.8.3	0	
	2.8.4		
	2.9	DEFINING INITIAL CONDITIONS	
	2.9.1		
	2.9.2		
	2.10	DEFINING THE MATERIAL PROPERTIES	
	2.11	SAVING AND RUNNING THE MODEL	
	2.11	1 Viewing Head Contours	
	2.11	2 Viewing a Water Table Iso-Surface	
	2.11		
	2.12	CONCLUSION	2-20
3	SEE	P2D - CONFINED	3-1
	3.1	DESCRIPTION OF PROBLEM	

5	UTC	СНЕМ	5-1
	4.17	CONCLUSION	
	4.16	VIEWING THE SOLUTION	
	4.15	RUNNING SEEP2D	
	4.14	SAVING THE SIMULATION	
	4.13	0 1	
	4.13		
	4.13		
	4.13	8	
	4.13	MODELING FLOW IN THE UNSATURATED ZONE	
	4.12	VIEWING THE SOLUTION	
	4.11	RUNNING SEEP2D	
	4.10	SAVING THE SIMULATION	
	4.9.2		
	4.9.1	-r-g	
	4.9	Assigning Boundary Conditions	
	4.8	Assigning Material Properties	
	4.7	INITIALIZING THE SEEP2D SOLUTION	
	4.6	RENUMBERING THE MESH.	
	4.5.8	0	
	4.5.7	0 0 11	
	4.5.6	0 10	
	4.5.5	0	
	4.5.4	0	
	4.5.3	0	
	4.5.2	0 0	
	4.5.1	-J	
	4.5	CREATING THE MESH	
	4.4	SETTING THE UNITS	
	4.3	REQUIRED MODULES/INTERFACES	
	4.2	GETTING STARTED	
	4.1	DESCRIPTION OF PROBLEM	
-			
4	SFF	P2D - UNCONFINED	⊿_1
	3.12	CONCLUSION	3-13
	3.11	RUNNING SEEP2D	
	3.10	SAVING THE SIMULATION	
	3.9.1		
	3.9	Assigning Boundary Conditions	
	3.8	ASSIGNING MATERIAL PROPERTIES	
	3.7	INITIALIZING SEEP2D	
	3.6	RENUMBERING THE MESH	
	3.5.7		
	3.5.6	0	
	3.5.5	0	
	3.5.4	0	
	3.5.3		
	3.5.2		
	3.5.1	-, -, -, -, -, -, -, -, -, -, -, -, -, -	
	3.5	CREATING THE MESH	
	3.4	SETTING THE UNITS	
	3.3	REQUIRED MODULES/INTERFACES	
	3.2	GETTING STARTED	

5.1 I	DESCRIPTION OF PROBLEM	5-1
	Getting Started	
5.3 I	Required Modules/Interfaces	5-3
5.4 (CREATING THE GRID	5-3
5.5 (CONTAMINATION PHASE	5-4
5.5.1	Initializing the UTCHEM Simulation	5-4
5.5.2	Saving the Project	
5.5.3	Time Options	
5.5.4	Output Control	
5.5.5	Reservoir Properties	
5.5.6	Physical Properties	
5.5.7	Boundaries	
5.5.8	Wells	
5.5.9	Saving the Model and Running UTCHEM	
5.5.10		
5.5.11		
5.5.11		
	8 1	
	DISSOLUTION PHASE	
5.6.1	Initializing the UTCHEM Simulation	
5.6.2	General Options	
5.6.3	Time Options	
5.6.4	Drainage Option	
5.6.5	Capillary Pressure	
5.6.6	Saving and Running the Model	
5.6.7	Viewing the Solution	
5.6.8	Additional Simulations	
5.7 I	PRE-FLUSH PITT PHASE	
5.7.1	Initializing the UTCHEM Simulation	
5.7.2	General Options	5-22
5.7.3	Time Options	5-23
5.7.4	Physical Properties	5-24
5.7.5	Wells	5-25
5.7.6	Saving and Running the Model	5-28
5.7.7	Viewing the Solution	
5.8 V	Water Flush Treatment Phase	
5.8.1	Initializing the UTCHEM Simulation	
5.8.2	General Options	
5.8.3	Injection Period for Flushing	
	Physical Properties	
5.8.5	Editing the Well Data	
5.8.6	Saving and Running the Model	
5.8.7	Viewing the Solution	
	SURFACTANT FLUSH TREATMENT PHASE	
5.9.1	Initializing the UTCHEM Simulation	
5.9.2	General Options	
5.9.3	Editing the Injection Periods	
5.9.4	Initial Conditions	
5.9.4	Editing the Phase Behavior Parameters	
5.9.5 5.9.6		
5.9.0 5.9.7	Interfacial Tension	
	Relative Permeability	
5.9.8	Viscosity	
5.9.9	Component Density	
5.9.10	Diffusion and Dispersion	

5.9.11	Boundaries	
5.9.12	Editing the Concentrations at Wells	
5.9.13	Saving and Running the Model	
5.9.14	Viewing the Solution	
5.9.15	Designing a More Effective System	
5.10 P	OST-FLUSH PITT (OPTIONAL)	
5.10.1	Initializing the UTCHEM Simulation	
5.10.2	General Options	
5.10.3	Time Options	
5.10.4	Tracer Properties	
5.10.5	Wells	
5.10.6	Saving and Running the Model	
5.10.7	Viewing the Solution	
5.11 C	ONCLUSION	
6 GIS M	IODULE	
6.1 P	ART 1 - WITHOUT ESRI [®] ArcObjects [®]	6.1
	ETTING STARTED	
	LEQUIRED MODULES/INTERFACES	
	EQUIKED MODULES/INTERFACES	
	ZEADING THE SHAPEFILE	
	IEWING THE SHAPEFILE	
	CONVERTING THE SHAPEFILE TO 2D SCATTER POINTS	
	ONVERTING THE SHAPEFILE TO FEATURE OBJECTS	
6.8.1	Creating the Conceptual Model	
6.8.2	Mapping the GIS Data	
6.8.3	Part 1 Conclusion	
	ART 2 - WITH ESRI [®] ArcObjects [®]	
	AKT2 - WITHLIGKT ARCOBILITS	
0.10	ONCLUSION	
0.11 C		

CHAPTER

Introduction

This document contains tutorials for the Department of Defense Groundwater Modeling System (GMS). Each tutorial provides training on a specific component of GMS. Since the GMS interface contains a large number of options and commands, you are strongly encouraged to complete the tutorials before attempting to use GMS on a routine basis.

The tutorials are not intended to teach groundwater modeling concepts. They are only meant to illustrate the use of GMS.

In addition to this document, the online GMS Help document also describes the GMS interface. Typically, the most effective approach to learning GMS is to complete the tutorials before browsing the GMS Help document.

1.1 Suggested Order Of Completion

In most cases, the tutorials can be completed in any desired order. However, some of the tutorials are pre-requisites for other tutorials. Tutorials that have other tutorials as pre-requisites will indicate it at the beginning of the tutorial.

1.2 Demo vs. Normal Mode

The interface for GMS is divided into eleven modules. Some of the modules contain interfaces to models such as MODFLOW. Such interfaces are typically contained within a single menu. Since some users may not require all of the modules or model interfaces provided in GMS, modules and model interfaces can be licensed individually. Modules and interfaces that have been

licensed are enabled using the *File* | *Register* command. The icons for the unlicensed modules or the menus for model interfaces are dimmed and cannot be accessed.

GMS provides two modes of operation: demo and normal. In normal mode, the modules and interfaces you have licensed are undimmed and fully functional and the items you have not licensed are dimmed and inaccessible. In demo mode, all modules and interfaces are undimmed and functional regardless of which items have been licensed. However, all of the print and save commands are disabled.

The modules and interfaces needed for the tutorial are listed at the beginning of each tutorial. While some of the tutorials may be completed in either normal or demo mode, many of them can only be completed in normal mode. If some of the required items have not been licensed, you will need to obtain an updated password or hardware lock before you complete the tutorial.

1.3 Format

Throughout the tutorials, interface objects like menus or buttons, are shown in italics. Menu commands are given by specifying the menu followed by a "|" symbol followed by the command, like this: "Select the *File* | *Open* command". Values that must be entered by the user are given in bold, like this: "Enter **2.0** for the *Hydraulic conductivity*."

CHAPTER

FEMWATER – Flow Model

FEMWATER is a three-dimensional finite element ground water model. It can be used to simulate flow and transport in both the saturated and the unsaturated zone. Furthermore, the flow and transport can be coupled to simulate density dependent problems such as salinity intrusion. This tutorial describes how to build a FEMWATER model to simulate flow only.

2.1 Description of Problem

The site to be modeled in this tutorial is shown in Figure 2-1. The site is a small coastal aquifer with three production wells, each pumping at a rate of 100,000 ft^3/day. The no flow boundary on the upper left corresponds to a parallel flow boundary and the no flow boundary on the left corresponds to a thinning of the aquifer due to a high bedrock elevation. A stream provides a specified head boundary on the lower left and the remaining boundary is a coastal boundary simulated with a specified head condition.

The stratigraphy of the site consists of an upper and lower aquifer. The upper aquifer has a hydraulic conductivity of 10 ft/day and the lower aquifer has a hydraulic conductivity of 30 ft/day. The wells extend to the lower aquifer. The recharge to the aquifer is about one foot per year. The objective of this tutorial is to create a steady state flow model of the site.

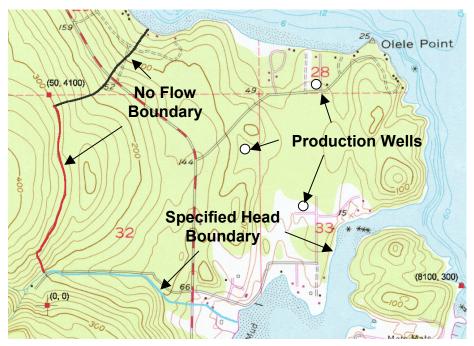


Figure 2-1 Site to be Modeled with FEMWATER Flow Model.

2.2 Getting Started

If you have not yet done so, launch GMS. If you have already been using GMS, you may wish to select the $File \mid New$ command to ensure the program settings are restored to the default state.

2.3 Required Modules/Interfaces

The license registration system used by GMS allows the components of GMS to be licensed individually, depending on the needs of the user. Before continuing, you may wish to check whether or not the GMS components used in this tutorial have been enabled in the copy of GMS you are using. This can be accomplished by selecting the *Register* | *File* command. On the left side of the *Register* dialog, the following components should have "ENABLED" displayed in the *Status* column to the right of each of the following components:

- Sub-surface characterization
- Mesh
- Geostatistics
- Map

FEMWATER

2.4 Building the Conceptual Model

FEMWATER models can be constructed using the direct approach or the conceptual model approach. With the direct approach, a mesh is constructed and the boundary conditions are assigned directly to the mesh by interactively selecting nodes and elements. With the conceptual model approach, feature objects (points, arcs, and polygons) are used to define the model domain and boundary conditions. The mesh is then automatically generated and the boundary conditions are automatically assigned. We will use the conceptual model approach for this tutorial.

2.4.1 Importing the Background Image

Before creating the feature objects, we will import a scanned image of the site. The image was generated by scanning a section of a USGS quadrangle map on a desktop scanner. The image has previously been imported to GMS and registered to real world coordinates. The registered image was saved to a GMS project file. To read the image:

- 1. Select the *Open* button $\stackrel{\frown}{\Longrightarrow}$.
- 2. Locate and open the directory entitled: tutfiles\femwater
- 3. Select the file entitled **start.gpr** and select the *Open* button.

2.4.2 Defining the Units

We will now define the units. GMS uses the units we select to plot helpful labels next to input edit fields.

- 1. Select the *Edit* | *Units* command.
- 2. Check to ensure that the default *Length* unit is **feet** and the default *Time* unit is **days**.
- 3. Change the *Mass* unit to **slug**. The remaining units are for a transport simulation and can be ignored.
- 4. Select the *OK* button to exit the *Units* dialog.

2.4.3 Initializing the FEMWATER Coverage

Before creating the feature objects, we first need to create a FEMWATER coverage.

- 1. Switch to the *Map* module \clubsuit .
- 2. Right-click on the *Map Data* folder in the *Data Tree* and, from the pop-up menu, select the *New Conceptual Model* command.
- 3. Change the *name* to "femmod".
- 4. Change the *model* to **FEMWATER** and click *OK*.
- 5. Right-click on the **femmod** conceptual model and select the *New Coverage* command from the pop-up menu.
- 6. Change the *Name* to "femwater".
- 7. Turn on the following properties:
 - Flow BC
 - Wells
 - Refinement
 - Meshing options
- 8. Select the *OK* button.

2.4.4 Creating the Boundary Arcs

We are now ready to begin creating the arcs defining the boundary of the model. Notice that the three boundaries on the left have been marked on the background image and are color-coded.

- 1. Select the *Create Arc* tool .
- 2. Using the boundary lines shown on the background image, create one arc for each of the three marked boundaries on the left side of the model. Click on a series of points along each line to trace the arc and double click at the end of the boundary to end the arc. Make sure the arcs are connected by starting one arc precisely at the ending point of the previous arc.
- 3. Create an arc for the coastline boundary. Once again, be sure the arc is connected to the other boundary arcs.

2.4.5 Redistributing the Arc Vertices

The two endpoints of each arc are called *nodes* and the intermediate points are called *vertices*. These arcs will be used to generate a 2D mesh that will be

converted into a 3D mesh. The spacing of the line segments defined by the vertices will control the size and number of elements. Thus, we need to redistribute the vertices along each arc to ensure that they are evenly spaced and of the correct length.

- 1. Select the *Select Arcs* tool **.**
- 2. Select all of the arcs by dragging a box that encloses all of the arcs.
- 3. Select the Feature Objects | Redistribute Vertices command.
- 4. Change the *Spacing* to **300**.
- 5. Select the *OK* button.

2.4.6 Defining the Boundary Conditions

Now that the arcs are defined, we can assign boundary conditions to the arcs. The two no-flow boundaries do not need to be altered since the default boundary type is no-flow. However, we need to mark the stream arc and the coastline arc as constant head arcs.

- 1. Select the *Select Arcs* tool **.**
- 2. While holding down the *Shift* key, click on both the stream arc and on the coastline arc.
- 3. Select the *Properties* button 😭.
- 4. In the *All* row in the spreadsheet, change the *Flow bc* to *spec. head*. This assigns this type to both arcs.
- 5. Select the *OK* button.

Note that no head values were assigned to the arcs. The head values are assigned to the nodes at the ends of the arc. This allows the head to vary linearly along the length of the arc. For the coastline arc, the head at both ends is the same. Since the default head value is zero, no changes need to be made. However, we do need to enter a head value for the upper end of the stream. The head will vary linearly along the stream from the specified value at the top to zero at the coast.

- 6. Select the Select Points/Nodes tool K.
- 7. Double click on the node at the top (left) end of the stream arc.
- 8. Enter a value of **200** for the head.
- 9. Select the *OK* button.

2.4.7 Building the Polygon

Now that the arcs are defined, we are ready to build a polygon defining the model domain. The polygon is necessary for two reasons: 1) it is used to define the model domain when the mesh is generated, and 2) it is used to assign the recharge. In many cases, the model domain is subdivided into multiple recharge zones, each defined by a polygon. In this case, we will use one polygon since we have a single recharge value.

1. Select the Feature Objects | Build Polygons command.

2.4.8 Assigning the Recharge

Next, we will assign the recharge value. There are two ways to assign recharge in FEMWATER: using a specified flux boundary or using a variable boundary. The variable boundary is more accurate but it is more time-consuming and less stable. To ensure that the tutorial can be completed in a timely fashion, we will use the simpler specified flux approach.

- 1. Select the *Select Polygons* tool \mathbb{E} .
- 2. Double click anywhere in the interior of the model domain.
- 3. Change the *Flow bc* to be **spec. flux**.
- 4. Enter a value of **0.003** for the flux (this value is in ft/d and corresponds to about 1.1 ft/yr).
- 5. Select the *OK* button.
- 6. Click anywhere outside the polygon to unselect it.

2.4.9 Creating the Wells

The final step in defining the conceptual model is to create the wells. To create the first well, do the following:

- 1. Select the *Create Point* tool
- 2. Click on a point anywhere in the upper right corner of the model.
- 3. Using the edit fields at the top of the screen, change the xyz coordinates of the point you just created to (52b90, **4206**, **45**). Hit the *Tab* or *Enter* key after entering each value.
- 4. With the point still selected, select the *Properties* button \square .

First, we will mark the point as a well point. For a well, we define the pumping rate, and the elevation of the screened interval. The screened interval is used to determine which nodes in the 3D mesh to assign the pumping rate to. The pumping rate is factored among all nodes lying within the screened interval. In our case, there will only be one node.

- 5. Change the *Type* to well.
- 6. Enter -185 for the *Top of screen*.
- 7. Enter -195 for the *Bottom of screen*.
- 8. Enter -100000 for the *Flow rate*.

Next, we will set the "*Refine*" option so that the mesh is refined around the well.

- 9. Turn on the Refine option.
- 10. Enter **150** for the *Element* size (this controls the element size at the well).
- 11. Select *OK* to exit the dialog.

Repeat this entire process to create two more wells with the following properties:

Well #	1	2
Х	3854	5026
Y	3034	1872
Z	75	45
Element size	150	150
Top of screen	-200	-240
Bottom of screen	-210	-250
Flux rate	-100000	-100000

2.5 Building the 3D Mesh

At this point, the conceptual model is complete and we are ready to build the 3D finite element mesh. The mesh will consist of two zones, one for the upper aquifer and one for the lower aquifer. The upper zone will consist of two layers of elements and the lower zone will consist of three layers of elements. To build the mesh, we will first create a 2D "projection" mesh using the feature objects in the conceptual model. We will then create three triangulated irregular networks (TINs): one for the top (terrain) surface, one for the bottom of the upper aquifer, and one for the bottom of the lower aquifer. We will then create the 3D elements by extruding each of the elements in the 2D mesh into a column of 3D elements.

2.5.1 Defining the Materials

Before building the mesh, we will define a material for each of the aquifers. The materials are assigned to the TINs and eventually to each of the 3D elements.

- 1. Select the *Edit* | *Materials* command.
- 2. Change the name of the default material to **Upper Aquifer**. To change the name click on the material name in the text window.
- 3. Change the material color to green.
- 4. Select the *New* button to create another material.
- 5. Change the name of the new material to Lower Aquifer.
- 6. Change the material color to red.
- 7. Select the *OK* button.

2.5.2 Building the 2D Projection Mesh

The 2D projection mesh can be constructed directly from the conceptual model:

- 1. Select the *Feature Objects* | $Map \rightarrow 2D$ Mesh command.
- 2. Select *OK* to accept the defaults in the *Map* \rightarrow 2*D Mesh* dialog.

After a few seconds, the mesh should appear.

2.5.3 Building the TINs

To build the TINs defining the stratigraphic horizons, we will make three TINs where each TIN is a copy of the 2D mesh. At first, these three TIN's will have the same elevations (zero) as the 2D mesh. We will then import a set of scatter points and interpolate the proper elevations to the TINs.

To create the top TIN:

- 1. Switch to the 2D Mesh module \blacksquare .
- 2. Select the *Build Mesh* | *Mesh* \rightarrow *TIN* command.
- 3. Enter terrain for the name of the TIN.
- 4. Select the list of materials, select *Upper Aquifer* (this defines the material below the TIN).

- 5. Select OK.
- 6. Select *No* at the prompt. We do not want to delete the 2D mesh.

To create the second TIN:

- 1. Select the *Build Mesh* | *Mesh* \rightarrow *TIN* command.
- 2. Enter **bottom upper aquifer** for the name of the TIN.
- 3. Select the list of materials, select Lower Aquifer.
- 4. Select OK.
- 5. Select *No* at the prompt.

To create the third TIN:

- 1. From the *Build Mesh* | *Mesh* \rightarrow *TIN* command.
- 2. Enter **bottom lower aquifer** for the name of the TIN.
- 3. Select the list of materials, select *Lower Aquifer* (this value is ignored for the bottom TIN).
- 4. Select OK.
- 5. Select *No* at the prompt.

2.5.4 Interpolating the Terrain Data

Next, we will use the scatter points defining the terrain elevations to interpolate to the top TIN. The terrain points were created by digitizing elevations from the contour map. Before interpolating to the TIN, we need to make sure the top TIN is the active TIN.

- 1. Switch to the *TIN* module \bigotimes .
- 2. From the Data Tree, select the TIN named terrain.

Before interpolating, we will make some adjustments to the interpolation options (based on our experience with these scatter point data).

- 3. Switch to the 2D Scatter Point module
- 4. Select the data set entitled terrain in the *Data Tree* to make it the active scatter point set.
- 5. From the Interpolation | Interpolation Options command.

- 6. Select the Options button next to the Inverse distance weighted item.
- 7. In the *Nodal function* section, select the *Constant* option.
- 8. Select the *OK* button and then the *OK* button to exit both dialogs.

To interpolate from the scatter points to the TIN.

- 9. Select the Interpolation | Interpolate \rightarrow Active TIN command.
- 10. Select the OK button.

To view the interpolated elevations:

- 11. Select the *Oblique View* macro
- 12. Select the Display | Settings command.
- 13. Enter a magnification factor of **4.0**.
- 14. Select the OK button.

2.5.5 Interpolating the Layer Elevation Data

Next, we will interpolate the elevations defining the bottom of the upper and lower aquifers. These elevations were obtained from a set of exploratory boreholes. Once again, before interpolating to the TIN, we need to make sure the desired TIN is the active TIN.

- 1. Switch to the *TIN* module \bigotimes .
- 2. Select the TIN named **bottom upper aquifer** from the *Data Tree*.

Before interpolating, we will switch back to the default interpolation method.

- 3. Switch to the 2D Scatter Point module
- 4. Select the Interpolation | Interpolation Options command.
- 5. Select the Options button next to the Inverse distance weighted item.
- 6. In the *Nodal function* section, select the *Gradient plane* option.
- 7. Select the *OK* button and then the *OK* button to exit both dialogs.

This scatter point set has two data sets: one set of elevations for the bottom of the upper aquifer and one set for the bottom of the lower aquifer. We will first interpolate the elevations for the bottom of the upper aquifer.

- 8. Select the data set entitled **elevs** in the *Data Tree* to make it the active scatter point set.
- 9. If necessary, expand the **elevs** item so you can see the data sets associated with the scatter point set.
- 10. Select the **bot of layer 1** data set to make it active.

To interpolate from the scatter points to the TIN.

- 11. Select the *Interpolation* | to Active TIN command.
- 12. Select the OK button.

Finally, we will interpolate the elevations for the bottom TIN.

- 13. Switch to the *TIN* module \bigotimes .
- 14. Select the TIN named bottom lower aquifer in the Data Tree.
- 15. Switch to the 2D Scatter Point module .
- 16. Select the data set named **bot of layer 2** in the *Data Tree*.
- 17. Select the Interpolation | to Active TIN command.
- 18. Select the OK button.

At this point, you should see the correct elevations on all three TINs. To simplify the display:

- 19. Switch to the *TIN* module \bigotimes .
- 20. Select the *Display Options* button
- 21. Turn off the Vertices option and turn on the Triangle faces option.
- 22. Select the OK button.

2.5.6 Building the 3D Mesh

We are now ready to build the 3D mesh. The 3D mesh is constructed by selecting a pair of TINs and then extruding elements between the TINs.

- 1. Select the *Select TINs* tool \mathfrak{W} .
- 2. Select the top and middle TINs by clicking on the icons for the TINs while holding down the *Shift* key.

- 3. Select the *Build TIN* | *Fill Between TINs* \rightarrow 3D Mesh command.
- 4. Enter 2 for the Number of interpolated mesh layers.
- 5. Select the *Specify material* option.
- 6. Select the material called Upper Aquifer.
- 7. Select the *OK* button.

Next, we will build the elements for the lower aquifer.

- 8. Select the bottom two TINs.
- 9. Select the *Build TIN* | *Fill Between TINs* \rightarrow 3D Mesh command.
- 10. Enter **3** for the Number of interpolated mesh layers.
- 11. Select the Specify material option.
- 12. Select the material called Lower Aquifer.
- 13. Select the *OK* button.

2.6 Hiding Objects

Before continuing, we will unclutter the display by hiding the objects we are finished with. We will hide everything but the feature objects and the 3D mesh.

To hide the TINs:

1. Uncheck all three TINs in the Data Tree.

We can also hide the scatter points:

- 2. Switch to the *2D Scatter Point* module
- 3. Uncheck both scatter point sets in the Data Tree.

To hide the 2D mesh:

- 4. Switch to the 2D Mesh module \mathbf{H} .
- 5. Hide the mesh by unchecking the 2D Mesh Data object in the Data Tree.

To unclutter the display of the 3D mesh:

- 6. Switch to the *3D Mesh* module \mathbf{II} .
- 7. Select the *Display Options* button
- 8. Turn off the Nodes option.
- 9. Select the OK button.

2.7 Converting the Conceptual Model

Now we are ready to convert the conceptual model to the 3D mesh model. This will assign all of the boundary conditions using the data defined on the feature objects.

- 1. Select the *FEMWATER* | *New Simulation* command. (this initializes the data structures for the FEMWATER simulation).
- 2. Select the *OK* button.
- 3. Switch to the *Map* module \clubsuit .
- 4. Select the *Feature Objects* | $Map \rightarrow FEMWATER$ command.
- 5. Select *OK* at the prompt (since we only have one coverage, the choice here does not matter).

A set of symbols should appear indicating that the boundary conditions have been assigned.

2.8 Selecting the Analysis Options

Next, we will switch to the 3D Mesh module and select the analysis options.

2.8.1 Entering the Run Options

First, we will indicate that we wish to run a steady state flow simulation:

- 1. Switch to the *3D Mesh* module \mathbf{II} .
- 2. Select the *FEMWATER* | *Run Options* command.
- 3. For the *Type of simulation*, ensure the *Flow only* option is selected.
- 4. In the Steady State vs. Transient section, select Steady state solution.

The problem we are solving has a very large partially saturated region, mainly in the upper left corner of the model. The larger the unsaturated zone, the more difficult it is to get FEMWATER to converge. For these types of problems, the *Nodal/Nodal* option is a qood choice for quadrature. It is not as accurate as the default option (*Gaussian/Gaussian*), but it is more stable.

- 5. In the *Quadrature selection* section, select the *Nodal/Nodal* option.
- 6. Select the *OK* button.

2.8.2 Setting the Iteration Parameters

Next, we will adjust the iteration parameters.

- 1. Select the *FEMWATER* | *Iteration Parameters* command.
- 2. Set the Max iterations for non-linear equation to 100.
- 3. Set the *Max iterations for linear equation* to **1000**.
- 4. Set the *Steady state convergence criterion* to **0.01**.
- 5. Select the *OK* button.

2.8.3 Selecting Output Control

Next, we will select the output options. We will choose to output a pressure head file only.

- 1. Select the *FEMWATER* | *Output Control* command.
- 2. Turn off the *Save nodal moisture content file*, *Save velocity file*, and *Save flux file* options.
- 3. Select the *OK* button.

2.8.4 Defining the Fluid Properties

Finally, we will define the fluid properties.

1. Select the *FEMWATER* | *Fluid Properties* command.

The items in this dialog are dependent on the units we have selected. Since this is a steady state solution, we can ignore the viscosity and compressibility options.

2. Enter **1.94** for the *Density of water*.

3. Select the *OK* button.

2.9 Defining Initial Conditions

Because of the non-linear equations used by FEMWATER to model flow in the unsaturated zone, FEMWATER is more sensitive to initial conditions than saturated flow models such as MODFLOW. If a set of initial conditions is defined that is significantly different than the final head distribution, FEMWATER may be slow or even unable to converge.

For a flow simulation, FEMWATER requires a set of pressure heads as an initial condition. The FEMWATER interface in GMS includes a command that can be used to automatically create a set of pressure heads from a userdefined water table surface. The water table surface is defined by a set of scatter points. A total head data set is generated by interpolating head values from the scatter points to the nodes of the 3D mesh. Finally, the pressure head data set is created by subtracting the node elevations from the total head values.

2.9.1 The Scatter Point Set

To define the initial condition, we will use a small set of points at the expected elevation of the computed water table surface. In the interest of time, these points have already been created for you and are already in the project. To learn more about how to create scatter points, refer to the tutorial in Volume I entitled *2D Geostatistics*.

Before digitizing the points, we will turn off the flux boundary condition display options.

- 1. Select the FEMWATER | BC Display Options command.
- 2. Turn off the *Flux* option.
- 3. Select the *OK* button.

To view the scatter point set.

- 4. Switch to *Plan View*
- 5. Switch to the 2D Scatter Point module
- 6. In the *Data Tree*, turn on the scatter point set named **Starting Heads**.

The scatter points should be located as shown in Figure 2-2. The values will not be visible by default, but you could turn them on if desired.

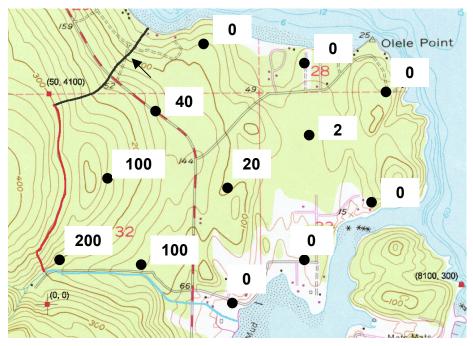


Figure 2-2 Locations and Elevations for New Points.

2.9.2 Creating the Data Set

Finally, to define the initial condition, we must create a pressure head data set. The data set will be saved to a data set file. The path to this file will be passed to FEMWATER when the simulation is launched.

- 1. Switch to the *3D Mesh* module \mathbf{II} .
- 2. Select the FEMWATER | Initial Conditions command.
- 3. In the *Cold start* section on the upper left side of the dialog, select the *Read from data set file* option.
- 4. Select the *Generate IC* button.
- 5. Select Starting_Heads for the Active 2D scatter point set.
- 6. Enter -200 for the *Minimum pressure head*.
- 7. Select the *OK* button.
- 8. When prompted for the file name, enter **starthd.phd** and select the *Save* button.
- 9. Select the OK button to exit the Initial Conditions dialog.

2.10 Defining the Material Properties

The final step in setting up the model is to define the material properties.

1. Select the *FEMWATER* | *Material Properties* dialog.

We need to enter a hydraulic conductivity and a set of unsaturated zone curves for each aquifer.

To define the material properties for the upper aquifer:

- 2. Select the *Upper aquifer material* from the list of materials.
- 3. Select the *FEMWATER Flow* tab.
- 4. Enter a value of **10.0** in the upper left edit field in the *Conductivity* section and select the *Isotropic* button. This should fill in all of the diagonal terms with a value of 10.0.
- 5. Select the Generate Curves button.
- 6. Set the *Curve type* to van Genuchten equations.
- 7. Enter **6.0** for the *Max. height above water table*.
- 8. Select the *Preset parameter values* section and select *Silt*.
- 9. Select the *Compute Curves* button.
- 10. Select the OK button.

To define the material properties for the lower aquifer:

- 11. Select the *Lower aquifer* item in the list at the top of the dialog.
- 12. Enter a value of **30.0** in the upper left edit field in the *Conductivity* section and select the *Isotropic* button
- 13. Select the Generate Curves button.
- 14. Select the Compute Curves button.
- 15. Select the *OK* button.
- 16. Select the OK button to exit the Material Properties dialog.

2.11 Saving and Running the Model

We are now ready to save and run the model.

- 1. Select the *File* | *Save As* command.
- 2. Enter **femmod.gpr** for the project name.
- 3. Select the *Save* button.

To run FEMWATER:

4. Select the *FEMWATER* | *Run FEMWATER* command.

The FEMWATER window should appear and you will see some information on the progress of the model convergence. The model should converge in a few minutes.

5. When the model converges, select the *Close* button.

2.11.1 Viewing Head Contours

First, we will view a color fringe plot.

- 1. Select the *Display Options* button .
- 2. Turn on the Contours option.
- 3. Select the *Options* button next to the *Contours* item.
- 4. Under the *Line* options section of the dialog change the color of the line to *blue*.
- 5. Select OK to exit the dialog.
- 6. Select the *FEMWATER* tab.
- 7. Turn off the *Head* option.
- 8. Select the *OK* button.

2.11.2 Viewing a Water Table Iso-Surface

Another way to view the solution is to generate an iso-surface at a pressure head of zero. This creates a surface matching the computed water table. Further, if we cap the iso-surface on the side greater than zero, we will get a color-shaded image of the pressure variation in the saturated zone.

- 1. Expand the **femmod** solution in the *Data Tree*.
- 2. Select **pressure_head** to make it the active data set.

- 3. Select the *Display Options* button
- 4. Turn off the *Element edges* and the *Contours* options.
- 5. Turn on the *Iso-surfaces* option.
- 6. Select the Options button next to the Iso-surfaces item.
- 7. Make sure that the number of iso-surfaces is 1.
- 8. For the upper value on the first line of the spreadsheet enter a value of **0.0**.
- 9. Turn on the *Fill between* toggle on the second line of the spreadsheet to fill between **0.0** and the maximum value.
- 10. Turn on the Iso-surface faces.
- 11. Turn on the Contour specified range option.
- 12. Set the *Minimum* to **0** and the *Maximum* to **456**.
- 13. Select the OK button to exit both dialogs.
- 14. Select the *Oblique View* macro 4.

2.11.3 Draping the TIFF Image on the Ground Surface

Finally, we will drape the TIFF image on the terrain surface to illustrate the spatial relationship between the computed water table surface and the ground surface. To do this, we will first unhide the top TIN.

- 1. Switch to the *TIN* module \bigotimes .
- 2. Check the box next to the terrain TIN to show it.
- 3. Select the terrain TIN in the *Data Tree* to make it active.

Next we will set the option to map the TIFF image to the TIN when shaded.

- 4. Switch to the *Map* module.
- 5. Select the *Display Options* button
- 6. Select the Images/Drawing tab.

<<< This option is not yet available >>>

After a short wait (this may take up to several minutes depending on the machine speed), the shaded image should appear. To view the image from the other side:

- 7. Select the *Rotate* tool \mathfrak{D} .
- 8. Click on the screen and drag horizontally to the left side of the screen. Repeat as necessary until the other side of the model is visible.

Finally, we will try the smooth shade option.

- 9. Select the *Display* | *Lighting Options* command.
- 10. Select the Smooth features option.
- 11. Select the *OK* button.

2.12 Conclusion

This concludes the *FEMWATER* – *Flow Model* tutorial. If you wish to exit GMS at this time:

- 1. Select the *File* | *Exit* command.
- 2. Select *No* at the prompt.

CHAPTER SEEP2D - Confined

SEEP2D is a 2D finite element, steady state, flow model. It is typically used for profile models, i.e., cross-section models representing a vertical slice through a flow system which is symmetric in the third dimension. Examples include earth dams, levees, sheet piles, etc.

SEEP2D can be used for both confined and unconfined problems. Accordingly, the SEEP2D tutorials are divided into two parts. The tutorial in this chapter describes how to set up and solve a confined seepage problem for SEEP2D using GMS. The steps required for simulating the unconfined condition are described in the following chapter. The two SEEP2D tutorials are entirely independent and can be completed in any order. However, it is recommended that the first tutorial be completed before the second tutorial since the motivation behind many of the steps in the model definition process is described in more detail in the first tutorial.

3.1 Description of Problem

The problem we will be solving in this tutorial is shown in Figure 3-1.

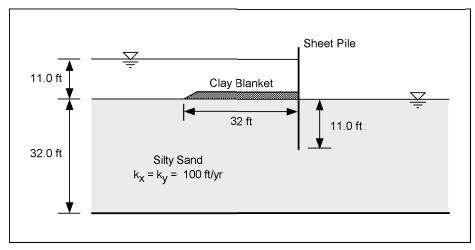


Figure 3-1 Confined Flow Problem.

The problem involves a partially penetrating sheet pile wall with an impervious clay blanket on the upstream side. The sheet pile is driven into a silty sand deposit underlain by bedrock at a depth of 32 feet.

From a SEEP2D viewpoint, this problem is a "confined" problem. For SEEP2D, a problem is confined if it is completely saturated. A problem is unconfined if it is partially saturated.

3.2 Getting Started

If you have not yet done so, launch GMS. If you have already been using GMS, you may wish to select the $File \mid New$ command to ensure the program settings are restored to the default state.

3.3 Required Modules/Interfaces

The license registration system used by GMS allows the components of GMS to be licensed individually, depending on the needs of the user. Before continuing, you may wish to check whether or not the GMS components used in this tutorial have been enabled in the copy of GMS you are using. This can be accomplished by selecting the *Register* | *File* command. On the left side of the *Register* dialog, the following components should have "ENABLED" displayed in the *Status* column to the right of each of the following components:

- Mesh
- Map
- SEEP2D

3.4 Setting the Units

We will start by setting the units we are using. GMS will display the units we select next to the input fields to remind us what they are.

- 1. Select the *Edit* | *Units* command.
- 2. Select **ft** for the *Length* units.
- 3. Select **yr** for the *Time* units.
- 4. Select *slug* for the *Mass* units.
- 5. Select the *OK* button.

3.5 Creating the Mesh

The first step in setting up the problem is to create the finite element mesh. Two types of elements can be used with SEEP2D: three node triangular elements and four node quadrilateral elements.

A variety of methods are available in GMS for constructing a 2D mesh. The approach we will use here will be to define the boundary of the mesh using map objects, and then use the $Map \rightarrow 2D$ Mesh command to automatically fill in the elements and nodes.

3.5.1 Defining a Coordinate System

Before we construct the mesh, we must first establish a coordinate system. We will use a coordinate system with the origin 90 feet upstream of the sheet pile at the top of the bedrock as shown in Figure 3-2.

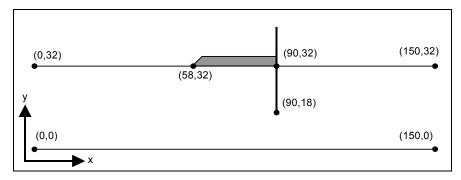


Figure 3-2 Coordinate System.

3.5.2 Creating the Conceptual Model

First we'll create a SEEP2D conceptual model. Then we'll create a coverage in that conceptual model.

- 1. Switch to the *Map* module $\mathbf{+}$.
- 2. In the *Data Tree*, right-click on the *Map Data* folder and select the *New Conceptual Model* command from the pop-up menu.
- 3. Change the *Name* to "Confined".
- 4. Change the *Model* to **SEEP2D**.
- 5. Click OK.
- 6. In the *Data Tree*, right-click on the **Confined** conceptual model and select the *New Coverage* command from the pop-up menu.
- 7. Turn on the following properties:
 - Refinement
- 8. Click OK.

3.5.3 Creating the Corner Points

We are now ready to create some points at key corner locations. These points will then be used to guide the construction of a set of arcs defining the mesh boundary.

- 1. Select the Create Point tool from the Tool Palette.
- 2. Click anywhere on the graphics window to create a point. Then edit the coordinates using the edit fields at the top of the GMS window. Change the *X*: value to **0.0** and the *Y*: value to **0.0**.
- 3. Create another point by clicking on the graphics window and change the x and y coordinates to **150.0** and **32.0** respectively.
- 4. Now select the *Frame* macro \Im_{K} .
- 5. Now create points at the following locations using the same steps as before:

Х	У
0	32
58	32
90	32
90	18
150	0

If you need to edit the node coordinates this can be done by using the *Select Points/Nodes* tool \bigwedge . When this tool is active you can select points and change the coordinates using the edit fields. You can also select points and delete them using the *Delete* key on the keyboard or the *Delete* command in the *Edit* menu.

The nodes you have created should resemble the nodes shown in Figure 3-3.

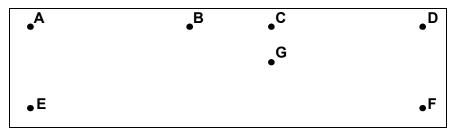


Figure 3-3 Points Created with the Create Point Tool

3.5.4 Creating the Arcs

Now that the corner nodes are created, the next step is to create the arcs. This can be accomplished as follows:

- 1. Select the *Create Arc* tool Γ .
- 2. Click on the existing points to create arcs between the points around the perimeter of the model. Start by clicking on point A, as shown in Figure 3-4, then B and so on to point F. Then double click on point A to finish creating the boundary.
- 3. Also create an arc for the sheet pile. Start by clicking on point C and double click on point G to finish.
- 4. Your model should now look like Figure 3-4.

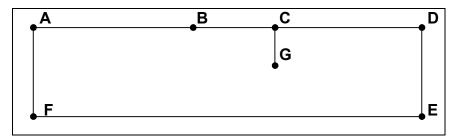


Figure 3-4 Arcs Connecting Points

3.5.5 Modeling the Sheet Pile

To model the sheet pile, we need a no-flow boundary. However, SEEP2D doesn't have a no-flow boundary condition that we can apply. Thus, we will put a break in the mesh at the location of the sheet pile, as shown in Figure 3-5.

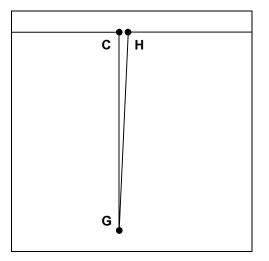


Figure 3-5 Sheet Pile Zoomed

To create the break, we need to add another point and another arc as shown in Figure 3-5. To create the point:

- 1. Use the *Zoom* tool \bigcirc to zoom up on the sheet pile area shown in Figure 3-5.
- 2. Choose the *Create Vertex* tool *.
- 3. Create point H by clicking anywhere on the arc to the right of node C.
- 4. With the vertex still selected, change the vertex coordinates to x = 90.25 and y = 32.0 using the x and y fields in the Edit Window.
- 5. With the vertex still selected, select the *Feature Objects* | *Vertices* $\leftarrow \rightarrow$ *Nodes* command.

This turns the vertex into a node and splits the arc into 2 arcs. Now we can delete the small arc between points C and H.

- 6. Select the *Select Arcs* tool **.**
- 7. Delete the small arc between points C and H by selecting it and hitting the Delete key.
- 8. Select the *Create Arc* tool .
- 9. Create the vertical arc between points G and H as shown in Figure 3-5 by clicking on point G and double-clicking on point H.
- 10. Select the *Frame* macro $\overrightarrow{\mathbf{A}}$ to see the entire model.

3.5.6 Redistributing Vertices

At this point, all of our arcs have one edge and zero vertices. When we issue the $Map \rightarrow 2D$ Mesh command, the density of the elements in the interior of the mesh is controlled by the edge spacing along the arcs. Thus, we will subdivide the arcs to create appropriately sized edges.

- 1. Choose the *Select Arcs* tool **.**
- 2. Select the *Edit* | *Select All* command.
- 3. Select the *Feature Objects* | *Redistribute Vertices* command.
- 4. Select the Specified spacing option.
- 5. Enter a value of **4.0** for the spacing.
- 6. Select the *OK* button.

Notice the arcs are divided into much smaller segments now.

3.5.7 Creating the Polygons and Building the Mesh

Before we can create the mesh, we first have to build a polygon. Simply creating the arcs does not create the polygon. We must explicitly create the polygons using the *Build Polygons* command.

1. Select the *Feature Objects* | *Build Polygons* command.

At this point, we are ready to construct the mesh.

2. In the *Feature Objects* | $Map \rightarrow 2D$ Mesh command.

3. Select *OK* at the prompt.

You should now see a 2D mesh.

3.6 Renumbering the Mesh

The next step in the model definition process is to renumber the nodes and elements. The sequence that the nodes are numbered has a dramatic impact on the amount of time required by SEEP2D to find a solution. The nodes and elements have been numbered in the order that they were created. This numbering is not optimal. The relative quality of the node numbering is indicated by the nodal half band width. The time required for a solution is quadratically proportional to the nodal half band width. To view the nodal half band width:

- 1. Switch to the 2D Mesh module \blacksquare .
- 2. In the *Data Tree*, right-click on the *2D Mesh Data* object and select the *Properties* command from the pop-up menu.
- 3. Note the Max node half band width.
- 4. Select the *Done* button.

The ID's of each of the nodes in the mesh can be displayed as follows:

- 5. Select the *Display Options* button **B**.
- 6. Turn on Node numbers.
- 7. Select the *OK* button.

To renumber the nodes and elements, we must first select a string of nodes on the boundary. This string of nodes defines a starting point for the renumbering process.

- 8. Choose the *Select Node String* tool ^.
- 9. Select the leftmost column of nodes in sequence from top to bottom. This can be done one of two ways:
- (a) Click on the top node, then the next node down and so on until all of the nodes in the column have been selected. Or,
- (b) Click on the top node in the column, and while holding down the *Control* key, click on the bottom node in the column. All of the intermediate nodes will automatically be selected.

10. Select the Modify Mesh | Renumber command.

Notice how the node numbering has changed. Bring up the *Get Info* dialog again to examine the new nodal half band width. Generally, the best node half band width occurs when a sequence of renumbering nodes is selected along the minor axis of the mesh. When in doubt, the mesh can be renumbered using several different strings of nodes to find the best numbering sequence.

To turn off the node numbers:

- 11. Select the *Display Options* button
- 12. Turn the Node numbers option off.
- 13. Select the *OK* button.

3.7 Initializing SEEP2D

Now that the mesh is constructed, we can begin to enter the SEEP2D data.

- 1. Select the SEEP2D | New Simulation command.
- 2. Select the Model Type section, select the Confined option.
- 3. Select the *OK* button to exit the dialog.

3.8 Assigning Material Properties

The next step in creating the model is to define material properties. There is one set of material properties for each zone of the mesh. The material properties are k_1 , k_2 , and an angle. The values k_1 and k_2 represent the two principal hydraulic conductivities and the angle is the angle from the x-axis to the direction of the major principle hydraulic conductivity measured counterclockwise as shown in Figure 3-6.

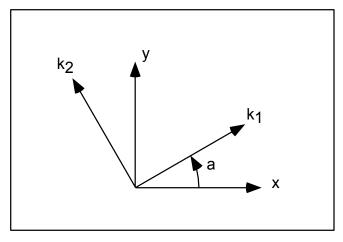


Figure 3-6 Definition of Hydraulic Conductivity Angle.

With most natural soil deposits, the major principal hydraulic conductivity is in the x direction, the minor principal hydraulic conductivity is in the y direction, and the angle is zero.

Each element in the mesh is assigned a material id. The material id is an index into a list of material properties. All of the elements we have created so far have a default material id of 1. This is sufficient since we only have one soil type in our problem. To enter the properties for material #1:

- 1. Select the SEEP2D | Material Properties command.
- 2. Enter a value of **100** for both *k1* and *k2*.
- 3. Select the *OK* button.

Note: The units for hydraulic conductivity are L/T (length / time). The length units should always be consistent with the units used in defining the mesh geometry. Any time units can be used. However, small time units (such as seconds) will result in very small velocity values and may make it difficult to display velocity vectors. It is recommended that time units of days or years be used.

3.9 Assigning Boundary Conditions

The final step in defining the model is to assign boundary conditions to the mesh. For the problem we are modeling there are two types of boundary conditions: constant head and no-flow (flow is parallel to the boundary). With the finite element method, not assigning a boundary condition is equivalent to assigning a no-flow boundary condition. Therefore, all of the boundaries have a no-flow boundary condition by default and all that is necessary in this case is to assign the constant head boundary conditions.

3.9.1 Constant Head Boundaries

h = 43 ft h = 32 ft 58 ft

The constant head boundary conditions for our mesh are shown in Figure 3-7.

Figure 3-7 Constant Head Boundary Conditions.

The region on the left in Figure 3-7 represents the top of the mesh on the upstream side that is not covered with the clay blanket. The region on the right represents the downstream side of the mesh. Using a datum of zero, the total head in either case is simply the elevation of the water. As mentioned above, all other boundaries on the mesh have a no-flow boundary condition by default.

To enter the constant head boundary conditions for the region on the left:

- 1. Choose the *Select Nodes* tool
- 2. Using the cursor and noting the cursor coordinates in the lower left corner of the screen, locate the node with the coordinates (58, 32). This node represents the left end of the clay blanket. Drag a box which just encloses this node and all of the other nodes on the top boundary to the left of this node, as shown in Figure 3-8.

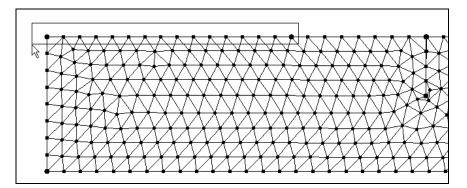


Figure 3-8 Selecting Nodes Where Head = 43.

- 3. Select the *SEEP2D* | *Node BC* command.
- 4. Select the *Head* option and enter a value of 43.

5. Select the *OK* button.

To enter the constant head boundary conditions for the region on the right:

- Using the cursor and noting the cursor coordinates in the lower left corner of the screen, locate the region of the mesh representing the top of the sheet pile. Recall that this is the location where we defined two nodes very close to each other. The coordinates of the nodes are (90, 32) and (90.25, 32).
- 7. Select the *Zoom* tool \bigcirc and zoom in on the top of the sheet pile until you can clearly distinguish the 2 nodes that are very close to each other.
- 8. Switch to the *Select Nodes* tool **•** and select the node on the right at the top of the sheet pile (the node with coordinates (90.25, 32).
- 9. Switch to the *Zoom* tool \bigcirc and zoom out until you can see all the nodes on the top boundary of the mesh to the right of the node you just selected.
- 10. Switch back to the *Select Nodes* tool **•**. While holding down the Shift key, drag a box that just encloses all of the nodes on the top boundary to the right of the sheet pile, as shown in Figure 3-9.

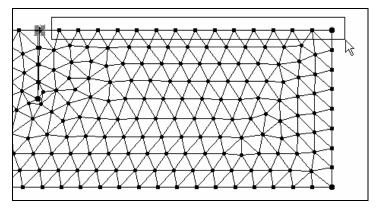


Figure 3-9 Selecting Nodes Where Head = 32.

- 11. Select the SEEP2D | Node BC command.
- 12. Select the *Head option* and enter a value of **32**.
- 13. Select the *OK* button.
- 14. Select the *Frame Image* macro

3.10 Saving the Simulation

We are now ready to save the simulation.

- 1. Select the *File* | *Save As* command.
- 2. Locate and open the directory entitled tutfiles\s2con.
- 3. Enter **blanket** for the file name.
- 4. Select the *Save* button.

3.11 Running SEEP2D

To run SEEP2D:

- 1. Select the *SEEP2D* | *Run SEEP2D* command. At this point SEEP2D is launched in a new window.
- 2. When the solution is finished, select the *Close* button.

GMS automatically reads in the SEEP2D solution. You should see the solution as a flow net. The flow net consists of equipotential lines (total head contours) and flow lines.

You can also view the total flow through the cross section. To turn on the display of the total flow through the cross section as do the following:

- 3. Select the *Display Options* button
- 4. Select the *SEEP2D* tab.
- 5. Turn on the *Title* and *Total flow rate* options.
- 6. Select the *OK* button.

3.12 Conclusion

This concludes the SEEP2D tutorial. If you wish to exit GMS at this time:

- 1. Select the *File* | *Exit* command.
- 2. Select *No* at the prompt.

CHAPTER SEEP2D - Unconfined

SEEP2D can be used for both confined and unconfined problems. The steps involved in performing a SEEP2D simulation for the unconfined condition are described in this tutorial.

Two approaches are available for unconfined problems with SEEP2D. With the first approach, the solution is only computed in the saturated zone and the mesh is truncated to the phreatic surface. The computed solution then consists of a new mesh geometry file and a solution file with the heads. With the second approach, the mesh is not deformed and the flow in both the saturated and unsaturated zones is computed. Both approaches will be illustrated in this tutorial.

It is recommended, but not required, that you complete the first SEEP2D tutorial (the previous chapter) before doing this tutorial.

4.1 Description of Problem

The problem we will be solving in this tutorial is shown in

Figure 4-1. The problem consists of an earth dam with anisotropic soil and a low permeability core in the interior.

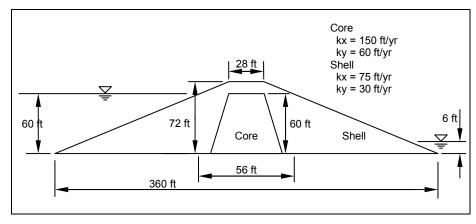


Figure 4-1 Unconfined Flow Problem

4.2 Getting Started

If you have not yet done so, launch GMS. If you have already been using GMS, you may wish to select the *File* | *New* command to ensure the program settings are restored to the default state.

4.3 Required Modules/Interfaces

The license registration system used by GMS allows the components of GMS to be licensed individually, depending on the needs of the user. Before continuing, you may wish to check whether or not the GMS components used in this tutorial have been enabled in the copy of GMS you are using. This can be accomplished by selecting the *Register* | *File* command. On the left side of the *Register* dialog, the following components should have "ENABLED" displayed in the *Status* column to the right of each of the following components:

- Mesh
- Map
- SEEP2D

4.4 Setting the Units

We will start by setting the units we are using. GMS will display the units we select next to the input fields to remind us what they are.

- 1. Select the *Edit* | *Units* command.
- 2. Select ft for the *Length* units.

- 3. Select **yr** for the *Time* units.
- 4. Select **slug** for the *Mass* units.
- 5. Select the *OK* button.

4.5 Creating the Mesh

The first step in defining the model is to create the finite element mesh. The mesh will be constructed using the $Map \rightarrow 2D$ Mesh command in the Map module. With this approach, we simply need to define the boundaries of the problem domain and GMS automatically constructs all of the interior nodes and elements.

4.5.1 Defining a Coordinate System

Before we construct the mesh we must first establish a coordinate system. We will use a coordinate system with the origin at the lower left corner of the dam as shown in Figure 4-2.

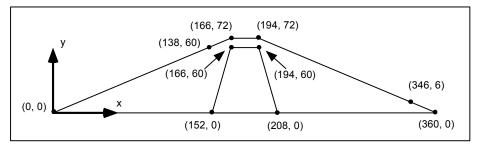


Figure 4-2 Coordinate System.

We will begin the mesh construction by creating some points at key locations in the mesh.

4.5.2 Creating a Coverage

Before we construct the feature objects defining the boundary of the mesh, we must first create a 2D mesh coverage.

- 1. Switch to the *Map* module +.
- 2. In the *Data Tree*, right-click on the *Map Data* item and select the *New Conceptual Model* command from the pop-up menu.
- 3. Change the name to SEEP2D Mesh.
- 4. Change the *Model* to **SEEP2D** and click *OK*.

- 5. Right-click on the **SEEP2D Mesh** conceptual model and select the *New Coverage* command from the pop-up menu.
- 6. In the list of Areal Properties, turn on Meshing options.
- 7. Select the *OK* button.

4.5.3 Creating the Corner Points

We are now ready to create some points at key corner locations. These points will then be used to guide the construction of a set of arcs defining the mesh boundary.

- 1. Select the *Create Point* tool from the *Tool Palette*.
- 2. Click anywhere on the graphics window to create a point. Then edit the coordinates using the edit fields at the top of the GMS window. Change the *X*: value to **0.0** and the *Y*: value to **0.0**.
- 3. Create another point by clicking on the graphics window and change the x and y coordinates to **194.0** and **72.0** respectively.
- 4. Create another point by clicking on the graphics window and change the x and y coordinates to **360.0** and **0.0** respectively.
- 5. Now select the *Frame* macro \Im_{K} .
- 6. Now create points at the following locations using the same steps as before:

х	У
138	60
166	72
166	60
194	60
152	0
208	0
346	6

If you need to edit the node coordinates this can be done by using the *Select Points/Nodes* tool \bigwedge . When this tool is active you can select points and change the coordinates using the edit fields. You can also select points and delete them using the *Delete* key on the keyboard or the *Delete* command in the *Edit* menu.

The nodes you have created should resemble the nodes shown in Figure 4-3 (without the labels).

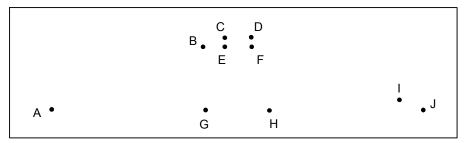


Figure 4-3 Points Created with the Create Point Tool

4.5.4 Creating the Arcs

Now that the corner nodes are created, the next step is to create the arcs defining the boundaries of both the shell and the core of the dam. This can be accomplished as follows:

- 1. Select the *Create Arc* tool .
- 2. Create a series of arcs around the perimeter of the dam by clicking on the following points in order (double click on the last point to end the sequence): A-B-C-D-I-J-H-G-A.
- 3. Create the remaining arcs around the core boundary by clicking on the following points in order (double click on the last point to end the sequence): G-E-F-H.

4.5.5 Redistributing Vertices

Arcs are composed of both nodes and vertices. The nodes are the two end points of the arc. The vertices are intermediate points between the nodes. The gaps between vertices are called edges. At this point, all of our arcs have one edge and zero vertices. When we issue the $Map \rightarrow 2D$ Mesh command, the density of the elements in the interior of the mesh is controlled by the edge spacing along the arcs. Thus, we will subdivide the arcs to create appropriately sized edges.

- 1. Choose the *Select Arcs* tool **.**
- 2. Select all of the arcs by dragging a box that encloses all of the arcs.
- 3. Select the *Feature Objects* | *Redistribute Vertices* command.
- 4. Select the *Specified spacing* option.
- 5. Enter a value of **8.0** for the *spacing*.
- 6. Select the *OK* button.

In this particular problem most of the head loss will occur in the core of the dam. To more accurately model the core we will make the mesh more dense in the core of the dam.

- 1. Select the arcs that make up the core of the dam (G-E, E-F, F-H, H-G).
- 2. Select the Feature Objects | Redistribute Vertices command.
- 3. Select the *Specified spacing* option.
- 4. Enter a value of **3.0** for the spacing.
- 5. Select the *OK* button.

4.5.6 Creating the Polygons

Now we are ready to create the polygons defining the two material zones. Simply creating the arcs does not create the polygons. We must explicitly create the polygons using the arcs.

1. Select the *Feature Objects* | *Build Polygons* command.

4.5.7 Assigning the Material Types

Now that the polygons are created, we need to define a material type to be associated with each polygon.

- 1. Select the *Edit* | *Materials* command.
- 2. Create a new material by clicking the *New* button.
- 3. Rename the materials to "Shell" and "Core". To change the name of a material simply double-click on the material in the list.
- 4. Click OK.
- 5. Choose the *Select Polygons* tool Σ .
- 6. Double click anywhere inside the polygon representing the shell of the dam.
- 7. Make sure the material associated with this polygon is the **Shell** material.
- 8. Select the *OK* button.

Now we will do the same for the other polygon.

- 9. Double click anywhere inside the polygon representing the core of the dam.
- 10. Make sure that **Core** is selected as the material for this polygon.
- 11. Select the OK button.
- 12. Click anywhere on the Graphics Window to unselect the polygon.

4.5.8 Constructing the Mesh

At this point, we are ready to construct the mesh.

- 1. In the *Feature Objects* | $Map \rightarrow 2D$ Mesh command.
- 2. Select *OK* at the prompt.

4.6 Renumbering the Mesh

The next step in the mesh construction process is to renumber the nodes and elements. The motivation behind the renumbering process and some tools for viewing node and element numbering are described in the previous tutorial and in the GMS *Online Help*.

To renumber the nodes and elements, we must first select a string of nodes on the boundary. This string of nodes defines a starting point for the renumbering process. In the case of a simple earth dam, the numbering is typically optimal if the renumbering begins at the leftmost or rightmost node in the mesh. Therefore, in this case, the string of nodes for renumbering will consist of only one node.

- 1. Switch to the 2D Mesh module \blacksquare .
- 2. Choose the *Select Node Strings* tool ^.
- 3. Select the leftmost node in the mesh (point A in Figure 4-3).
- 4. Select the *Modify Mesh* | *Renumber* command.

4.7 Initializing the SEEP2D Solution

Now that the mesh is constructed, we can begin to enter the SEEP2D data.

1. Select the *SEEP2D* | *New Simulation* command.

We will select the option to deform the mesh to the phreatic surface. This will model flow in the saturated zone only.

- 1. In the Model Type section, select the Unconfined option.
- 2. Select the Saturated with deforming mesh option.
- 3. Select the *OK* button to exit the dialog.

4.8 Assigning Material Properties

The next step is to define material properties. Each element in the mesh is assigned a material. The materials were automatically assigned to the elements using the polygons when the mesh was constructed. At this point, all that is left is to enter the hydraulic conductivity.

- 1. Select the SEEP2D | Material Properties command.
- 2. Highlight the material entitled Shell.
- 3. Enter a value of **150** for k_1 and **60** k_2 .
- 4. Highlight the material entitled **Core**.
- 5. Enter a value of 15 for k_1 and 6 k_2 .
- 6. Select the *OK* button.

4.9 Assigning Boundary Conditions

The final step in defining the model is to assign boundary conditions to the mesh. For the problem we are modeling there are three types of boundary conditions: (1) no-flow (flow is parallel to the boundary), (2) specified head, and (3) exit face. With the finite element method, not assigning a boundary condition is equivalent to assigning a no-flow boundary condition. Therefore, all of the boundaries have a no-flow boundary condition by default and all that is necessary is to assign the specified head and exit face boundary conditions.

4.9.1 Specified Head Boundary Conditions

The specified head boundary conditions for our mesh are shown in Figure 4-4.

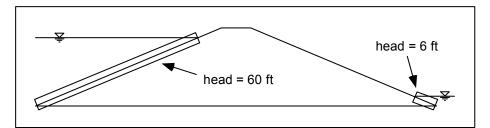


Figure 4-4 The Specified Head Boundary Conditions.

To enter the specified head boundary conditions for the region on the left:

- 1. Choose the *Select Node Strings* tool ^.
- 2. Select the node on the left face of the dam at y = 60 ft (where the water surface touches the dam on the upstream side). If you select the wrong node by mistake, press the ESC key.
- 3. While holding down the *Control* key, select the leftmost node on the mesh (at y = 0).
- 4. Select the *SEEP2D* | *Node BC* command.
- 5. Select the *Head* option and enter a value of **60**.
- 6. Click on the OK button.

To enter the specified head boundary conditions for the region on the right:

- 7. Select the rightmost node on the dam (at y = 0).
- 8. While holding down the *Control* key, select the node at y = 6 ft (where the water surface touches the dam on the downstream side).
- 9. Select the *SEEP2D* | *Node BC* command.
- 10. Select the *Head* option and enter a value of 6.
- 11. Click on the OK button.

4.9.2 Exit Face Boundary Conditions

The remaining type of boundary condition to enter is the exit face definition. Since we are using the deforming mesh option, SEEP2D will iterate to find the location of the phreatic surface. During this iteration, the geometry of the mesh will be altered so that the top of the mesh coincides with the phreatic surface. To guide the iteration process, we need to mark all of the nodes on the mesh where the phreatic surface may exit as exit face nodes. The region of the mesh where the phreatic surface may exit is illustrated in Figure 4-5.

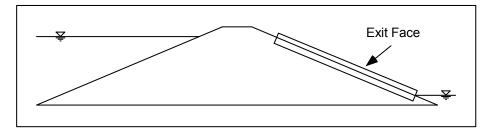


Figure 4-5 The Exit Face Boundary Condition.

To define the exit face boundary conditions:

- 1. Select the node just above the tail water level (the node just above the top specified head node) on the right side of the dam.
- 2. Holding down the *Control* key, select the node at approximately y = 60 ft on the right side of the dam.
- 3. Select the *SEEP2D* | *Node BC* command.
- 4. Select the *Exit Face* option.
- 5. Click on the *OK* button.

4.10 Saving the Simulation

We are now ready to save the simulation.

- 1. Select the *File* | *Save As* command.
- 2. Locate and open the directory entitled tutfiles\s2unc.
- 3. Enter **dam1** for the file name.
- 4. Select the *Save* button.

4.11 Running SEEP2D

We are now ready to run SEEP2D.

1. Select the *SEEP2D* | *Run SEEP2D* command.

At this point SEEP2D is launched in a new window. When the solution is finished, select the *Close* button. GMS will automatically read in the SEEP2D solution when this dialog is closed.

2. Select *OK* at the prompt to delete the existing mesh.

4.12 Viewing the Solution

You should now see a plot of the flow net. To better view the flow net, we will turn off the display of nodes and elements.

- 1. Select the *Display Options* button
- 2. Turn off the Nodes and Element edges options.
- 3. Turn on the Mesh boundary option.
- 4. Select the *OK* button.

Note that there are only a small number of flow lines. GMS determines the number of flow lines to display based on how closely spaced the equipotential lines are in one of the materials. By default, the interval is computed based on the Shell material. To base the number of flow lines on the Core material:

- 5. Select the *Display Options* button
- 6. Select the *SEEP2D* tab.
- 7. Select the Base Material pull-down list, select the Core material.
- 8. Select the *OK* button to exit the dialog.

You should now see a more flow lines through your model.

4.13 Modeling Flow in the Unsaturated Zone

For the last stage of the tutorial, we will compute a solution using a different approach. Rather than deforming the mesh and computing the solution in the saturated zone only, we will compute the flow in both the saturated and the unsaturated zone.

4.13.1 Reading in the Original Model

Before making the required changes to the model, we need to read the undeformed model back into memory.

- 1. Select the *File* | *Open* command.
- 2. Select *No* at the prompt to confirm we don't want to save changes if it appears.
- 3. Change the filter to be *Model Super Files*.
- 4. Select the file entitled dam1.sps.
- 5. Select the *Open* button.
- 6. Select *OK* at the prompt.

4.13.2 Changing the Mesh Display

Next, we will turn on the display of the nodes and elements.

- 1. Select the *Display Options* button
- 2. Turn on the *Element edges* option.
- 3. Select the *OK* button.

4.13.3 Changing the Analysis Options

Next, we will change the analysis options. Two methods are provided in SEEP2D for computing the relative conductivity in the unsaturated zone: the linear front method and the Van Genuchten method. With the linear front method, the relative conductivity varies linearly from the saturated value down to a user specified minimum at a given negative pressure head. With the Van Genuchten method, the Van Genuchten parameters are used to define the variation of the relative conductivity in the unsaturated zone. Both methods are described in detail in the SEEP2D Primer. We will use the linear front option.

- 1. Select the SEEP2D | Analysis Options command.
- 2. Enter Sample Unconfined Problem, Part II for the title.
- 3. In the *Model type* section, change the unconfined type to *Saturated/Unsaturated with linear front*.
- 4. Select the *OK* button.

4.13.4 Editing the Material Properties

Next, we need to define a minimum relative conductivity and a threshold pressure head for each material.

- 1. Select the SEEP2D | Material Properties command.
- 2. Select the material entitled Shell.
- 3. Enter a value of **-1.0** for *ho*.
- 4. Enter a value of **0.001** for *kro*.
- 5. Select the material entitled Core.
- 6. Enter a value of **-4.0** for *ho*.
- 7. Enter a value of **0.001** for *kro*.
- 8. Select the *OK* button.

4.14 Saving the Simulation

We are now ready to save the simulation and compute a new solution.

- 1. Select the *File* | *Save As* command.
- 2. Enter dam2.sps for the file name.
- 3. Select the *Save* button.

4.15 Running SEEP2D

To run SEEP2D:

1. Select the SEEP2D | Run SEEP2D command.

At this point SEEP2D is launched in a new window. When the solution is finished, select the *Close* button. GMS will automatically read in the SEEP2D solution when this dialog is closed.

4.16 Viewing the Solution

You should see a display of the equipotential lines and flow lines. To make the lines more visible:

- 1. Select the *Display Options* button **B**.
- 2. Turn off the *Element edges* option.

Another useful way to view a sat/unsat solution is to create a plot of the phreatic surface.

- 3. Select the *SEEP2D* tab.
- 4. Turn off the *Flow lines* option.
- 5. Turn on the *Phreatic surface* option.
- 6. Select the *OK* button.

The displayed line corresponds to the boundary between the saturated and unsaturated zones.

4.17 Conclusion

This concludes the SEEP2D tutorial. If you wish to exit GMS at this time:

- 1. Select the *File* | *Exit* command.
- 2. Select *No* at the prompt.

CHAPTER UTCHEM

UTCHEM is a highly sophisticated, multi-phase flow and multi-constituent, reactive transport model capable of performing a wide variety of groundwater simulations. UTCHEM was developed at the *Center for Petroleum and Geosystems Engineering* at the *University of Texas at Austin* as a chemical flood simulator for enhanced oil recovery design. In recent years, UTCHEM has been adapted for a variety of environmental applications as well, particularly surfactant-enhanced aquifer remediation (SEAR). The steps involved in setting up, running, and visualizing the results of a UTCHEM simulation are described in this tutorial.

5.1 Description of Problem

The problem to be solved in this tutorial is shown in Figure 20.1. This problem is a modified and expanded version of the ex21 and ex22 sample problems described in the UTCHEM documentation, which, in turn, are based on the SEAR demonstration at the Borden site (Brown and Jin, circa 1993). The problem is a single slice model in the X-Z plane with one PCE (perchloroethylene or, more accurately, tetrachloroethene) spill in the center. The evaluation and remediation are performed with one extraction well at the spill location and an injection well on either side. The regional gradient creates a flow from left to right.

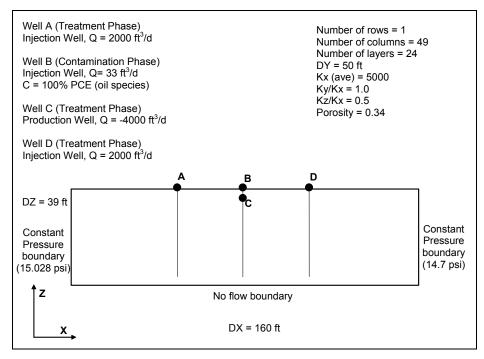


Figure 5-1 Sample Problem to be Solved with UTCHEM.

The problem is divided into six simulation phases, each designed to highlight particular aspects of UTCHEM. These simulation phases are described briefly as follows:

- **Contamination**. Define media and contaminant properties, initial and boundary conditions, and PCE release well. Simulate release of 1000 ft³ of PCE DNAPL (33.33 ft³/day for 30 days) at point C (Fig-1), followed by 60 days of redistribution. UTCHEM file: *UTC-contam.gpr*.
- **Dissolution**. Equilibrium PCE dissolution (only) from DNAPL and conservative transport over a 20 year period are simulated as a modification of simulation #1. UTCHEM file: *UTC-dissol.gpr*.
- **Pre-flush PITT**. A partitioning interwell tracer test (PITT) to assess DNAPL saturations is simulated. Injection and withdrawal wells are defined. This 60 day simulation is a modification of simulation #1. UTCHEM file: *UTC-prePITT.gpr*.
- **Water Flush**. A "pump and treat" simulation of 270 days of flushing using water. The results of this flush can be compared with the surfactant flush simulation. This is a restart from the UTC-contam.gpr simulation. UTCHEM file: *UTC-flush.gpr*.
- **Surfactant Flush**. A SEAR simulation using a surfactant to enhance dissolution and recovery; the 60 day simulation is a restart from the UCT-contam.gpr simulation. UTCHEM file: *UTC-SEAR.gpr*.

Post-flush PITT (optional). Same as simulation #3, but post-flush (i.e. restarting from simulation #4) to assess the success of the water flush. UTCHEM file: *UTC-postPITT.gpr*.

Although the six phases of this tutorial are designed to be run in sequence, they can be completed in any order using a set of provided sample files. A set of model files (with solutions) for each of the six phases can be found in the *gms\tutfiles\utchem\samples* directory.

5.2 Getting Started

If you have not yet done so, launch GMS. If you have already been using GMS, you may wish to select the *File* | *New* command to ensure the program settings are restored to the default state.

The user may select either metric or English units, which must be used consistently (mixing can be perilous). Several model parameters and their units may be unfamiliar to users accustomed to more traditional groundwater models. The units in UTCHEM reflect its roots in petroleum and chemical engineering disciplines. All time units are in days. Chemical concentrations are expressed in either volume fractions or mg/L (see UTCHEM documentation for details). We will be working in English units throughout these tutorials. Lengths will be in feet.

5.3 Required Modules/Interfaces

The license registration system used by GMS allows the components of GMS to be licensed individually, depending on the needs of the user. Before continuing, you may wish to check whether or not the GMS components used in this tutorial have been enabled in the copy of GMS you are using. This can be accomplished by selecting the *Register* | *File* command. On the left side of the *Register* dialog, the following components should have "ENABLED" displayed in the *Status* column to the right of each of the following components:

- Grid
- UTCHEM

5.4 Creating the Grid

The first step in setting up the flow simulation is to create the grid. Since this is a profile model in the xz plane, there will be only one cell width in the y-direction. To create the grid:

- 1. Switch to the *3D Grid* module \mathbb{H} .
- 2. Select the Grid | Create Grid command.
- 3. In the section entitled X-dimension, enter **160.0** for the *Length* value, and **49** for the *Number Cells* value. (dX = 160/49 = 3.265 ft)
- 4. In the section entitled Y-dimension, enter **50.0** for the *Length* value, and **1** for the *Number Cells* value.
- 5. In the section entitled Z-dimension, enter **39.0** for the *Length* value, and **24** for the *Number Cells* value. (dZ = 39/24 = 1.625 ft).
- 6. Keep *Orientation/type* set to *MODFLOW*. Keep *Rotation about Z-axis* at **0.0**. These are the default values.
- 7. Select the *OK* button.

A grid should appear in the *Graphics Window*. The grid appears as a single row since we are looking down the z axis at the xy plane. To view the xz plane:

8. Select the *View I Axis* macro 🗟 .

5.5 Contamination Phase

The first phase of our simulation will be to model the spill and dispersal of a pure PCE DNAPL from near the surface. The spill will be simulated using a single injection well in the center of the model that injects a steady stream of the DNAPL over a thirty-day period.

5.5.1 Initializing the UTCHEM Simulation

To initialize a new UTCHEM simulation:

1. Select the UTCHEM | New Simulation command.

First, we will enter the Titles and other basic information.

- 2. For the *Run* number, enter "EX21-1"
- 3. For *Title 1*, enter: "2D (X-Z) PCE DNAPL Release in Saturated Heterogeneous Media (EX21)".
- 4. For *Title 2*, enter: "30 day PCE spill 60-day redistribution"
- 5. For *Title 3*, enter your name and the current date.

- 6. For the *Numerical dispersion* control, choose the **Improved TVD 3rd order** method from the dropdown menu.
- 7. This is not a restart simulation, so leave the *Use Restart* option unselected (we will make use of this later).
- 8. Ensure that the default units are *English*.

Next, we will define the species used in the simulation. This simulation will model two species: water and PCE.

- 9. Select the *Define Species* button.
- 10. Unselect the *Surfactant*, *Chloride*, *Calcium*, *Alcohol 1*, *Air/Gas* species toggles. At this point, only two names should show up in the names list window (water and oil).
- 11. Select the *oil* species and change the name to PCE.

We also need to define four water/oil tracers. We will not be using these tracers in the contamination phase of the simulation. However, we will be using the tracers for the PITT simulation later in the tutorial. If any supplemental species are used (NAPLs, tracers, or bio species) in a restartbased simulation, UTCHEM requires that these species be defined in the original run used to generate the restart file. Thus, in order to use the contamination simulation as a restart file for later runs, we need to have the tracers defined in this simulation. These species will not be injected into the model for this simulation, so they essentially act as "dummy" species.

- 12. Change the number of *Water/Oil Tracers* to 4. Four *wot* (water/oil tracer) entries should appear in the *Names* list.
- 13. Rename the *wot* entries to **1Pr**, **2Pr**, **Hex**, and **Hep**. In subsequent dialogs, these tracers will be listed as *1Pr_wo*, *2Pr_wo*, *Hex_wo*, and *Hep_wo*.
- 14. Select the OK button twice to exit both dialogs.

5.5.2 Saving the Project

Before continuing, we will save the files associated with the simulation.

- 1. Select the *File* | *Save As* command.
- 2. Locate the **gms\tutorials\utchem**\ directory.
- 3. Enter "UTC-contam.gpr" for the file name.
- 4. Select the *Save* button.

Having saved and named the project, you can now select the *Save* macro is save your changes as you go along through the tutorial.

5.5.3 Time Options

The next step is to set up the time options for the UTCHEM output and the time step control.

- 1. Select the UTCHEM | Time Options command.
- 2. Ensure that **Days** is selected as the option for both the *Output* and *Max* & *Inject* option controls.
- 3. For the *Time step size* option, choose Automatic.

Injection Periods

The time domain of a UTCHEM simulation is subdivided into *Injection Periods*. Pumping rates and boundary condition values can only change at the beginning of an injection period. For the contamination phase of this simulation, we will create a 30-day injection period, followed by 60-day redistribution period.

1. Select the *Injection Periods*... button.

By default, GMS creates one injection period so we will simply change the length of the first period (PCE injection) and then insert a second period (PCE redistribution).

2. Enter **30.0** [days] as the *Length* value for *Injection period* #1.

Before creating the second injection period, we will complete the input for the first injection period. By doing so, all of the values defined for the first period will be the default values when we create the second period.

Time steps

When using the automatic time step option, UTCHEM allows the minimum and maximum time steps to be governed by *Courant numbers* or *Days*. For injection periods where the flow rate in one or more wells is non-zero, the *Courant number* option is generally preferable. For injection periods with no well activity, the *Days* option must be used. Since the first injection period corresponds to a spill event simulated with a well, we will use the *Courant number* option. The initial time step size always has units of days. A description of these options can be found in *Appendix E* of the *UTCHEM User's Guide*.

1. Enter a value of **0.001** for the *Initial time step size* value.

- 2. Enter a value of **0.003** for the *Tol. for conc. change* value.
- 3. In the *Time steps* section, choose *Courant Numbers* as the units for the min and max time steps.
- 4. Enter a value of **0.15** for the *Max time step size* value.
- 5. Enter a value of **0.01** for the *Min time step size* value.

Output Intervals

The *Output Intervals* determine when values will be saved from UTCHEM. The most important of these is the *Profiles* value. This determines at what intervals concentration values will be output to GMS data set solution files.

- 1. Enter a value of **15.0** for the *Print data* value.
- 2. Enter a value of **15.0** for the *Prod. data* value.
- 3. Enter a value of **5.0** for the *Prod. histories* value.
- 4. Enter a value of **5.0** for the *Profiles* value.

Second Injection Period

Next, we will define a second Injection Period of 60 days, during which the PCE injected in the first 30 day period is allowed to redistribute.

- 1. Select the *Insert Right* button to create the second injection period. Note that all of the *Time steps* and *Output intervals* from the first period are retained as initial settings for this period.
- 2. Make sure that the *Injection period field counter* is at **2** and enter a value of **60** for the *Length*.

Since this injection period does not include any injection or extraction via wells, we must use the *Days* option for the min and max time step values.

- 3. In the *Time steps* section, choose *Days* as the units for the *min and max time steps*.
- 4. Enter a value of **0.28** for the *Max time step size* value.
- 5. Enter a value of **0.014** for the *Min time step size* value.

This concludes the input for the Injection Periods dialog.

6. Select *OK* button twice to exit both dialogs.

5.5.4 Output Control

Output Control allows us to choose what data will be saved from UTCHEM.

1. Select the UTCHEM | Output Control command.

The *Profiles* section includes data that can be saved in GMS dataset solution format, and should be checked on by default. The *Print* section includes other important data output from UTCHEM that can be viewed in a text editor. In the *Profiles* section, we want to output *Phase pressures, Phase saturations,* and *Component concentrations.* In the *Print* section, we want all options to be off. This should correspond to the default options in the dialog so no changes need to be made.

2. Select the *OK* button the exit the *Output Control* dialog.

5.5.5 Reservoir Properties

In the *Reservoir Properties* section, we will define the aquifer characteristics. Some properties, such as porosity and pressure, will be entered as an array of values (one for each cell). The other properties, like the hydraulic conductivity ratios, are single values applied to the aquifer as a whole.

- 1. Select the UTCHEM | Reservoir Properties command.
- 2. Make sure that the *Rock Compressibility* value is **0.0** and the *Reference pressure* value is **14.7**.

Porosity

To define the porosity:

- 1. Select the *Porosity* button.
- 2. Select the *Constant* \rightarrow *Grid* button and enter a value of **0.34**.
- 3. Select *OK* on both dialogs to return to the *Reservoir Properties* dialog.

Initial Conditions

To define the initial conditions:

- 1. Select the *Pressure* button.
- 2. Select the *Constant* \rightarrow *Grid* button and enter a value of 14.7.
- 3. Select OK on both dialogs to return to the Reservoir Properties dialog.
- 4. Select the *Water Sat* button.

- 5. Select the *Constant* \rightarrow *Grid* button and enter a value of **1.0** (default).
- 6. Select OK on both dialogs to return to the Reservoir Properties dialog.

Permeability (k)

The average permeability at the Borden test site was approximately 8300 millidarcies (md). For this tutorial, we will use a somewhat lower value (5000 md) for most of the domain, with four lower-*k* layers (3000 md) at grid layers 5, 10, 15, and 20. The lower permeability prevents the PCE from dropping straight to the bottom. The simple heterogeneities demonstrate model stability, but also make for a more interesting and realistic tutorial. For those unfamiliar with Darcy units of intrinsic permeability, 1 Darcy is equivalent to 1 μ m² or 10⁻⁸ cm² or, if the fluid is water, a hydraulic conductivity of 10⁻³ cm/s.

- 1. Select the *Kx* button.
- 2. Select the *Constant* \rightarrow *Grid* button.
- 3. Enter a value of **5000**; Press *OK*.
- 4. Move the *Layer* counter to 5.
- 5. Select *Constant* \rightarrow *Layer* button (**not** the *Constant* \rightarrow *Grid* button this time).
- 6. Enter a value of **3000**.
- 7. Repeat steps 4-6 for layer 10, 15, and 20.
- 8. Click OK on both dialogs to return to the Reservoir Properties dialog.
- 9. Ensure that the Ky/Kx value is set at 1.0.
- 10. Change the Kz/Kx value to **0.5**.
- 11. Select OK to exit the Reservoir Properties dialog.

Notice that the values defined by arrays can also be edited on a cell-by-cell basis if necessary. One quick way to perform such editing is to select the cells and use the *UTCHEM* | *Cell Properties* command.

5.5.6 Physical Properties

Next, we will enter the *Physical Property* data. These data include relative permeability, viscosity, density, compressibility, dispersion, and sorption parameters. These items are organized in a submenu in the *UTCHEM* menu.

Phase Behavior

The phase behavior properties are related to surfactants and cosolvents, which are not being used in this case. We will edit these values in a later tutorial.

Interfacial Tension

These values are also related to surfactant properties.

Organic Mass Transfer

To edit the organic mass transfer parameters:

- 1. Select the UTCHEM | Physical Properties | Organic Mass Transfer command.
- 2. Select the *Allow solubility of oil in water in absence of surfactant* option.
- 3. Enter a value of **0.00015** for the *Equilibrium conc. of oil in water*. [Note: These are volume fraction units. PCE liquid density is 1.623 g/cm³ or 1.623E+06 mg/L. In more familiar units, this equilibrium concentration is 243.45 mg/L, within the reported solubility range for PCE at 20C (150-250 mg/L)].
- 4. Click OK to exit the Organic Mass Transfer dialog.

Relative Permeability

To edit the relative permeability data:

- 1. Select the UTCHEM | Physical Properties | Relative Permeability command.
- 2. Choose the *First drainage corey* option.

Note: When simulating an initial spill, the *First drainage corey* option is preferable. Studies have shown that it best simulates gravity drainage of DNAPLs. However, for flushing simulations, the *Imbibition corey* option produces the best results. We will use the *First drainage corey* option for this phase and use the *Imbibition corey* option later in the tutorial for the flushing simulations.

In the Aqueous column, do the following:

- 3. Select the *Residual Saturation* button.
- 4. Select the *Constant* \rightarrow *Grid button* and enter a value of **0.24**.
- 5. Select *OK* on both dialogs to return to the *Relative Permeability* dialog.

- 6. Select the Kr Endpoint button.
- 7. Select the *Constant* \rightarrow *Grid* button and enter a value of **0.486**.
- 8. Select OK on both dialogs to return to the *Relative Permeability* dialog.
- 9. Select the Kr Exponent button.
- 10. Select the *Constant* \rightarrow *Grid* button and enter a value of **2.85**.
- 11. Select OK on both dialogs to return to the Relative Permeability dialog.

In the *Oleic* column, do the following:

- 12. Select the Residual Saturation button.
- 13. Select the *Constant* \rightarrow *Grid* button and enter a value of **0.17**.
- 14. Select OK on both dialogs to return to the Relative Permeability dialog.
- 15. Select the Kr Endpoint button.
- 16. Select the *Constant* \rightarrow *Grid* button and enter a value of **0.65**.
- 17. Select OK on both dialogs to return to the *Relative Permeability* dialog.
- 18. Select the Kr Exponent button.
- 19. Select the *Constant* \rightarrow *Grid* button and enter a value of 2.7.
- 20. Select OK on both dialogs to return to the Relative Permeability dialog.

We're now done with the *Relative Permeability* dialog.

21. Select the OK button to exit the Relative Permeability dialog.

Viscosity

Next, we will enter the viscosity data:

- 1. Select the UTCHEM | Physical Properties | Viscosity command.
- 2. Change the *Water viscosity* value to 1.0.
- 3. Change the *Oil viscosity* value to **0.89**.
- 4. Make sure the *Reference temp*. is set to **0.0**.
- 5. Select the OK button to exit the Viscosity dialog.

Component Density

Next, we will enter the component density data [Units: g/cm³ or psi/ft; 1 g/cm³ = $62.428 \text{ lbs/ft}^2 = 0.4335 \text{ psi/ft}$]

- 1. Select the UTCHEM | Physical Properties | Component Density command.
- 2. Enter a value of **0.433** for the *Water value* (0.998 g/cm3).
- 3. Enter a value of **0.7036** for the *Oil value* (1.623 g/cm3).
- 4. Select the *Consider gravity effect* option.
- 5. Click OK to exit the Component Density dialog.

Fluid Compressibility

We will assume the fluids are incompressible in this simulation so the default values of **0.0** for fluid compressibility will be fine.

Capillary Pressure

To edit the capillary pressure data:

- 1. Select the UTCHEM | Physical Properties | Capillary Pressure command.
- 2. Choose the Strongly water wet option from the Wettability section.
- 3. Select the Cap. Press. Endpoint button.
- 4. Select the *Constant* \rightarrow *Grid* button and enter a value of **1.4**.
- 5. Select OK on both dialogs to return to the Capillary Pressure dialog.
- 6. Select the Cap. Press. Exponent button.
- 7. Select the *Constant* \rightarrow *Grid* button and enter a value of -0.52.
- 8. Select OK on both dialogs to return to the Capillary Pressure dialog.
- 9. Click OK to exit the Capillary Pressure dialog.

Diffusion and Dispersion

We will neglect molecular diffusion (use default diffusion coefficients of 0.0 ft^2/d) and edit the dispersion coefficients.

1. Select the UTCHEM | Physical Properties | Diffusion/Dispersion command.

- 2. In the *Dispersivity* section, change the *Aqueous phase*, *Longitudinal value* to 0.1 [ft2/d].
- 3. Change the *Aqueous phase*, *Transverse value* to the value **0.03**.
- 4. Repeat the last two steps (2 and 3) for the *Oleic* phase.
- 5. Click OK to exit the Diffusion & Dispersion dialog.

Adsorption

We will neglect sorption for this simulation.

Tracer Properties

There are no partitioning tracers in this simulation.

5.5.7 Boundaries

Our simulation will contain a flow field from left to right that models only the saturated zone. Both the left and right sides will be specified; all other sides are no-flow boundaries.

- 1. From the UTCHEM | Boundaries command.
- 2. Ensure that the *Saturated only* option is selected in the *Zone to be modeled* section.
- 3. Select the *Left boundary is specified* and *Right boundary is specified* options.

Left

For the parameters in the *Left* column, do the following:

- 1. Select the *Pressure at top layer* curve.
- 2. Under the pressure heading, enter 15.028 into both edit fields.
- 3. Click OK to return to the Boundaries dialog.
- 4. Select the *Conc. of water* curve.
- 5. Under the concentration heading, enter **1.0** (phase volume fraction) into both edit fields.
- 6. Click OK to return to the Boundaries dialog.

Right

For the parameters in the *Right* column, do the following:

- 1. Select the *Pressure at top layer* curve.
- 2. Under the pressure heading, enter 14.7 into both edit fields.
- 3. Click OK to return to the Boundaries dialog.
- 4. Edit the water concentration values for the right side so that they match what was entered for the left side.
- 5. Click *OK* to exit the Boundaries dialog.

5.5.8 Wells

For this simulation, we will only be using one well: an injection well simulating the PCE spill. However, in subsequent model runs we will be simulating flushing using two injection wells and an extraction well. In order to use the results of the spill simulation as a "restart" for the flushing and SEAR simulations, the first simulation must contain the same number of wells as all subsequent simulations. Thus, we will create all four wells now but only define a non-zero flow rate for the spill well.

PCE Spill Well

First, we will create a single well in the center of the model to simulate the PCE spill at the surface.

- 1. Select the UTCHEM | Wells command.
- 2. Select the *New* button.
- 3. Enter "PCE spill" into the Name field.
- 4. Change the Column value to **25**. Leave the *Starting layer* and *Ending layer* at **1**.
- 5. Select the *oleic* option from the *Phases* list.
- 6. Select the Q curve.
- Under the flow rate heading, enter 33.33 into the first edit field (0-30 days); leave the second field at 0.0. (Total: ~1000 ft3 or 6428.3 gal or 28.316 m3 or 28,316 L of PCE)
- 8. Click *OK* to return to the *Wells* dialog.

- 9. Select the **PCE** component from the *Components* list (with oleic selected in the Phases list)
- 10. Select the Conc. curve.
- 11. Under the concentration heading, enter **1.0** on the first line; leave **0.0** in the second line.
- 12. Click OK to return to the Wells dialog.

Left Injection Well

Next we will create the left injection well (corresponding to an infiltration trench) to be used in subsequent flushing simulations. We will leave the flow rate at zero for all phases.

- 1. Select the *New* button.
- 2. Change the text in the Name field to "Left Injection Well"
- 3. Enter a value of **16** for the *Column* entry. We will leave the *Row* with a value of **1**.
- 4. Enter a value of **24** for the *Ending layer* value.

Production Well

Likewise, we will create a production will at the center of the grid at the location of the spill to simulate the extraction well during the subsequent flushing simulations.

- 1. Select the *New* button.
- 2. Change the text in the Name field to "Center Production Well".
- 3. Change the *Type* to **Rate Constrained Production Well**.
- 4. Enter a value of **25** for the *Column* value. We will leave the *Row* with a value of **1**.
- 5. Enter a value of **24** for the *Ending layer* value.

Right Injection Well

Finally, we will create the right injection well (corresponding to an infiltration trench) to be used in the subsequent flushing simulations:

- 1. Select the *New* button.
- 2. Change the text in the Name field to "Right Injection Well"

- 3. Enter a value of **34** for the *Column* entry. We will leave the *Row* with a value of **1**.
- 4. Enter a value of 24 for the *Ending layer* value.
- 5. Select the OK button to exit the Wells dialog.

5.5.9 Saving the Model and Running UTCHEM

We are now ready to save the model and launch UTCHEM.

- 1. Select the *File* | *Save* command.
- 2. Select the UTCHEM | Run UTCHEM command.

At this point, UTCHEM will begin execution. You will see a message displayed after each time step reporting the time elapsed in days, the step, the time step in days, and the time step courant number.

When UTCHEM has finished, a message will report the time that elapsed and that UTCHEM terminated successfully. Select the *Close* button to close the window and return to GMS.

5.5.10 Viewing the Solution

Next, we will view the computed solution. After closing the UTCHEM window, GMS should have automatically read in the computed UTCHEM solution. The UTCHEM solution is organized into a folder in the GMS *Data Tree*. The UTCHEM solution contains concentration data sets for each component along with pressure and saturation data sets for each phase. We are most interested in the PCE concentration.

- 1. Expand the folder titled "UTC-contam (UTCHEM)" in the Data Tree.
- 2. Select the UTC1-contam_pce item in the UTCHEM solution folder in the *Data Tree*.
- 3. Select one of the latter time steps from the *Time Steps* list at the bottom of the *Data Tree*.

You may wish to experiment with the different time step values. As you view the solution, notice that since the PCE is a DNAPL, it rapidly drops to the bottom of the aquifer.

5.5.11 Changing the Contouring Options

You should see a set of contours representing the contaminant plume. To better illustrate the relative concentrations, we will turn on color ramp.

- 1. Select the *Data* | *Contour Options* command.
- 2. Turn on the Use color ramp option.
- 3. Select the *OK* button.

5.5.12 Setting Up the Animation

Finally, we will observe how the solution changes during the flushing simulation by generating a film loop animation. To set up the animation:

- 1. Select the *Display* | *Animate* command.
- 2. Make sure the Data set option is on and click Next.
- 3. Select the *Match time steps* option.
- 4. Turn on the *Display clock* option.
- 5. Select the *Finish* button.

You should see some images appear on the screen. These are the frames of the film loop which are being generated. When the film loop is completely generated, it will appear in a separate window for playback.

- 6. After viewing the animation, select the *Stop* button to stop the animation.
- 7. Select the *Step* \blacktriangleright button to move the animation one frame at a time.
- 8. You may wish to experiment with some of the other playback controls. When you are finished, close the window and return to GMS.

5.6 Dissolution Phase

In this simulation we consider the non-enhanced dissolution of the PCE DNAPL starting with the conditions predicted at the end of the 30 day DNAPL spill period and 60 day redistribution. To dissolve the entire 1000 ft³ (28.316 m³) PCE DNAPL under the regional flow gradient would require approximately 17 years (~6200 days). This estimate assumes local equilibrium partitioning and is conditioned on a DNAPL distribution as simulated. These are highly idealized conditions.

We will assume local equilibrium partitioning. An equilibrium partitioning concentration of oil (PCE) in water was set to 0.00015 in the *Organic mass transfer* section above. We will retain this parameter.

This simulation will be run as a restart of the contamination phase. We will create a third injection period and change the drainage option to *Imbibition Corey*. So, rather than start from scratch, it is expedient simply to edit the file upon which this simulation builds. The initial contamination phase file ("UTC-contam.gpr") should be edited and saved under a new name indicative of this dissolution phase.

Project File: ("UTC-dissol.gpr").

5.6.1 Initializing the UTCHEM Simulation

If the **UTC-contam.gpr** simulation is currently loaded into GMS, you can skip the next two steps and proceed with the tutorial. Otherwise, read in the simulation as follows:

- 1. Select the *File* | *Open* command.
- 2. Select and open the **UTC-contam.gpr** file (from the directory to which it had been saved).

Before editing this file for the current simulation phase, save it under a new name:

- 3. Select the *File* | *Save As* command.
- 4. Rename the project to UTC-dissol.gpr.
- 5. Select Save.

Now, we can proceed with modifications.

5.6.2 General Options

First, we will edit the general options. These options include the problem title and the restart option.

1. Select the UTCHEM | General Options command.

Titles

First, we will enter the titles and other basic information.

1. For the *Run* number, enter "UTC-dissol-run1"

- 2. For *Title 1*, enter: "2D (X-Z) PCE DNAPL spill in Saturated Heterogeneous Media".
- 3. For *Title 2*, enter: "30-day PCE spill 60-day Redistribution 20year dissolution."
- 4. For *Title 3*, enter your name and the current date.
- 5. Ensure that the default units are *English*.

Restart

The objective of this phase is to simulate DNAPL dissolution following the initial spill simulation. We will run the dissolution phase in restart mode. There are two reasons for running in restart mode: 1) we save a little time by not having to re-run the first 90 days of the simulation, and 2) it allows us to use a different drainage option for the dissolution simulation.

- 1. Select the Use restart option.
- 2. Click on the *Browse* button.
- 3. Select the file titled "UTC-contam.RESTAR" and select *Open*.
- 4. Select the OK button to exit the General Options dialog.

5.6.3 Time Options

Next, we will create a third injection period:

- 1. Select the UTCHEM | Time Options command.
- 2. Select the *Injection Periods* button.
- 3. Select the second injection period by either clicking on the appropriate segment on the time line or by selecting "2" in the *Injection Period* counter.
- 4. Select the *Insert Right* button to create a third period. Note that all of the time steps and output intervals from the second period are retained as initial settings for this period.
- 5. Make sure that the *Injection period* field counter is at 3 and change the length of the injection period to **7300** days (20 years).
- 6. Within the *Output intervals* section, set the *Print data* and *Prod. data* values to **1460** days.
- 7. Enter a value of **365** days for the *Prod. histories* and *Profiles*.

8. Select *OK* twice to exit both dialogs.

5.6.4 Drainage Option

Next, we will edit the drainage option. The contamination phase was simulated using the *First Drainage Corey* option. We will use the *Imbibition Corey* option to simulate the dissolution phase.

- 1. Select the UTCHEM | Physical Properties | Relative Permeability command.
- 2. Select the Imbibition Corey option.
- 3. Select the *OK* button to exit the dialog.

5.6.5 Capillary Pressure

For the *Imbibition Corey* option, we need to change the *Capillary Pressure* parameters.

- 1. Select the UTCHEM | Physical Properties | Capillary Pressure command.
- 2. Select the Cap. Press. Endpoint button.
- 3. Select the *Constant* \rightarrow *Grid* button.
- 4. Enter a value of **2.9** and select the *OK* button twice to return to the *Capillary Pressure* dialog.
- 5. Select the Cap. Press. Exponent button.
- 6. Select the *Constant* \rightarrow *Grid* button.
- 7. Enter a value of **2.0** and select the *OK* button repeatedly to exit all dialogs.

5.6.6 Saving and Running the Model

We are now ready to save the model and launch UTCHEM.

- 1. Select the *File* | *Save* command.
- 2. Select the UTCHEM | Run UTCHEM command.

This simulation takes much longer to run than the first simulation due to the fact that it covers a much longer period.

3. Once the simulation is finished, click on the *Close* button.

5.6.7 Viewing the Solution

Next, we will view the computed component concentration values for the dissolution phase.

- 1. Select UTC1-dissol_PCE from the Data Tree.
- 2. Select one of the latter time steps from the *Time Steps* window.

You may wish to experiment with the different time step values and other postprocessing options.

5.6.8 Additional Simulations

Consider running these following additional (optional) scenarios:

(1) Non-equilibrium partitioning. Equilibrium partitioning probably is an optimistic assumption in that dissolution is effectively accelerated.

5.7 Pre-Flush PITT Phase

In this tutorial we demonstrate the forward modeling of a partitioning interwell tracer test (PITT). The three wells created in the first phase of this simulation will be used – one withdrawal well in the DNAPL zone and two injection wells (Figure 5-1). The UTCHEM technical documentation presents the concepts and mathematical descriptions for partitioning tracers.

Ideally, one may use a suite of partitioning tracers to detect and semi-quantify the amount of DNAPL present within the swept zone. We will use two pairs of tracers (4 alcohols) of contrasting hydrophobicity – a different pair in each of the two injection wells. Through one well, we will inject 1-propanol (n-propanol) and 1-heptanol. Through the second well, we will inject 2-propanol (a.k.a. isopropyl alcohol or isopropanol) and 1-hexanol.

1-propanol (*1Pr*) and 2-propanol (*2Pr*) are highly hydrophilic with partitioning coefficients (K_p) of 0.0. Thus, partitioning into any DNAPL would be minimal and they should pass through the media with a minimum of retardation.

1-hexanol (*Hex*) and 1-heptanol (*Hep*) are relatively hydrophobic tracers with K_p 's of 30.0 and 141.0, respectively. The retardation of these strongly hydrophobic (lipophilic) tracers should be in direct proportion to the amount of DNAPL encountered.

The DNAPL encountered by the tracer plumes should selectively retard the more lipophilic tracer, while the hydrophilic tracer behaves conservatively. Negligible biodegradation of the tracers is assumed.

This phase will be simulated as a restart of the 90 day contamination phase simulation. We will do a 41 day PITT test where the tracers are injected during the first day followed by a water flush for the next 40 days. We will create two new injection periods for the tracer slug and the flushing and we will switch the drainage option to *Imbibition Corey*.

GMS Project File: UTC-prePITT.gpr

5.7.1 Initializing the UTCHEM Simulation

We will build the input for this problem by modifying the input used in the contamination phase. If the *UTC-contam.gpr* simulation is currently loaded into GMS, you can proceed with the tutorial. Otherwise, read in the simulation as follows:

- 1. Select the *File* | *New* command.
- 2. Select the *File* | *Open* command.
- 3. Select and open the **UTC-contam.gpr** file (from the directory to which it had been saved).

Before editing this file for the current simulation phase, save it under a new name:

- 4. Select the *File* | *Save As* command.
- 5. Rename the project to UTC-prePITT.gpr.
- 6. Select Save.

Now, we can proceed with modifications.

5.7.2 General Options

First, we will set up the general options. These options include the problem title, the restart option, and the species involved in the simulation.

1. Select the UTCHEM | General Options command.

Titles

First, we will enter the titles and other basic information.

1. For the *Run* number, enter "UTC-prePITT-run1"

- 2. For *Title 2*, enter: "**30-day PCE spill 60-day Redistribution 41day PITT**".
- 3. For *Title 3*, enter your name and the current date.

Restart

To turn on the restart option:

- 1. Select the *Use restart* option.
- 2. Click on the *Browse* button.
- 3. Select the file titled "UTC-contam.RESTAR" and select Open.

Species

At this point, we would normally define the four tracers used in the simulation. However, we already defined these species (1Pr, 2Pr, Hex, Hep) in the contamination phase, so no changes need to be made.

1. Select the *OK* button to exit the dialog.

5.7.3 Time Options

The next step is to set up the time options for the UTCHEM output and the time step control. We will create two new injection periods, a one day period for the tracer slug and a 40 day period for the water flush.

- 1. Select the UTCHEM | Time Options command.
- 2. Select the *Injection Periods* button.
- 3. Select the second injection period by either clicking on the appropriate segment on the time line or by selecting "2" in the *Injection Period* counter.
- 4. Select the *Insert Right* button to create a third injection period. Note that all of the *Time steps* and *Output intervals* from the second period are retained as initial settings for this period.
- 5. Make sure that the *Injection period field counter* is at **3** and enter a value of **1.0** for the *Length* item.
- 6. In the *Time Steps* section, change the time step size option from *Days* to *Courant numbers*.
- 7. Change the *Max time step size* to **0.2**.

- 8. Change the *Min time step size* to **0.04**.
- 9. Within the *Output intervals* section, change all of the output intervals to **1.0**.
- 10. Select the *Insert Right* button to create a fourth injection period.
- 11. Make sure that the *Injection period field counter* is at **4** and enter a value of **40.0** for the *Length* item.
- 12. Within the *Output intervals* section, change the *Print data* and *Prod. data* values to **10.0**.
- 13. Enter a value of **2.0** for the *Prod. histories* and *Profiles*.
- 14. Select *OK* twice to exit both dialogs.

5.7.4 Physical Properties

Now, we will edit the *Physical Property* data. We will change the drainage option to *Imbibition Corey* since it better simulates flushing situations. We will also edit the tracer properties.

Drainage Option

To change the drainage option:

- 1. Select the UTCHEM | Physical Properties | Relative Permeability command.
- 2. Select the *Imbibition Corey* option.
- 3. Select the *OK* button to exit the dialog.

Capillary Pressure

For the *Imbibition Corey* option, we need to change the *Capillary Pressure* parameters.

- 1. Select the UTCHEM | Physical Properties | Capillary Pressure command.
- 2. Select the Cap. Press. Endpoint button.
- 3. Select the *Constant* \rightarrow *Grid* button.
- 4. Enter a value of **2.9** and select the *OK* button twice to return to the *Capillary Pressure* dialog.

- 5. Select the Cap. Press. Exponent button.
- 6. Select the *Constant* \rightarrow *Grid* button.
- 7. Enter a value of **2.0** and select the *OK* button three times to exit all dialogs.

Tracer Properties

We will edit the tracer properties to define the partitioning coefficients.

- 1. Select the UTCHEM | Physical Properties | Tracer Properties command.
- 2. Select **1PR_wo** (1-propanol) from the *Tracers* list.
- 3. Make sure all the coefficients are set to the default value of **0.0**.
- 4. Select **2Pr** (2-propanol) from the *Tracers* list.
- 5. Make sure all the coefficients are set to the default value of **0.0**.
- 6. Select **Hex_wo** (1-hexanol) from the *Tracers* list.
- 7. Enter a value of **30.0** for the *Partition coefficient*. Accept the default values of **0.0** for the other coefficients.
- 8. Select Hep_wo (1-heptanol) from the Tracers list.
- 9. Enter a value of **141.0** for the *Partition coefficient*. Accept the default values of **0.0** for the other coefficients.
- 10. Select OK.

5.7.5 Wells

The wells will have been defined in the original simulation (*UTC-contam.gpr*). Only the pump rates and compositions for the third and fourth injection periods must be edited here.

1. Select the UTCHEM | Wells command.

Left Injection Well

To define the flow rates for the left well:

- 1. Select the Left Injection Well from the wells list.
- 2. Select the *aqueous* option from the *Phases* list.

- 3. Select the Q curve.
- 4. Under the *flow rate* heading, enter **1000.0** into the third edit field (representing the third injection period) and enter a value of **2000.0** into the fourth edit field (representing the fourth injection period).
- 5. Click OK to return to the Wells dialog.

To define the component concentrations for the left well:

- 6. Select the *Water component* from the *Components* list.
- 7. Select the *Conc*. curve.
- 8. Under the *concentration* heading, enter **1.0** into both the third and fourth edit fields.
- 9. Click OK to return to the Wells dialog.
- 10. Select the **1PR_wo** component from the *Components* list.
- 11. Select the Conc. curve.
- 12. Assign a concentration of 1000 mg/L (∞ solubility; miscible) only in the third injection period line.
- 13. Click OK to return to the Wells dialog.
- 14. Select the **Hex_wo** component from the *Components* list.
- 15. Select the Conc. curve.
- 16. Assign a concentration of **500** mg/L only in the third injection period (1-hexanol has an aqueous solubility of about 6000 mg/L).
- 17. Click OK to return to the Wells dialog.

Production Well

To modify the variables for the center production well:

- 1. Select the Center Production Well item from the Wells list.
- 2. Note that the *Phases* list is dimmed because the pump rate is lumped (vs. for individual phases). Note that the *Components* field is also dimmed for production wells.
- 3. Select the Q curve.

- 4. Enter a value of **-2000.0** for the third injection period. The values should be zero in the earlier periods.
- 5. Enter a value of **-4000.0** for the fourth injection period.
- 6. Click OK to return to the Wells dialog.

Right Injection Well

To define the flow rates for the right well:

- 1. Select the *Right Injection Well* from the wells list.
- 2. Select the **aqueous** option from the *Phases* list.
- 3. Select the *Q* curve.
- 4. Under the *flow rate* heading, enter **1000.0** into the third edit field and enter a value of **2000.0** into the fourth edit field and click *OK*.

To define the component concentrations for the right well:

- 5. Select the *Water* component from the *Components* list.
- 6. Select the *Conc.* curve.
- 7. Under the *concentration* heading, enter **1.0** into both the third and fourth edit fields.
- 8. Click OK to return to the Wells dialog.
- 9. Select the **1PR_wo** component from the *Components* list.
- 10. Select the Conc. curve.
- 11. Assign a concentration of **1000** mg/L (∞ solubility; miscible) only in the third injection period line.
- 12. Click OK to return to the Wells dialog.
- 13. Select the **Hep_wo** component from the *Components* list.
- 14. Select the Conc. curve.
- 15. Assign a concentration of **500** mg/L only in the third injection period (1-heptanol has an aqueous solubility of about 2000 mg/L).
- 16. Click OK twice to exit all dialogs.

5.7.6 Saving and Running the Model

We are now ready to save the model and launch UTCHEM.

- 1. Select the *File* | *Save* command.
- 2. Select the UTCHEM | Run UTCHEM command.
- 3. Once the simulation is finished, click on the *Close* button.

5.7.7 Viewing the Solution

Next, we will view the computed component concentration values for the dissolution phase.

- 1. Select one of the tracers from the *Data Tree*.
- 2. Select one of the latter time steps from the *Time Step* window.

View each of the tracers at the later time steps. Notice how the Hex and Hep tracers partition to the PCE and the 1Pr and 2Pr tracers do not. Also, notice that at the end of the simulation, the Hex tracer from the left injection well is primarily trapped by the PCE that is settled at the very bottom of the aquifer. However, the Hep tracer from the right injection well at the end of the simulation is distributed both at the bottom and just to the right of the center production well. The difference is due to the left to right background flow gradient. After the 90 day spill and redistribution, the center production well. Furthermore, the background flow gradient assists the flushing from the left injection well.

Another important type of output from a PITT simulation is the concentration of the tracers at the production well. GMS does not include a post-processing tool for this output, but it can be viewed as part of the text output from UTCHEM (the "history" files) in a text editor.

5.8 Water Flush Treatment Phase

The next phase of this tutorial involves using the injection and extraction wells defined previously to simulate water flushing of the PCE plume. One extraction well was added at the location of the spill and two injection wells were added on each side of the spill. We will use the restart option to start the flushing simulation at the end of the previously defined spill simulation. The wells will then run for 280 days (nine months). In the next simulation, we will simulate surfactant flushing and compare the results.

UTCHEM file: UTC-flush.gpr

5.8.1 Initializing the UTCHEM Simulation

To build this simulation we will read in and modify the contamination simulation:

- 1. Select the *File* | *New* command.
- 2. Select the *File* | *Open* command.
- 3. Select and open the **UTC-contam.gpr** file (from the directory to which it had been saved).

Before editing this file for the current simulation phase, save it under a new name:

- 4. Select the *File* | *Save As* command.
- 5. Rename the project UTC-flush.gpr
- 6. Select Save.

Now, we can proceed with modifications.

5.8.2 General Options

First, we will set up the general options. We will edit the problem title and the restart option.

1. Select the UTCHEM | General Options command.

Titles

First, we will enter the titles and other basic information.

- 1. For the *Run number*, enter "UTC-flush-run1"
- 2. For *Title 2*, enter: "**30-day PCE spill 60-day redistribution 9 mo.** flush".
- 3. For *Title 3*, enter your name and the current date.

Restart

To turn on the restart option:

- 1. Select the Use restart option.
- 2. Click on the Browse button.
- 3. Select the file titled "UTC-contam.RESTAR" and select Open.

4. Select the OK button to exit the General Options dialog.

5.8.3 Injection Period for Flushing

Next, we will create a third injection period to simulate the flushing phase. This injection period will last for 280 days.

- 1. Select the UTCHEM | Time Options command.
- 2. Select the *Injection Periods* button.
- 3. Select the second injection period by either clicking on the appropriate segment on the time line or by selecting "2" in the *Injection Period* counter.
- 4. Select the *Insert Right* button to create a third injection period
- 5. Change the *Length* of the new injection period to **280** days.
- 6. In the *Time Steps* section, change the time step size option from *Days* to *Courant numbers*.
- 7. Change the *Max time step size* to **0.2**.
- 8. Change the *Min time step size* to **0.04**.

In the Output Intervals section, do the following:

- 9. Enter a value of **56.0** for the *Print data value*.
- 10. Enter a value of **56.0** for the *Prod. data value*.
- 11. Enter a value of **14.0** for the *Prod. histories* value.
- 12. Enter a value of **14.0** for the *Profiles* value.
- 13. Select the *OK* button twice to exit both dialogs.

5.8.4 Physical Properties

In the *Physical Properties* section, we will change the drainage option to *Imbibition Corey*, which better simulates flushing conditions.

Drainage Option

To change the drainage option:

1. Select the UTCHEM | Physical Properties | Relative Permeability command.

- 2. Select the Imbibition Corey option.
- 3. Select the *OK* button.

Capillary Pressure

For the *Imbibition Corey* option, we need to change the *Capillary Pressure* parameters.

- 1. Select the UTCHEM | Physical Properties | Capillary Pressure command.
- 2. Select the Cap. Press. Endpoint button.
- 3. Select the *Constant* \rightarrow *Grid* button.
- 4. Enter a value of **2.9** and select the *OK* button twice to return to the *Capillary Pressure* dialog.
- 5. Select the Cap. Press. Exponent button.
- 6. Select the *Constant* \rightarrow *Grid* button.
- 7. Enter a value of **2.0** and select the *OK* button three times to exit all dialogs.

5.8.5 Editing the Well Data

Next, we will edit the well data to turn on the injection and extraction wells for the flushing injection period.

1. Select the UTCHEM | Wells command.

Injection Wells

To set up the injection wells:

- 1. Select the *Left Injection Well* item from the list of wells.
- 2. In the list of phases, select the *aqueous* item.
- 3. Click on the curve labeled *Q*.
- 4. Under the *flow rate* heading, enter **2000.0** into the third edit field representing the third injection period.
- 5. Click OK to return to the Wells dialog.
- 6. In the Components section, select the water item.

- 7. Click on the curve labeled Conc.
- 8. In the *concentration* column, enter a value of **1.0** for the third injection period.
- 9. Click OK to return to the Wells dialog.
- 10. Select the *Right Injection Well* item from the list of wells.
- 11. Repeat steps 2-9 to enter the appropriate values for the right injection well.

Extraction Well

To set up the extraction well:

- 1. Select the Center Production Well item from the list of wells.
- 2. Click on the curve labeled *Q*.
- 3. Under the *flow rate* heading, enter **-4000.0** into the third edit field representing the third injection period.
- 4. Click *OK* twice to exit both dialogs.

5.8.6 Saving and Running the Model

We are now ready to save the model and launch UTCHEM.

- 1. Select the *File* | *Save* command.
- 2. Select the UTCHEM | Run UTCHEM command.

This simulation takes several minutes to run.

3. Once the simulation is finished, click on the *Close* button.

5.8.7 Viewing the Solution

Next, we will view the computed PCE concentrations for the water-flushing phase.

- 1. Select UTC4-flush_PCE from the *Data Tree*.
- 2. Select one of the latter time steps using the *Time Steps* window.

You may wish to experiment with the different time step values.

5.9 Surfactant Flush Treatment Phase

The next phase of this tutorial involves modifying the flushing simulation defined in the previous phase to include the injection of surfactants to accelerate the dissolution of the PCE. Instead of flushing for nine months, this simulation will only cover a period of 21 days (7 days of surfactant flood followed by 14 days of water flood). During the water flood, we will increase the flow rate in each injection well to 3000 ft^3/day .

UTCHEM file: UTC-SEAR.gpr

5.9.1 Initializing the UTCHEM Simulation

If the **UTC-flush.gpr** simulation is currently loaded into GMS, you can skip the next three steps and proceed with the tutorial. Otherwise, read in the simulation as follows:

- 1. Select the *File* | *New* command.
- 2. Select the *File* | *Open* command.
- 3. Select and open the UTC-flush.gpr file (from the directory to which it had been saved).

Before editing this file for the current simulation phase, save it under a new name:

- 4. Select the *File* | *Save As* command.
- 5. Rename the project UTC-SEAR.gpr and click Save.

Now, we can proceed with modifications.

5.9.2 General Options

First, we will set up the general options. We will edit the problem title and add the surfactant and electrolyte species.

1. Select the UTCHEM | General Options command.

Titles

To change the titles:

- 1. For the *Run* number, enter "UTC-SEAR-run1"
- 2. For *Title 2*, enter: "30-day PCE spill 60-day redistribution 21 day surfactant flush".

3. For *Title 3*, enter your name and the current date.

Species

Next, we will add three new species: surfactant, chloride, and calcium:

- 1. Select the *Define Species* button.
- 2. Turn on the *Surfactant*, *Chloride*, and *Calcium* options.
- 3. Select the *OK* button twice to exit both dialogs.

5.9.3 Editing the Injection Periods

Next, we will edit the injection periods. With the surfactant, the PCE is removed much more rapidly. Rather than nine months, we will only run the simulation for 21 days. This will require two injection periods: a 7 day period for the surfactant flood, and a 14 day period for the water flood. We will change the length of the existing third injection period to 7 days for the surfactant flood and add a new fourth injection period for the water flood.

Surfactant Injection Period

To edit the surfactant injection period:

- 1. Select the UTCHEM | Time Options command.
- 2. Select the *Injection Periods* button.
- 3. Select the third injection period and change the *Length* to 7 days.

In the Output Intervals section, do the following for the third period:

- 4. Enter a value of **3.5** for the *Print data* value.
- 5. Enter a value of **3.5** for the *Prod. data* value.
- 6. Enter a value of **1.0** for the *Prod. histories* value.
- 7. Enter a value of **1.0** for the *Profiles* value.

Water Injection Period

To create a new injection period for the water flood:

- 1. Make sure the third injection period is selected and select the *Insert Right* button.
- 2. Change the *Length* of the new injection period to **14** days.

In the Output Intervals section, do the following:

- 3. Enter a value of **7.0** for the *Print data* value.
- 4. Enter a value of **7.0** for the *Prod. data* value.
- 5. Enter a value of **1.0** for the *Prod. histories* value.
- 6. Enter a value of **1.0** for the *Profiles* value.
- 7. Select the *OK* button twice to exit both dialogs.

5.9.4 Initial Conditions

Next, we will use the *Reservoir Properties* dialog to define an initial condition for chloride and calcium.

- 1. Select the UTCHEM | Reservoir Properties command.
- 2. Enter a value of **0.009** for the initial condition for both *Chloride* and *Calcium*.
- 3. Select the *OK* button to exit the dialog.

5.9.5 Editing the Phase Behavior Parameters

Next, we will edit the surfactant properties in the *Phase Behavior* dialog. These properties define the behavior of the surfactant.

1. Select the UTCHEM | Physical Properties | Phase Behavior command.

Concentration

To edit the concentrations:

- 1. Select the Concentrations tab.
- 2. Change the *Oil concentration at plait point(+)* value to **0.0**.
- 3. Change the *Oil concentration at plait point(-)* value to **1.0**.
- 4. Change the *Critical micelle concentration* value to **0.0001**.

Binodal Curve

To edit the binodal curve:

1. Select the *Binodal Curve* tab.

- 2. Enter **0.1** for the *Intercept at zero salinity*.
- 3. Enter **0.0267** for the *Intercept at optimal salinity*.
- 4. Enter **0.1** for the *Intercept at twice optimal salinity*.

Salinity

To edit the salinity parameters:

- 1. Select the *Salinity* tab.
- 2. Enter 0.0198 for the Lower effective salinity limit.
- 3. Enter **0.0231** for the Upper effective salinity limit.
- 4. Enter **1.0** for the *Effective salinity slope param. for calcium.*
- 5. Select the *OK* button to exit the dialog.

5.9.6 Interfacial Tension

The interfacial tension parameters are also related to the behavior of the surfactant. To edit the interfacial tension parameters:

- 1. Select the UTCHEM | Physical Properties | Interfacial Tension command.
- 2. Select the *Healy & Reed's correlation* option.

For the *Water/micro-emulsion* parameters:

- 3. Under the *G11* heading, enter a value of **13.0**.
- 4. Under the *G12* heading, enter a value of **-14.8**.
- 5. Under the *G13* heading, enter a value of **0.007**.

For the Oil/micro-emulsion parameters:

- 6. Under the *G21* heading, enter a value of **13.0**.
- 7. Under the *G22* heading, enter a value of -14.5.
- 8. Under the G23 heading, enter a value of 0.01.

Finally,

9. Change the *XIFTW* value to **1.65**.

10. Click OK to exit the Interfacial Tension dialog.

5.9.7 Relative Permeability

Next, we will edit the relative permeability data related to the microemulsion phase:

1. Select the UTCHEM | Physical Properties | Relative Permeability command.

In the Microemulsion column, do the following:

- 2. Select the *Residual Saturation* button.
- 3. Select the *Constant* \rightarrow *Grid* button and enter a value of **0.24**.
- 4. Select OK on both dialogs to return to the Relative Permeability dialog.
- 5. Select the *Kr Endpoint* button.
- 6. Select the *Constant* \rightarrow *Grid* button and enter a value of **0.486**.
- 7. Select OK on both dialogs to return to the Relative Permeability dialog.
- 8. Select the Kr Exponent button.
- 9. Select the *Constant* \rightarrow *Grid* button and enter a value of **2.85**.
- 10. Select *OK* to exit all three dialogs.

5.9.8 Viscosity

We also need to edit the viscosity data related to the microemulsion phase:

1. Select the UTCHEM | Physical Properties | Viscosity command.

In the Microemulsion viscosity section, do the following:

- 2. Change the *Alpha 1* property to a value of **3.4**.
- 3. Change the *Alpha 2* property to a value of **1.0**.
- 4. Change the *Alpha 3* property to a value of **3.0**.
- 5. Change the *Alpha 4* property to a value of **1.0**.
- 6. Change the *Alpha 5* property to a value of **1.0**.
- 7. Click *OK* to exit the *Viscosity* dialog.

5.9.9 Component Density

Next, we need to enter a value of component density for the surfactant:

- 1. Select the UTCHEM | Physical Properties | Component Density command.
- 2. Enter a value of **0.7036** for the *Coef. of oil in microemulsion* value.
- 3. Enter a value of **0.498** for in the *Surfactant* edit field.
- 4. Select *OK* to exit the dialog.

5.9.10 Diffusion and Dispersion

Next, we will edit the dispersion coefficients related to the microemulsion phase:

- 1. Select the UTCHEM | Physical Properties | Diffusion/Dispersion command.
- 2. In the *Dispersivity* section, change the *Microemulsion phase*, *Longitudinal* value to **0.1** $[ft^2/d]$.
- 3. Change the *Microemulsion phase*, *Transverse* value to the **0.03**.
- 4. Click OK to exit the Diffusion & Dispersion dialog.

5.9.11 Boundaries

Now that we have added the chloride and calcium components, we must edit the boundary condition data.

1. Select the UTCHEM | Boundaries command.

Left

For the parameters in the *Left* column, do the following:

- 1. Select the *Conc. of chloride* curve.
- 2. Under the *cholorine conc* heading, enter **0.009** into all the edit fields.
- 3. Click *OK* to return to the *Boundaries* dialog.
- 4. Select the Conc. of calcium curve.
- 5. Under the *calcium conc* heading, enter **0.009** into all the edit fields.

6. Click OK to return to the Boundaries dialog.

Right

- 1. Repeat the previous steps to enter the chloride and calcium values to the right side.
- 2. Exit the *Boundaries* dialog when finished.

5.9.12 Editing the Concentrations at Wells

Finally, we will edit the component densities at the injection wells to ensure that the surfactant is injected during the third injection period and that water is injected during the fourth injection period.

1. Select the UTCHEM | Wells command.

Left Injection Well

To edit the left injection well:

- 1. In the list of *Wells*, select the Left Injection Well item.
- 2. In the *Phases* section, make sure the *aqueous* item is selected.
- 3. Click on the curve labeled *Q*:
- 4. In the *flow rate* column, enter a value of **1125** for **injection period #3** and **3000** for **injection period #4**.
- 5. Select the OK button to return to the Wells dialog.
- 6. In the *Components* section, select the *water* item.
- 7. Click on the curve labeled Conc.
- 8. In the *concentration* column, enter a value of **0.96** for the third injection period and a value of **1.0** for the fourth injection period.
- 9. Select the OK button to return to the Wells dialog.
- 10. In the Components section, select the Surfactant item.
- 11. Click on the curve labeled Conc.
- 12. In the *concentration* column, enter a value of **0.04** for the third injection period and leave the other values at **0.0**.
- 13. Select the OK button to return to the Wells dialog.

- 14. Select the **Chloride** component from the *Components* list.
- 15. Select the *Conc*. curve.
- 16. Under the concentration heading, enter **0.009** into both the third and fourth edit fields.
- 17. Click OK to return to the Wells dialog.
- 18. Select the Calcium component from the Components list.
- 19. Select the *Conc*. curve.
- 20. Under the *concentration* heading, enter **0.009** into the both the third and fourth edit fields.
- 21. Click OK to return to the Wells dialog.

Right Injection Well

Repeat each of the steps in the previous section to edit the well data for the right injection well.

Center Production Well

To edit the pumping rate for the center production well:

In the list of wells, select the Center Production Well item

- 1. Click on the curve labeled *Q*:
- 2. In the *flow rate* column, enter a value of **-2250** for **injection period #3** and **-6000** for **injection period #4**.
- 3. Select the *OK* button twice to exit both dialogs.

5.9.13 Saving and Running the Model

We are now ready to save the model and launch UTCHEM.

- 1. Select the *File* | *Save* command.
- 2. Select the UTCHEM | Run UTCHEM command.

This simulation takes several minutes to run.

3. Once the simulation is finished, click on the *Close* button.

5.9.14 Viewing the Solution

Next, we will view the computed PCE concentrations for the surfactant-flushing phase.

- 1. Select UTC5-SEAR_PCE from the Data Tree.
- 2. Select one of the later time steps using the *Time Steps* window.

You may wish to experiment with the different time step values.

5.9.15 Designing a More Effective System

As you view the solution, notice that only a portion of the PCE is removed. Most of the PCE is concentrated at the bottom of the aquifer. To achieve a more effective remediation design, you may wish to try the following and rerun the model:

- 1. Change the screened interval for the wells. Since most of the PCE is concentrated at the bottom of the aquifer, try changing the screened interval for the injection and extraction wells so that the screened interval is focused on the bottom of the aquifer. This can be accomplished by editing the *Starting layer* and *Ending layer* values in the *Wells* dialog.
- 2. Change the pumping rates and/or lengths of the injection periods for the wells. However, keep in mind that surfactants are expensive. If you inject surfactants for a long time period, you can completely remediate the PCE. But you may bankrupt your client!

5.10 Post-Flush PITT (optional)

One of the purposes of a PITT is to assess the effectiveness of a cleanup effort. Repeating the tracer tests, presumably in the absence of DNAPL, should show little retardation of the hydrophobic tracers. In this phase, we will simulate a PITT following the surfactant flush. We will follow the same basic steps we followed in setting up the pre-flush PITT simulation. This simulation will be a restart of the surfactant flush (SEAR) simulation.

UTCHEM file: UTC-postPITT.gpr

5.10.1 Initializing the UTCHEM Simulation

We will build the input for this problem by modifying the input used in the SEAR phase. If the *UTC-SEAR.gpr* simulation is currently loaded into GMS, you can proceed with the tutorial. Otherwise, read in the simulation as follows:

- 1. Select the *File* | *Open* command.
- 2. Select and open the UTC-SEAR.gpr file (from the directory to which it had been saved).

Before editing this file for the current simulation phase, save it under a new name:

- 3. Select the *File* | *Save As* command.
- 4. Rename the project UTC-postPITT.gpr.
- 5. Select OK.

Now, we can proceed with the modifications.

5.10.2 General Options

First, we will set up the general options. These options include the problem title and the species involved in the simulation.

1. Select the UTCHEM | General Options command.

Titles

First, we will enter the titles and other basic information.

- 1. For the *Run number*, enter "UTC-postPITT-run1"
- 2. For *Title 2*, enter: "**30-day PCE spill 60-day redistribution –21 day SEAR 61-day PITT**".
- 3. For *Title 3*, enter your name and the current date.
- 4. Ensure that the default units are *English*.

Restart

This simulation will be a restart of the SEAR simulation.

- 1. Click on the *Browse* button in the *Restart Option* section.
- 2. Select the file titled "UTC-SEAR.RESTAR" and select *Open*.

Species

Next, we will define the species used in the simulation. However, since the four tracers were already created in the contamination phase simulation, no changes need to be made.

1. Select the *OK* button to exit the dialog.

5.10.3 Time Options

The next step is to set up the time options for the UTCHEM output and the time step control. A fifth injection period of one day will be defined, during which the tracer slug will be injected at the distal wells and recovered via the central well. A sixth injection period of sixty days will be defined to flush the tracer slug through the system.

- 1. Select the UTCHEM | Time Options command.
- Select the *Injection Periods* button. Select the fourth injection period by either clicking on the appropriate segment on the time line or by selecting "4" in the *Injection Period* counter.
- 3. Select the *Insert Right* button to create a fifth injection period.
- 4. Make sure that the *Injection period field counter* is at **5** and enter a value of **1.0** for the *Length* item.
- 5. Within the *Output intervals* section, enter a value of **1.0** for all of the output intervals.
- 6. Select the *Insert Right* button to create a sixth injection period.
- 7. Make sure that the *Injection period field counter* is at **6** and enter a value of **60.0** for the *Length* item.
- 8. Within the *Output intervals* section, set the *Print data* and *Prod. data* values to **20.0**.
- 9. Enter a value of **6.0** for the *Prod. histories* and *Profiles*.
- 10. Select *OK* twice to exit both dialogs.

5.10.4 Tracer Properties

Now, we will edit the tracer properties to define the partitioning coefficients.

- 1. Select the UTCHEM | Physical Properties | Tracer Properties command.
- 2. Select **Hex_wo** (1-hexanol) from the *Tracers* list.
- 3. Enter a value of **30.0** for the *Partition coefficient*. Accept the default values of **0.0** for the other parameters.

- 4. Select **Hep_wo** (1-heptanol) from the *Tracers* list.
- 5. Enter a value of **-141.0** for the *Partition coefficient*. Accept the default values of **0.0** for the other parameters.
- 6. Select OK.

5.10.5 Wells

The well pump rates and compositions for the two new injection periods must be edited.

1. Select the UTCHEM | Wells command.

Left Injection Well

To define the flow rates for the left well:

- 1. Select the *Left Injection Well* from the *wells* list.
- 2. Select the *aqueous* option from the *Phases* list.
- 3. Select the Q curve.
- 4. Under the *flow* heading, enter **1000.0** into the fifth edit field (representing the fifth injection period) and enter a value of **2000.0** into the sixth edit field (representing the sixth injection period).
- 5. Click OK to return to the Wells dialog.

To define the component concentrations for the left well:

- 6. Select the *Water* component from the *Components* list.
- 7. Select the *Conc. curve*.
- 8. Under the *concentration* heading, enter **1.0** into both the fifth and sixth edit fields.
- 9. Click *OK* to return to the *Wells* dialog.
- 10. Select the Chloride component from the Components list.
- 11. Select the Conc. curve.
- 12. Under the *concentration* heading, enter **0.009** into both the fifth and sixth edit fields.
- 13. Click OK to return to the Wells dialog.

- 14. Select the *Calcium* component from the *Components* list.
- 15. Select the Conc. curve.
- 16. Under the *concentration* heading, enter **0.009** into both the fifth and sixth edit fields.
- 17. Click OK to return to the Wells dialog.
- 18. Select the **1PR_wo** component from the *Components* list.
- 19. Select the Conc. curve.
- 20. Assign a concentration of 1000 mg/L (∞ solubility; miscible) only in the fifth injection period line.
- 21. Click OK to return to the Wells dialog.
- 22. Select the **Hex_wo** component from the *Components* list.
- 23. Select the Conc. curve.
- 24. Assign a concentration of **500** mg/L only in the fifth injection period (1-hexanol has an aqueous solubility of about 6000 mg/L).
- 25. Click OK to return to the Wells dialog.

Production Well

To modify the variables for the center production well:

- 1. Select the *Center Production Well* item from the *Wells* list.
- 2. Select the *Q* curve.
- 3. Enter a value of **-2000** for the fifth injection period.
- 4. Enter a value of **-4000** for the sixth injection period.
- 5. Click *OK* to return to the *Wells* dialog

Right Injection Well

To define the flow rates for the right well:

- 1. Select the *Right Injection Well* from the wells list.
- 2. Select the *aqueous* option from the *Phases* list.
- 3. Select the Q curve.

4. Under the *flow* heading, enter **1000.0** into the fifth edit field and enter a value of **2000.0** into the sixth edit field.

To define the component concentrations for the right well:

- 5. Select the *Water* component from the *Components* list.
- 6. Select the *Conc.* curve.
- 7. Under the *concentration* heading, enter **1.0** into both the fifth and sixth edit fields.
- 8. Click OK to return to the Wells dialog.
- 9. Select the *Chloride* component from the *Components* list.
- 10. Select the Conc. curve.
- 11. Under the concentration heading, enter **0.009** into both the fifth and sixth edit fields.
- 12. Click OK to return to the Wells dialog.
- 13. Select the Calcium component from the Components list.
- 14. Select the Conc. curve.
- 15. Under the concentration heading, enter **0.009** into both the fifth and sixth edit fields.
- 16. Click OK to return to the Wells dialog.
- 17. Select the **1PR_wo** component from the *Components* list.
- 18. Select the *Conc.* curve.
- 19. Assign a concentration of 1000 mg/L (∞ solubility; miscible) only in the fifth injection period line.
- 20. Click OK to return to the Wells dialog.
- 21. Select the **Hep_wo** component from the *Components* list.
- 22. Select the Conc. curve.
- 23. Assign a concentration of **500** mg/L only in the fifth injection period (1-heptanol has an aqueous solubility of about 2000 mg/L).
- 24. Click *OK* twice to exit both dialogs.

5.10.6 Saving and Running the Model

We are now ready to save the model and launch UTCHEM.

- 1. Select the *File* | *Save* command.
- 2. Select the UTCHEM | Run UTCHEM command.
- 3. Once the simulation is finished, click on the *Close* button.

5.10.7 Viewing the Solution

Next, we will view the computed component concentration values for the dissolution phase.

- 1. Select one of the tracers from the Data Tree.
- 2. Select one of the latter time steps using the *Time Steps* window.

View each of the tracers at the later time steps. Notice how the Hex and Hep tracers partition to the PCE and the 1Pr and 2Pr tracers do not.

Another important type of output from a PITT simulation is the concentration of the tracers at the production well. GMS does not include a post-processing tool for this output, but it can be viewed as part of the text output from UTCHEM (the "history" files) in a text editor.

5.11 Conclusion

This concludes the UTCHEM tutorial. If you wish to exit GMS at this time:

- 1. Select the *File* | *Exit* command.
- 2. Select No at the prompt.

CHAPTER GIS Module

The GIS module can be used to display data from a GIS database directly in GMS without having to convert that data to GMS data types. Native GMS data such as grids and boreholes can be displayed along with the GIS data. The GIS module can also be used to select a portion of the GIS data and convert it to GMS data types to be used in constructing a groundwater model. Currently the GIS module can only be used for steady state data.

If you have a license of ArcObjects[®] installed on your computer, many features available in ESRI[®] software (such as ArcMap[®]) become available in GMS. If you do not have a license of ArcObjects[®] installed, you can still use the GIS module, but many features will not be available. You can still import and display shapefiles and convert them to GMS feature objects. For a full list of the features available in the different modes, refer to the GMS Help.

This tutorial will introduce you to the GIS module. There are two parts to the tutorial. The first part shows the features available to you if you don't have a license of ArcObjects[®] installed on your computer. The second part shows the features available if you do. You will not be able to complete the second part if you do not have a license of ArcObjects[®] installed on your computer.

6.1 Part 1 - Without ESRI[®] ArcObjects[®]

We will import a point shapefile containing well data. Then we will create scatter points from the shapefile points. Next we will create a GMS MODFLOW conceptual model in the Map module, and create a coverage with well attributes. Then we will convert the shapefile to GMS wells that we could

use to help build a model. This will illustrate how GIS data can be imported and converted to GMS data.

6.2 Getting Started

If you have not yet done so, launch GMS. If you have already been using GMS, you may wish to select the *File* | *New* command to ensure the program settings are restored to the default state.

6.3 Required Modules/Interfaces

The license registration system used by GMS allows the components of GMS to be licensed individually, depending on the needs of the user. Before continuing, you may wish to check whether or not the GMS components used in this tutorial have been enabled in the copy of GMS you are using. This can be accomplished by selecting the *Register* | *File* command. On the left side of the *Register* dialog, the following components should have "ENABLED" displayed in the *Status* column to the right of each of the following components:

- *Map*
- GIS

6.4 Reading the Shapefile

The first step is to read the shapefile.

- 1. Select the *Open* button \overrightarrow{P} .
- 2. Locate and open the directory entitled: tutfiles\gismodule
- 3. In the **Open** dialog, change the *Files of type* to **Shapefiles (*.shp)**.
- 4. Select the file entitled **arcmap.shp** and select the *Open* button.

6.5 Viewing the Shapefile

You should not see a number of points displayed on the screen. These are the wells in the shapefile.

- 1. Switch to the GIS module 🥩.
- 2. In the Data Tree, expand the GIS Layers folder if necessary.

Notice the **arcmap.shp** object in the data tree. This is the shapefile we just opened.

Without ESRI[®] ArcObjects[®], we have only a limited set of options for displaying the shapefile.

- 3. Select the *Display Options* button
- 4. Click on the button displaying the point symbol style.
- 5. Change the point radius and color. Click OK to exit all dialogs.

Notice that the point color has changed.

6.6 Viewing the Attribute Table

The shapefile we opened has a number of attributes associated with each point. Let's take a look at them.

- 1. In the *Data Tree*, right-click on the **arcmap.shp** object.
- 2. Select the *Attribute Table* command from the pop-up menu.
- 3. Resize the dialog by dragging the bottom right corner out so you can see more of the data.

There are number of attributes (columns) associated with each point. Notice the data is not editable.

4. Click *OK* to exit the dialog.

6.7 Converting the Shapefile to 2D Scatter Points

Now we will convert the GIS data to 2D scatter points that we could use to do interpolation with.

- 1. In the Data Tree, right-click on the arcmap.shp object.
- 2. Select the *Convert to 2D Scatter Points* command from the pop-up menu.

You should see some new symbols appear on the screen. These are the new 2D scatter points.

- 3. Switch to the 2D Scatter Points module 🛄
- 4. If necessary, expand the 2D Scatter Data folder.

Notice the arcmap.shp 2D scatter point that we just created.

5. Expand the arcmap.shp object.

Notice that GMS automatically created a data set from each numeric attribute in the attribute table. You could use this procedure to create scatter points and then interpolate from the scatter points to a grid. If you had water level information for each point, for example, you could create a starting head data set for your model.

We won't do anything more with the scatter points, so we'll delete them now.

6. Select the *Edit* | *Delete All* command.

6.8 Converting the Shapefile to Feature Objects

Now we will convert the GIS data to GMS feature objects that we could use to build a conceptual model. First we must create a default conceptual model and coverage with the appropriate attributes.

6.8.1 Creating the Conceptual Model

- 1. Switch to the Map module *****.
- 2. In the *Data Tree*, right click on the *Map Data* folder and select the *New Conceptual Model* command from the pop-up menu.
- 3. Change the *Name* to **Model1**.
- 4. Make sure the *Model* is set to **MODFLOW** and click *OK*.
- 5. In the *Data Tree*, right click on the **Model1** folder and select the *New Coverage* command from the pop-up menu.
- 6. Rename the new coverage **coverage1**.
- 7. Select the **Wells** option in the list of *Sources/Sinks/BCs* and click *OK*.

6.8.2 Mapping the GIS Data

- 1. Switch to the GIS module \heartsuit .
- 2. Select the *Mapping* | *Shapes -> Feature Objects* command.
- 3. Click *Yes* to confirm that we want to use all visible shapes.

At this point, the GIS to Feature Objects Wizard appears.

- 4. Click Next.
- 5. In the WELLNAME column, change the mapping to Name.
- 6. In the PUMPRATE column, change the mapping to Flow rate.
- 7. Click Next.
- 8. Click Finish.

Feature points now exist in the same location as the GIS points, but since they're in the same locations, you probably won't notice any difference in the display.

- 9. Uncheck the arcmap.shp object in the Data Tree.
- 10. Switch to the Map module +.
- 11. In the *Data Tree*, right-click on **coverage1** and select the *Attribute Table* command from the pop-up menu.

This dialog shows the properties of all the feature points in the coverage. Notice that the names and flow rates were transferred from the GIS attributes, just like we specified. However, the points are all of type NONE. We need to make them wells.

- 12. Find the spreadsheet cell corresponding to the *All* row and the *Type* column. Change the type to **Well**. Since this is the *All* row, all of the points are changed to wells.
- 13. Click OK.

6.8.3 Part 1 Conclusion

At this point we have well points that we could use as we further construct a MODFLOW conceptual model. This topic is further discussed in the tutorial entitled *MODFLOW – Conceptual Model Approach* and will not be discussed further here.

6.9 Part 2 - With ESRI[®] ArcObjects[®]

If you have a license of ArcObjects[®] installed on your computer or on your network, you can proceed through part 2 of this tutorial If you have ESRI[®] software like ArcGIS[®] installed then you should have a license of ArcObjects[®] available. If you don't know if you have a license of ArcObjects[®], the tutorial will show you how you can tell.

Many more features in the GIS module are available if you have a license of $ArcObjects^{$ [®].</sup> This part of the tutorial introduces those features.

6.10

We will delete everything we have done so far and read in a new file.

1. Select the New button \square .

<THIS TUTORIAL IS NOT YET COMPLETED>

6.11 Conclusion

<THIS TUTORIAL IS NOT YET COMPLETED>