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PetraSim Example Manual

July 2007

TOUGH2 Example Guide

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Chapter 1. Five Spot Geothermal Production and Injection (EOS1)

Description

This example is Problem 4 - Five Spot Geothermal Production and Injection (EOS1, EOS2) described in the TOUGH2 User's Manual [Pruess, Oldenburg, and Moridis, 1999]. This example models a five-spot pattern of injection and production from a geothermal reservoir. Only 1/4 of the reservoir is modeled, since the solution is symmetric, as shown in Figure 1.1. The mesh uses cells of uniform 50 x 50 m size.

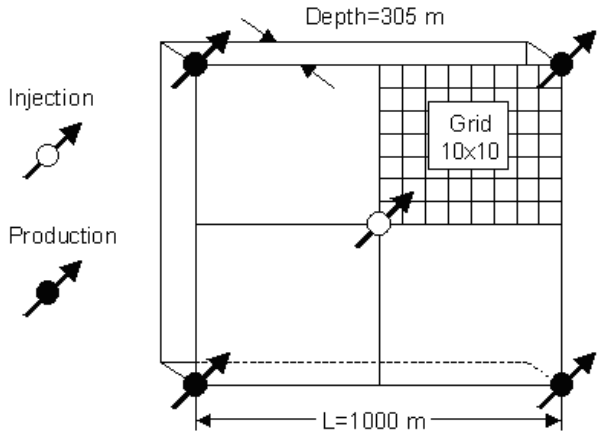

Figure 1.1. Five spot geothermal production and injection model (after [Pruess, Oldenburg, and Moridis, 1999])

We will solve this example using a porous media assumption for the formation.

Specify the Equation of State (EOS)

To ensure that PetraSim uses EOS1, edit your PetraSim preferences using the **Preferences** dialog.

1. On the **File** menu, click **Preferences...** .
2. In the **Simulator Mode** list, select **TOUGH**.
3. In the **Default EOS** list, select **EOS1**.
4. Click **OK**.

Your preferences have now been updated, but you will need to create a new model or restart PetraSim before they become active. If you already have a model open, it will not be affected by the preference change.

On the **File** menu, click **New**.

Create the Model Boundary

To create the boundary for this model, use the **Define Model Boundary** dialog. The boundary parameters for this model are shown in Table 1.1.

Table 1.1. Model Boundary Dimensions

Axis	Min (m)	Max (m)
x	0.0	500.0
y	0.0	500.0
z	0.0	305.0

To create the model boundary

1. On the **Model** menu, click **Define Boundary...** (or click on the toolbar).
2. Enter the values from Table 1.1.
3. Click **OK** to create the model boundary.

The resulting boundary is shown in Figure 1.2. You can rotate, pan, and zoom the model using the mouse and **Shift** and **Alt** keys.

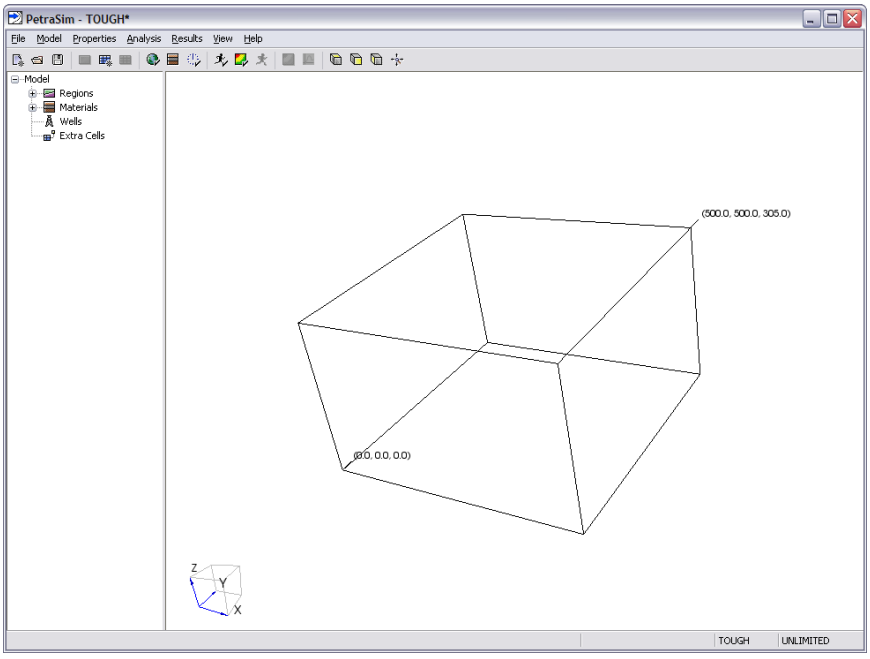

Figure 1.2. Boundary of model

Create the Grid

To create the solution grid

1. On the **Model** menu, click **Create Grid...** (or click on the toolbar).
2. In the **Division Method** box, select **Regular**.
3. In the **X Cells** box, type `10`.
4. In the **Y Cells** box, type `10`.
5. In the **Z Cells** box, type `1`.
6. Click **OK** to create the grid.

Global Properties

Global properties are those properties that apply to the entire model. In this example, the only thing we will change is the analysis name. To edit global properties, you use the **Global Properties** dialog.

On the **Properties** menu, click **Global Properties...** (or click on the toolbar).

Simulation Name

1. In the **Global Properties** dialog, select the **Analysis** tab.
2. In the **Name** box, type `Five Spot Production and Injection`.

EOS Data

The EOS (Equation of State) tab displays options for the active EOS (EOS1). In this example, the **Water, Non-isothermal** option is appropriate, so we do not need to make any changes.

Click **OK** to close the **Global Properties** dialog.

Material Properties

To specify the material properties, use the **Material Data** dialog. This example requires one material.

1. On the **Properties** menu, click **Materials** (or click on the toolbar).
2. In the **Name** box, type **POMED**.

3. In the **Density** box, type `2650.0`.
4. In the **Porosity** box, type `0.01`.
5. In all three **Permeability** boxes (X, Y, and Z), type `6e-15`.
6. In the **Wet Heat Conductivity** box, type `2.1`.
7. In the **Specific Heat** box, type `1000.0`.
8. Click **Apply** to save the changes.

In addition to the physical rock parameters, we also need to specify the relative permeability and capillary pressure functions for this material. These options can be found in the **Additional Material Data** dialog. To open this dialog, click the **Relative Perm...** button.

To specify the relative permeability function

1. Select the **Relative Perm** tab.
2. In the **Relative Permeability** list, select **Corey's Curves**.
3. In the **Slr** box, type `0.3`.
4. In the **Sgr** box, type `0.05`.

The default capillary pressure (none) is correct for this example.

Click **OK** to exit the **Advanced Material Data** dialog.

Click **OK** again to save your settings and exit the **Material Data** dialog.

Initial Conditions

The initial state of each cell in the model must be defined. The **Default Initial Conditions** dialog is used to define initial conditions that will be applied to the entire model. You can also specify initial conditions by cell, by region, or by importing the results of a previous analysis. For any analysis, the specific initial conditions will depend on several factors including EOS selection, simulator mode, and the initial state of the simulation.

Correct specification of initial conditions is essential for proper convergence and obtaining a correct result. The initial conditions must be physically meaningful. Often this requires an initial state analysis in which a model is run to obtain initial equilibrium conditions before the analysis of interest (geothermal production, VOC spill, etc.) is run.

To edit global initial conditions, on the **Properties** menu, click **Initial Conditions...**

(or click on the toolbar).

To set the initial conditions

1. Select the **Two-Phase (T, Sg)** state option.
2. In the **Temperature** box, type `300.0`.
3. In the **Gas Saturation** box, type `0.01`.
4. Click **OK**.

Selecting a two-phase initial state with a very small gas saturation is an appropriate simplification for this geothermal analysis. Since we have only one element in the vertical direction, we have selected a temperature of 300 C as a typical for this reservoir. The pressure will be calculated to correspond to the small gas saturation. Having all cells in a two-phase state will also reduce the number of state transitions (two-phase to single-phase or single-phase to two-phase) that make convergence more difficult.

Define Production Cell

The total injection/production from each five spot pattern is 30 kg/sec. Since we are using quarter symmetry, the production and injection mass flow rates will be 7.5 kg/sec. In this analysis, we will define injection and production in specific cells using the **Grid Editor**. To open the **Grid Editor**, on the **Model** menu, click **Edit Grid** (or click on the toolbar).

To define the production cell

1. Using the **Selection** tool, Right-click on the upper right cell.
2. Click **Edit Properties...**.
3. In the **Cell Name** box, type **Production**.
4. Click the **Sources/Sinks** tab.
5. Under, **Production**, select the **Mass Out** checkbox.
6. In the **Rate** box, type `7.5`.
7. Click the **Print Options** tab.
8. Select the **Print Cell Time Dependent Data** check box.
9. Click **OK** to close the **Edit Cell Data** dialog.

You will now see **Production** as the cell name and also **S** and **P**. The S indicates that the cell is a source/sink. The P indicates that detailed 2D cell history results plots will be available for this cell.

Define Injection Cell

The procdure to define the injection cell is similar

1. In the **Grid Editor**, click the **Selection** tool and then right-click on the lower left cell.
2. Click **Edit Properties...**.
3. In the **Cell Name** box, type **Injection**.
4. Click the **Sources/Sinks** tab.
5. Under, **Injection**, select the **Water/Steam** checkbox.
6. In the **Rate** box, type `7.5`.
7. In the **Enthalpy** box, type `5.0E5`.
8. Click the **Print Options** tab.
9. Select the **Print Cell Time Dependent Data** check box.
10. Click **OK** to close the **Edit Cell Data** dialog.

The **Grid Editor** display after both production and injection have been defined is shown in Figure 1.3.

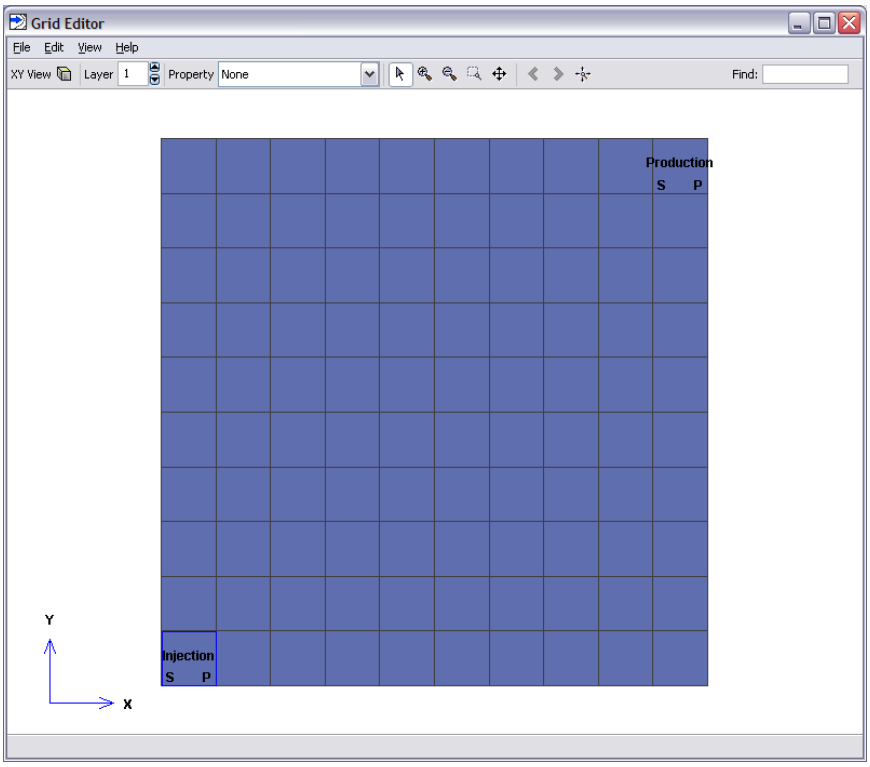

Figure 1.3. Grid Editor after injection and production has been defined

On the **File** menu, click **Close** to exit the grid editor.

Solution Controls

We will now define the solution options. Options relating the time step and other solution controls can be found in the **Solution Controls** dialog.

To open the **Solution Controls** dialog, on the **Analysis** menu, click **Solution Controls...** (or click on the toolbar).

For this example, we will set the end time and initial time step size.

1. In the **End Time** box, type `1.15185e9`.
2. In the **Time Step** list, ensure that `Single Value` is selected.
3. In the **Time Step** box, type `100`.
4. Select **Enable Automatic Time Step Adjustment**.

Click **OK** to exit the **Solution Controls** dialog.

Output Controls

By default, the simulation will print output every 100 time steps. We can increase the frequency of the output in the **Output Controls** dialog.

1. On the **Analysis** menu, click **Output Controls...** (or click on the toolbar).
2. In the **Print and Plot Every # Steps** box, type `5`.
3. Click **OK** to exit the **Output Controls** dialog.

Save and Run

The input is complete and you can run the simulation. If you haven't already, you may want to save your model in a directory specifically intended for the simulation results. For example

1. On the **File** menu, click **Save** (or click on the toolbar).
2. Create a new folder named **Five Spot** and in the **File Name** box, type **five_spot.sim**.
3. Click **Save**.

To run the simulation, on the **Analysis** menu, click **Run TOUGH2** (or click on the toolbar).

View 3D Results

To view the 3D results for a simulation, on the **Results** menu, click **3D Results** (or click on the toolbar). The data for the current simulation will be automatically loaded and displayed.

To show temperature data for the last time step

1. In the **Scalar** list, select **T**.
2. In the **Time(s)** list, select the last entry (**1.152E09**).

To add a slice plane on which contours will be displayed, click **Slice Planes...**. For this example we will show one slice plane. To configure the slice plane

1. In the **Axis** list, select **Z**.
2. In the **Coord** box, type `100.0`.
3. Select the **Scalar** check box.
4. Click **Close**.

To turn off the isosurfaces, click to clear the **Show Isosurfaces** check box.

The resulting contour plot is shown in Figure 1.4.

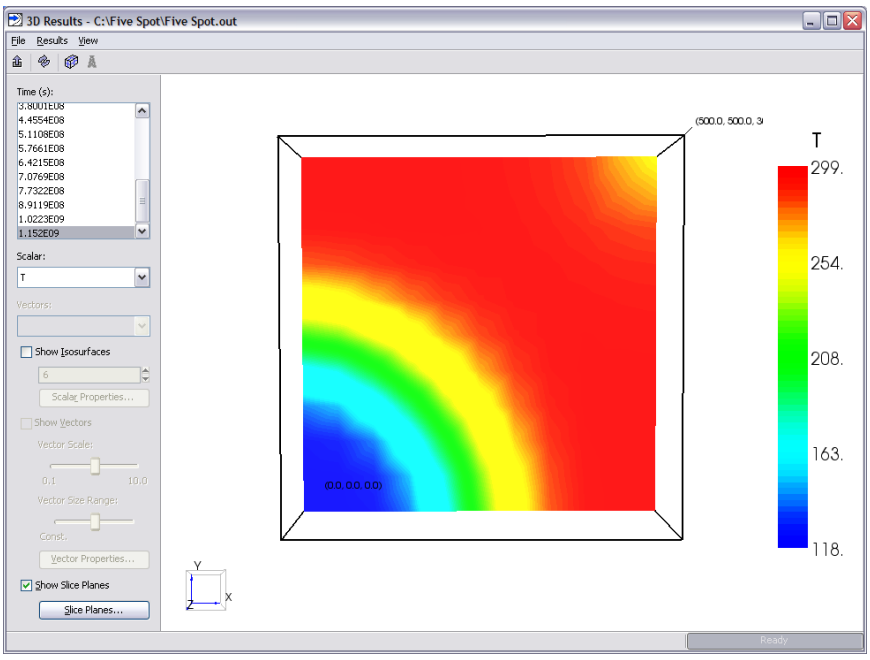

Figure 1.4. Temperature contours at end of simulation

On the **File** menu, click **Close** to close the 3D Results window

View Cell History Plots

You can view time history plots with the Cell History dialog. On the **Results** menu, click **Cell History Plots....** (or click on the toolbar).

The **Cell History** dialog will be displayed. In this window, you can display time history data using a plotting parameter and a list of cells. For example, to view the temperature in the Injection cell (cell #1)

1. In the **Variable** list, select **T**.

2. In the **Cell Name (Id#)** list, select **Injection (#1)**.

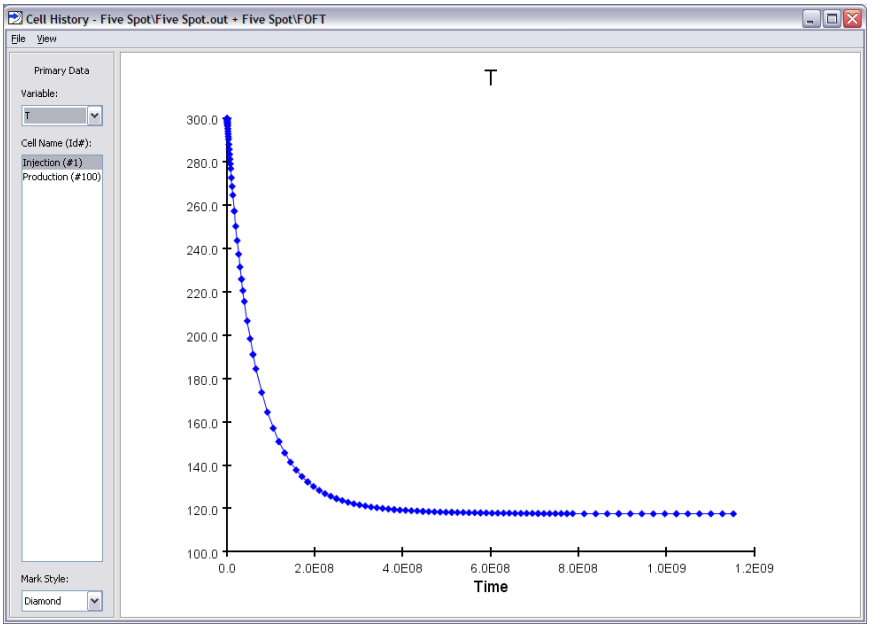

Figure 1.5. Temperature history of injection cell

In the **File** menu, click **Close** to close the Cell History window.

Chapter 2. 3D Five Spot Geothermal Production and Injection (EOS1)

Description

This example is a 3D variation of the five-spot example in Chapter 1. In this analysis, we use a 3D mesh and model the injection and production wells. We model 1/2 of the repeating five-spot pattern.

In the following descriptions, we use the full menu selection hierarchy. Optionally, many of the input dialogs can be accessed directly using the toolbar.

Specify the Equation of State (EOS)

To ensure that PetraSim uses EOS1, you may need to edit your PetraSim preferences. To edit preferences, you can use the **Preferences** dialog.

1. On the **File** menu, click **Preferences...** .
2. In the **Simulator Mode** list, select **TOUGH**.
3. In the **Default EOS** list, select **EOS1**.
4. Click **OK**.

Your preferences have now been updated, but you will need to create a new model or restart PetraSim before they become active. If you already have a model open, it will not be affected by the preference change.

On the **File** menu, click **New**.

Create the Model Boundary

To create the boundary for this model, use the **Define Model Boundary** dialog. The boundary parameters for this model are shown in Table 2.1.

Table 2.1. Model Boundary Dimensions

Axis	Min (m)	Max (m)
x	-500.0	500.0
y	0.0	500.0
z	-305.0	0.0

To create the model boundary

1. On the **Model** menu, click **Define Boundary...** (or click on the toolbar).
2. Enter the values from Table 1.1.
3. Click **OK** to create the model boundary.

You can rotate, pan, and zoom the model using the mouse and **Shift** and **Alt** keys.

Create the Grid

To create the grid

1. On the **Model** menu, click **Create Grid...** (or click on the toolbar).
2. In the **Division Method** box, select **Regular**.
3. In the **X Cells** box, type `21`.
4. In the **Y Cells** box, type `11`.
5. In the **Z Cells** box, type `6`.
6. Click **OK** to create the grid.

Global Properties

Global properties are those properties that apply to the entire model. In this example, the only thing we will change is the analysis name. To edit global properties, you use the **Global Properties** dialog.

On the **Properties** menu, click **Global Properties...** (or click on the toolbar).

1. In the **Global Properties** dialog, select the **Analysis** tab
2. In the **Name** box, type `3D Five Spot Production and Injection`

Click **OK** to close the **Global Properties** dialog.

Material Properties

To specify the material properties, you use the **Material Data** dialog. This example requires one material.

1. On the **Properties** menu, click **Materials** (or click on the toolbar).
2. In the **Name** box, type **POMED**.

3. In the **Density** box, type `2650.0`.
4. In the **Porosity** box, type `0.01`.
5. In all three **Permeability** boxes (X, Y, and Z), type `6e-15`.
6. In the **Wet Heat Conductivity** box, type `2.1`.
7. In the **Specific Heat** box, type `1000.0`.
8. Click **Apply** to save the changes.

In addition to the physical rock parameters, we also need to specify the relative permeability and capillary pressure functions for this material. These options can be found in the **Additional Material Data** dialog. To open this dialog, click the **Relative Perm...** button.

To specify the relative permeability function

1. Select the **Relative Perm** tab.
2. In the **Relative Permeability** list, select **Corey's Curves**.
3. In the **Slr** box, type `0.3`.
4. In the **Sgr** box, type `0.05`.

The default capillary pressure (none) is correct for this example.

Click **OK** to exit the **Advanced Material Data** dialog.

Click **OK** again to save your settings and exit the **Material Data** dialog.

Initial Conditions

The initial state of each cell in the model must be defined. To specify global initial conditions that will be used as the default for all cells in the model, on the **Properties** menu, click **Initial Conditions...** (or click on the toolbar).

To set the initial conditions

1. Select the **Two-Phase (T, Sg)** state option.
2. In the **Temperature** box, type `300.0`.
3. In the **Gas Saturation** box, type `0.01`.
4. Click **OK**.

Define Production Wells

In this model, we will use the well option in PetraSim. This is not a true well model with flow through cells that represent the well, it is just a way to quickly identify cells that intersect a well and then create independent sources and sinks in each intersected cell. This well will be straight, with the geometry coordinates shown in Table 2.2. For a curved well, you can use more coordinates, but they must be given in order from either the top or bottom of the well.

Table 2.2. Geometry of the first production well

X (m)	Y (m)	Z (m)
-475.0	475.0	0.0
-475.0	475.0	-305.0

To create a well, on the **Model** menu, click **Add Well...**.

1. In the **Name** box, type **ProdUL**.
2. In the **Coordinates** boxes, type the values shown in Table 2.2.
3. Click **OK** to save the changes.

Now expand the **Wells** in the **Tree View** and double-click on **ProdUL** to define the flow properties of the well. The completion interval is the length of the well from which fluid can be produced (or injected) into the reservoir.

1. Click the **Geometry** tab.
2. In the **Top Completion Depth** box, type **-200.0**.
3. In the **Bottom Completion Depth** box, type **-305.0**.

The boundary condition options for a well are similar to those for individual cells. The flow into (or from) each cell intersected by the well can be apportioned either by the cell intersection length divided by the total completion length or using the permeability-length product (k*h). This proportions flow taking into account the different permeabilities of the intersected cells. For this model, we will produce at a rate of 7.5 kg/s from each production well.

1. Click the **Flow** tab.
2. Select the **Mass Out** check box.
3. In the **Rate** box, type **7.5**.

4. Select the **Using k*h**.

5. Click **OK** to save the changes.

Create a second production well named **ProdUR** with the coordinates shown in Table 2.3. Use the same completion interval and production rates as for the **ProdUL** well.

Table 2.3. Geometry of the second production well

X (m)	Y (m)	Z (m)
475.0	475.0	0.0
475.0	475.0	-305.0

Define Injection Well

We will model one injection well. Create the well using the coordinates in Table 2.4. Use the name **Inject**.

Table 2.4. Geometry of the injection well

X (m)	Y (m)	Z (m)
0.0	25.0	0.0
0.0	25.0	-305.0

Double-click on **Inject** to define the flow properties of the well. Define the completion interval.

1. Click the **Geometry** tab.

2. In the **Top Completion Depth** box, type **0.0**.

3. In the **Bottom Completion Depth** box, type **-200.0**.

This is an injection well with a flow rate of 15.0 kg/s.

1. Click the **Flow** tab.

2. Under **Injection**, select the **Water/Steam** check box.

3. In the **Rate** box, type **15.0**.

4. In the **Enthalpy** box, type **5.0E5**. Using a steam table, this corresponds to subcooled water at a temperature of about 119 C.

5. In the **Apportion** box, select **Using k*h**.

6. Click **OK** to save the changes.

A display of the wells is shown in Figure 2.1. To turn off the grid

1. On the **View** menu, click **Grid**.

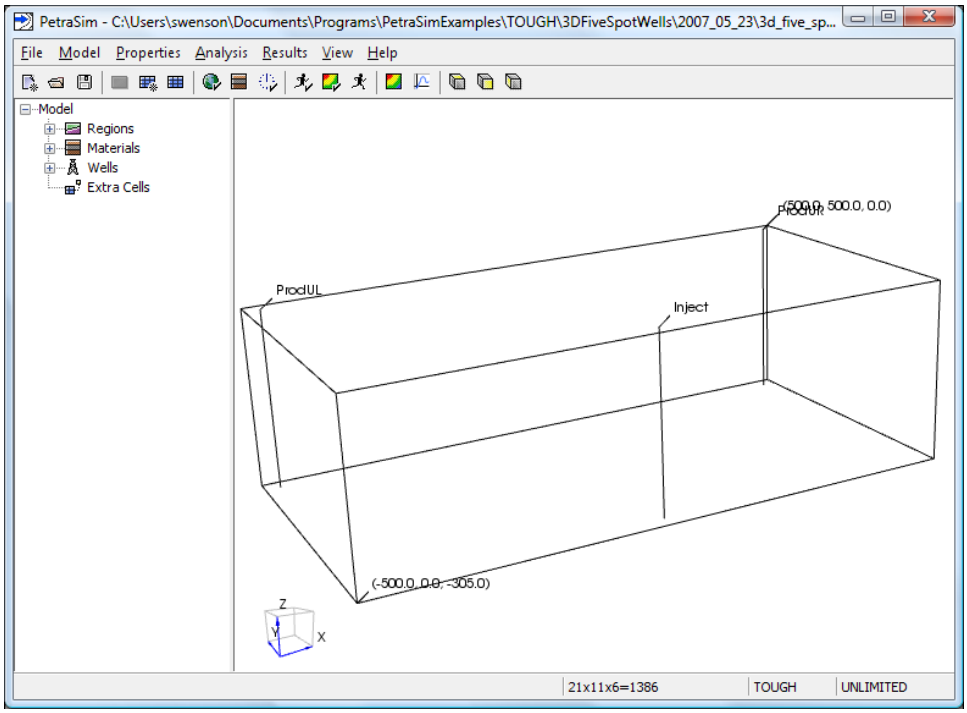

Figure 2.1. Wells in the model

Solution Controls

We will now define the solution options. Options relating the time step and other solution controls can be found in the **Solution Controls** dialog.

To open the **Solution Controls** dialog, on the **Analysis** menu, click **Solution Controls...** (or click on the toolbar).

For this example, we will set the end time and the initial time step size.

1. In the **End Time** box, type `1.15185e9`.

2. In the **Time Step** list, ensure that `Single Value` is selected.

3. In the **Time Step** box, type `100`.

4. Select **Enable Automatic Time Step Adjustment**.

Click **OK** to exit the **Solution Controls** dialog.

Output Controls

By default, the simulation will print output every 100 time steps. We can change the frequency of the output in the **Output Controls** dialog.

1. On the **Analysis** menu, click **Output Controls...** (or click on the toolbar).

2. In the **Print and Plot Every # Steps** box, type `5`.

3. Select the **Fluxes and Velocities** check box.

4. Click **OK** to exit the **Output Controls** dialog.

Save and Run

The input is complete and you can run the simulation. If you haven't already, you may want to save your model in a directory specifically intended for the simulation results. For example

1. On the **File** menu, click **Save** (or click on the toolbar).

2. Create a new folder named **3D Five Spot Wells** and in the **File Name** box, type **five_spot_wells.sim**.

3. Click **Save**.

To run the simulation, on the **Analysis** menu, click **Run TOUGH2** (or click on the toolbar).

View 3D Results

To view the 3D results for a simulation, on the **Results** menu, click **3D Results** (or click on the toolbar). The data for the current simulation will be automatically loaded and displayed.

To show temperature data for the last time step

1. In the **Time(s)** list, select the last entry (**1.152E09**).

2. In the **Scalar** list, select **T**.

To show water flow vectors

1. In the **Vectors** list, select **FLOF**.
2. Select the **Show Vectors** checkbox.

To add a slice plane on which contours will be displayed, click **Slice Planes...**. For this example we will show one slice plane. To configure the slice plane

1. In the **Axis** list, select **Z**.
2. In the **Coord** box, type `-200.0`.
3. Select the **Scalar** check box.
4. In the **Axis** list, select **X**.
5. In the **Coord** box, type `0.0`.
6. Select the **Scalar** check box.
7. Click **Close**.

The resulting contour plot is shown in Figure 2.2.

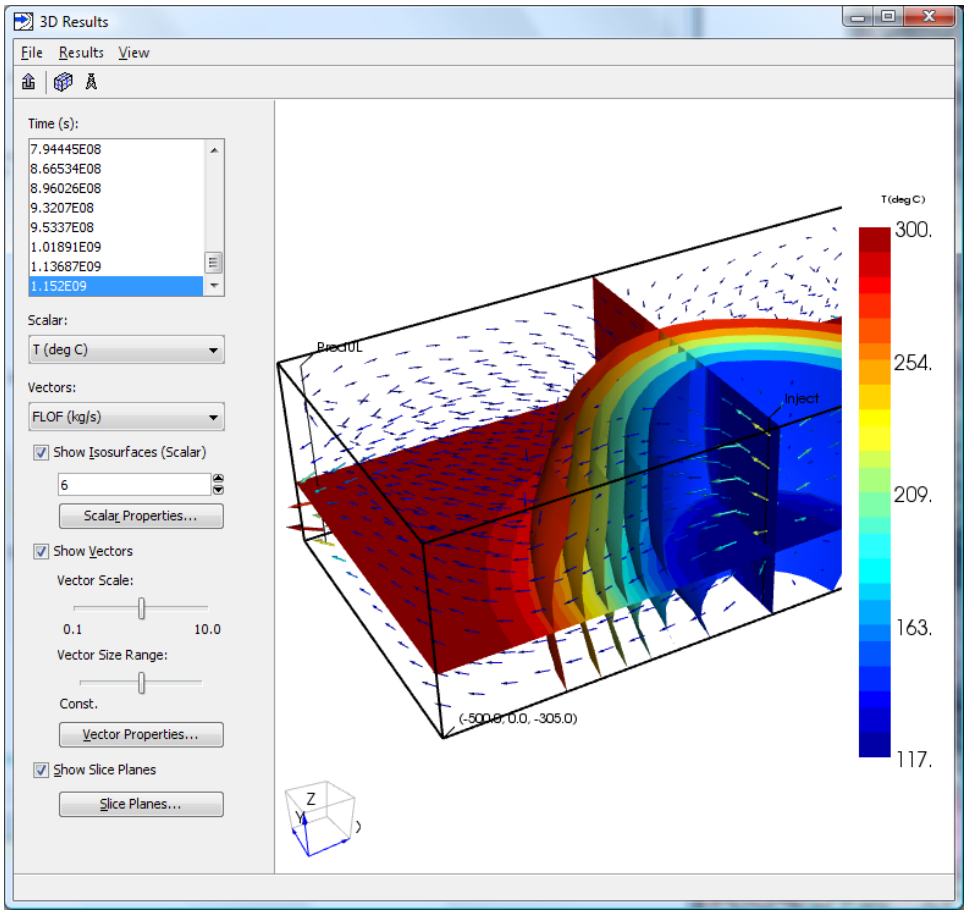

Figure 2.2. Temperature contours and water flow vectors at end of simulation

On the **File** menu, click **Close** to close the 3D Results window.

Chapter 3. 3D Contour Example (EOS1)

Description

This example demonstrates a basic reservoir analysis, including an initial state calculation and then a production analysis. The example also demonstrates the use of contours to define the model surface, so that the surface represents a varying topography. Surface boundary conditions are also specified.

It is assumed that the user has obtained familiarity with PetraSim by working the examples in Chapter 1 and Chapter 2.

Specify the Equation of State (EOS)

To ensure that PetraSim uses EOS1, edit your PetraSim preferences using the **Preferences** dialog.

1. On the **File** menu, click **Preferences...** .
2. In the **Simulator Mode** list, select **TOUGH**.
3. In the **Default EOS** list, select **EOS1**.
4. Click **OK**.

Your preferences have now been updated, but you will need to create a new model or restart PetraSim before they become active. If you already have a model open, it will not be affected by the preference change. On the **File** menu, click **New**.

Create the Model Boundary

To create the boundary, use the **Define Model Boundary** dialog. The boundary parameters for this model are shown in Table 3.1.

Table 3.1. Model boundary dimensions

Axis	Min (m)	Max (m)
x	-1000.0	1000.0
y	0.0	1000.0
z	-1500.0	200.0

To create the model boundary

1. On the **Model** menu, click **Define Boundary...** (or click on the toolbar).

2. Enter the values from Table 3.1.

3. Click **OK** to create the model boundary.

You can rotate, pan, and zoom the model using the mouse and **Shift** and **Alt** keys.

Define Contour of Model

We next define the top contour of the model. This is done using a file that defines the surface contour levels in the format described in the PetraSim User Manual

To specify the top surface contour

1. Download the contour file for this example under **Support** at http://www.thunderheadeng.com). Save the file with the name `top.ctr`.

2. On the **Model** menu, click **Set Top and Bottom...**.

3. In the **Top Surface** list, click **Contour** and then click **Choose** to select the **top.ctr** file, Figure 3.1.

4. Click **OK** to save the data.

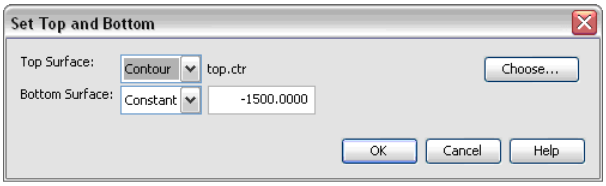

Figure 3.1. Defining the top contour of the model

Create the Grid

To create the solution grid

1. On the **Model** menu, click **Create Grid...** (or click on the toolbar).

2. In the **Division Method** box, select **Regular**.

3. Click **Cells Above Top and Below Bottom are Inactive**. This removes the cells outside of the boundaries from the model.

4. Click **XYZ Grid**.

5. In the **X Cells** box, type `20`.

6. In the **Y Cells** box, type `10`.

7. In the **Z Cells** box, type `17`.

8. Click **OK** to create the grid.

The resulting mesh is displayed in Figure 3.2. Click on the model and spin it so that it is displayed as shown below. Hold the **Shift** key and drag to pan; hold the **Alt** key and drag to zoom. The display shows the cells that have been disabled as a result of defining a top contour. This capability allows the user to define more complex surface features in detailed models.

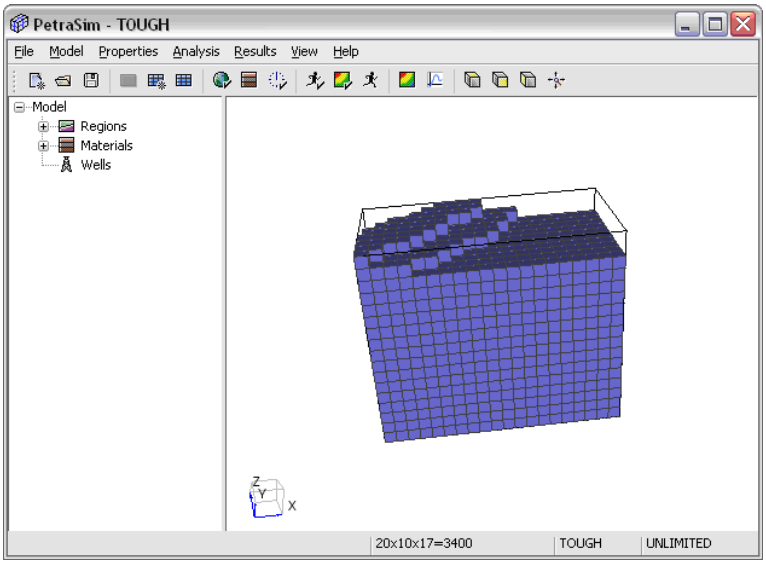

Figure 3.2. Creating grid for the model

Global Properties

None of the global properties need to be changed. We use the default EOS1 option of water, non-isothermal.

Material Properties

To specify the material properties, use the **Material Data** dialog. This example requires three materials.

1. On the **Properties** menu, click **Materials** (or click on the toolbar).

2. In the **Name** box, type **POMED**.

3. In the **Density** box, type `2650.0`.

4. In the **Porosity** box, type `0.01`.

5. In all three **Permeability** boxes (X, Y, and Z), type `6e-15`.

6. In the **Wet Heat Conductivity** box, type `2.1`.

7. In the **Specific Heat** box, type `1000.0`.

8. Click **Apply** to save the changes.

In addition to the physical rock parameters, we can also specify the relative permeability and capillary pressure functions by clicking the **Relative Perm...** button. for this example, we will just use the default functions and so will not make any changes.

We will now create a new cap rock material, based on POMED

1. In the **Material Data** dialog, click **New**.

2. In the **Tough Name** box, type **CAPRK**.

3. In the **Description** box, type **Cap Rock**.

4. In the **Based On** list, select **POMED**.

5. Click **OK** to create the new material.

The **CAPRK** will represent a material with low permeability near the top of the reservoir. Because it was based on the **POMED** material, it has inherited all the properties we previously defined for that material. To modify the **CAPRK** material

1. On the **Materials** list, select **CAPRK**.

2. In all three **Permeability** boxes (X, Y, and Z), type `6e-16`.

3. Click **Apply** to save the changes.

Finally, we will create one material to be used to represent an aquifer boundary condition. This material will allow the flow of water, but not heat.

1. In the **Material Data** dialog, click **New**.

2. In the **Tough Name** box, type **AQUIF**.

3. In the **Description** box, type **Aquifer**.

4. In the **Based On** list, select **POMED**.

5. Click **OK** to create the new material.

The **AQUIF** will represent a material with zero heat conduction. To modify the **AQUIF** material

1. On the **Materials** list, select **AQUIF**.
2. In the **Wet Heat Conductivity** box, type `0.0`, Figure 3.3.
3. Click **OK** to save the changes and close the **Material Data** dialog.

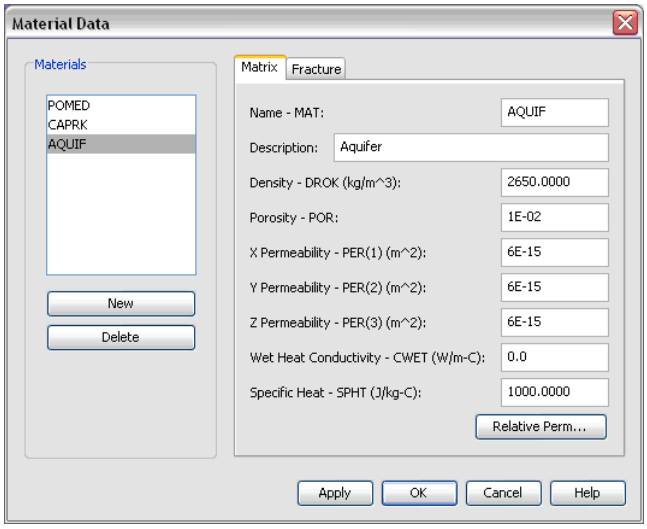

Figure 3.3. Changing the conductivity for the material AQUIF

Initial Conditions

The initial state of each cell in the model must be defined. For this analysis, we will define linear pressure and temperature gradients. At the surface (200 m), the pressure will be 1E5 Pa (1 bar) and the temperature 10 C. At the bottom of the reservoir (-1500 m), the pressure will be the approximate hydraulic head 15E6 Pa and a temperature of 200 C. These initial conditions approximate the steady state solution, so they help speed convergence.

To define the global initial conditions, on the **Properties** menu, click **Initial Conditions...** (or click on the toolbar).

To define the pressure gradient

1. Select the **Single-Phase (P, T)** state option.
2. In the **Pressure** type list, select **Function**.
3. In the **Edit Linear Function** dialog in the **A** box, type `1.853E6`.
4. In the **D** box, type `-8765.0`.

To define the temperature gradient

1. In the **Temperature** type list, select **Function**.
2. In the **Edit Linear Function** dialog in the **A** box, type `32.353`.
3. In the **D** box, type `-0.1117`.
4. Click **OK** to close the **Edit Linear Function** dialog.
5. Click **OK** to close the **Default Initial Conditions** dialog.

The **Default Initial Conditions** dialog after the functions have been defined is shown in Figure 3.4.

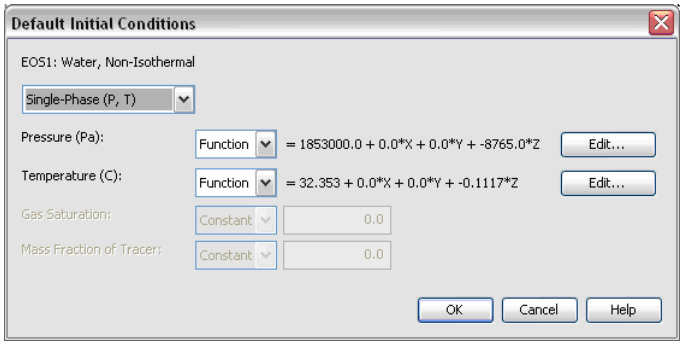

Figure 3.4. Defining the initial conditions

Grid Operations

Delete Gridlines

We will first delete some gridlines to reduce the number of cells in the solution. To edit the grid or individual cell properties, use the **Grid Editor**.

To delete gridlines in the model

1. Open the **Grid Editor**. On the **Model** menu, click **Edit Grid** (or click on the toolbar).
2. Click on the **View** icon to select the **XZ View**.
3. Right-click on the 5th gridline down from the top.
4. Click **Delete Selected Line**.
5. Repeat for the 7th, 9th, and 11th gridlines from the top.

When completed, the side view should be as shown in Figure 3.5. We leave the more refined grid to represent the reservoir from -1500 to -1000 m.

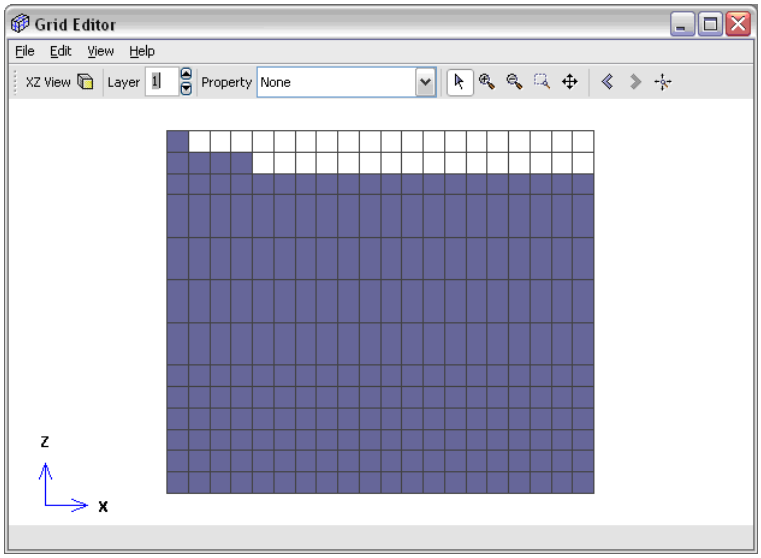

Figure 3.5. The view after removing gridlines 5, 7, 9, 11

Insert Gridline

We will also insert a gridline that will give a thin layer of cells on the side of the reservoir. These will be used to define boundary conditions. To insert a gridline

1. In the **Grid Editor**, click on the **View** icon to select the **XZ View**.
2. On the **Edit** menu, click **Add Vertical Line...**.
3. In the **Add Vertical Line** dialog, in the **X Position** box, type `990.0`.
4. Click **OK** to close add the line.

The new gridline will be inserted on the right side of the grid.

Change Material Properties of a Layer

We will assign the relatively impermeable material properties to a layer of cells near the top of the model. To do this

1. In the **Grid Editor**, click on the **View** icon to select the **XY View**.
2. In the **Layer** box, type `10` and then press the **ENTER** key.
3. On the **Edit** menu, click **Select Layer** (or press and drag the mouse to select all cells). In the 3D view, the selected layer will be highlighted.
4. Right-click on any of the selected cells and click **Properties**.

5. In the **Material** list, select **CAPRK**.

6. Click **OK** to close the **Edit Multi-Cell Data** dialog.

To confirm that the material has been assigned

1. In the **Grid Editor**, click on the **View** icon to select the **XZ View**.

2. In the **Property** list, select **Material**.

3. The display will show two materials, Figure 3.6. Note that the material name is displayed in the lower information bar as the cursor hovers over each cell.

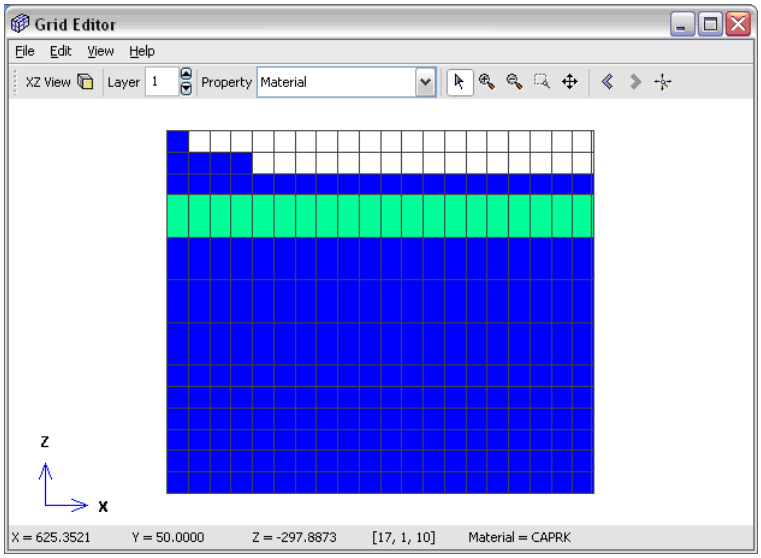

Figure 3.6. Displaying the different materials in different colors

Surface Boundary Conditions

We now want to define surface boundary conditions for the model. These will be a pressure of 1E5 Pa (1 bar) and a temperature of 10 C.

1. In the **Grid Editor**, click on the **View** icon to select the **XZ View**.

2. In the **Layer** box, scroll to layer `1`.

3. Select the top cells in the layer, Figure 3.7. To select multiple cells, press the **CTRL** key and then either drag or click on individual cells.

4. Right-click on any of the selected cells and click **Properties**.

5. In the **Type** list, select **Fixed State**.

6. Click the **Initial Conditions** tab.

7. Click **Specify Initial Conditions by Cell**. The initial conditions for the individual cells override the global values.

8. In the **Pressure** box, type `1E5`.

9. In the **Temperature** box, type `10.0`.

10. Click **OK** to close the **Edit Multi-Cell Data** dialog.

11. You will see an **F** indicating these cells are **Fixed State**.

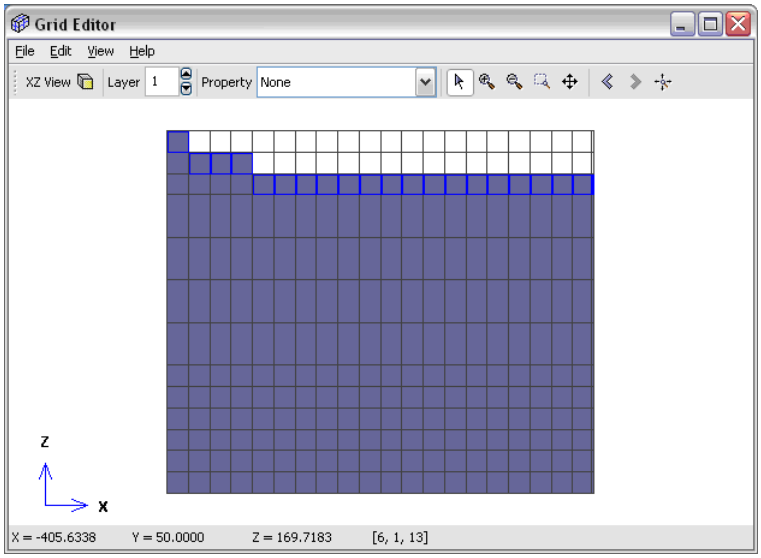

Figure 3.7. Selecting multiple cells to be edited

Repeat this operation for all 10 layers in the **XZ View**, remembering to select only the top cells for each layer.

When completed, you can verify your specification by looking at the mesh in different views. For example, click on the **View** icon to select the **XY View**. In the **Layer** box, scroll to layer `12`. You should see the fixed cells displayed as in Figure 3.8.

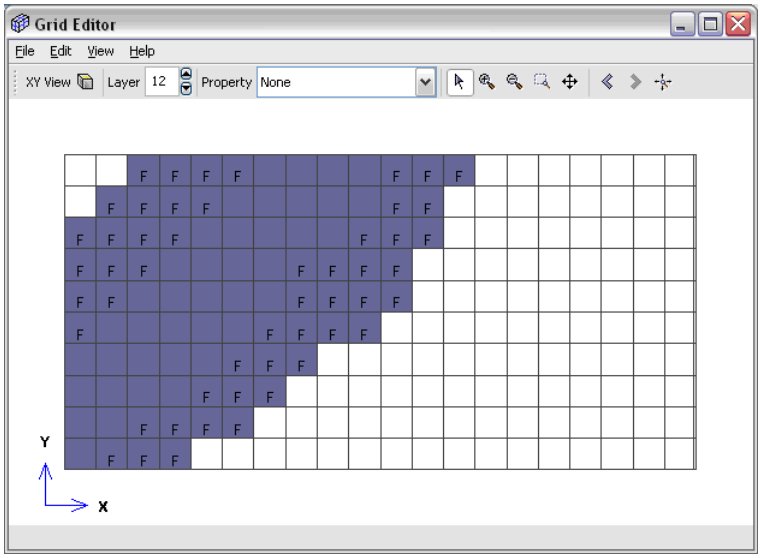

Figure 3.8. The result after changing the top cells in each layer

Define Heat Source

We will assume that there is a heat source at the bottom of the reservoir. To define this source

1. In the **Grid Editor**, click on the **View** icon to select the **XY View**.
2. In the **Layer** box, scroll to layer `1`.
3. In this view, click and drag to select the cells shown in Figure 3.9. We will define a total flow of 25 kg/s for these 50 cells, or 0.5 kg/s for each cell.
4. Right-click on any of the selected cells and click **Source/Sink...**.
5. Under **Injection**, select the **Water/Steam** check box..
6. In the **Rate** box, type `0.5`.
7. In the **Enthalpy** box, type `1.085E6`.
8. Click **OK** to close the **Edit Multi-Cell Data** dialog.
9. You will see an **S** indicating these cells are **Sources**.

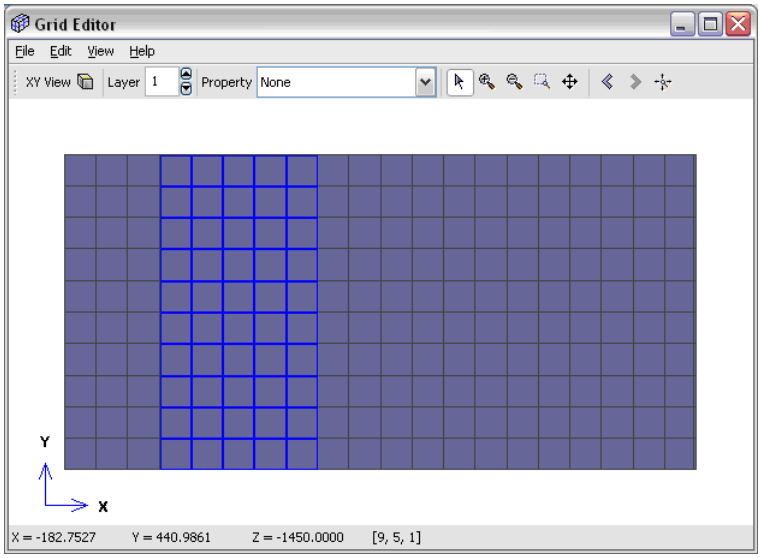

Figure 3.9. The cells to select in Layer 1

Define Outflow Aquifer

We will define a fixed pressure aquifer on the side of the reservoir. We previously defined a mass upflow from the bottom of the reservoir. By setting a fixed pressure on selected cells on the side of the reservoir, this will represent an aquifer that receives outflow from the reservoir. We will also change the material type of the aquifer cells to AQUIF.

1. In the **Grid Editor**, click on the **View** icon to select the **YZ View**.
2. In the **Layer** box, scroll to layer `21` (or enter `21` and press **ENTER**.
3. In this view, click and drag to select the cells shown in Figure 3.10.
4. Right-click on any of the selected cells and click **Properties**.
5. In the **Type** list, select **Disabled**.
6. Click **OK** to close the **Edit Multi-Cell Data** dialog.
7. The disabled cells will not be drawn.

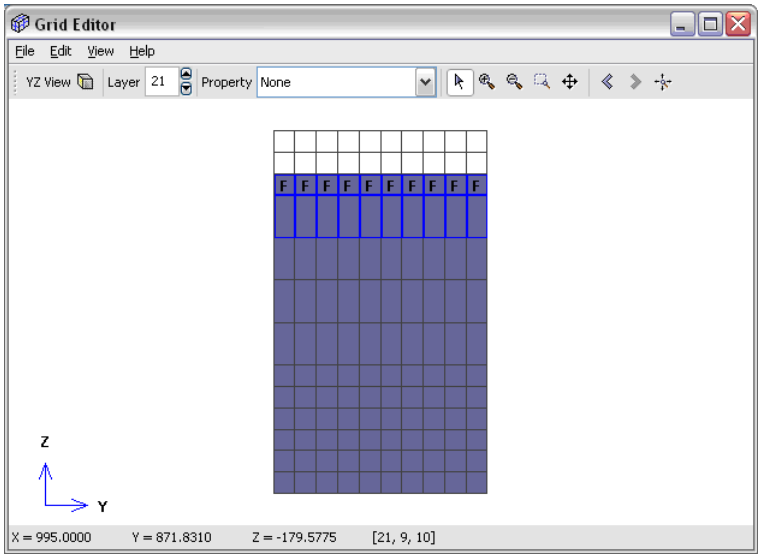

Figure 3.10. The cells to select for Layer 21

Repeat to disable the cells shown in Figure 3.11

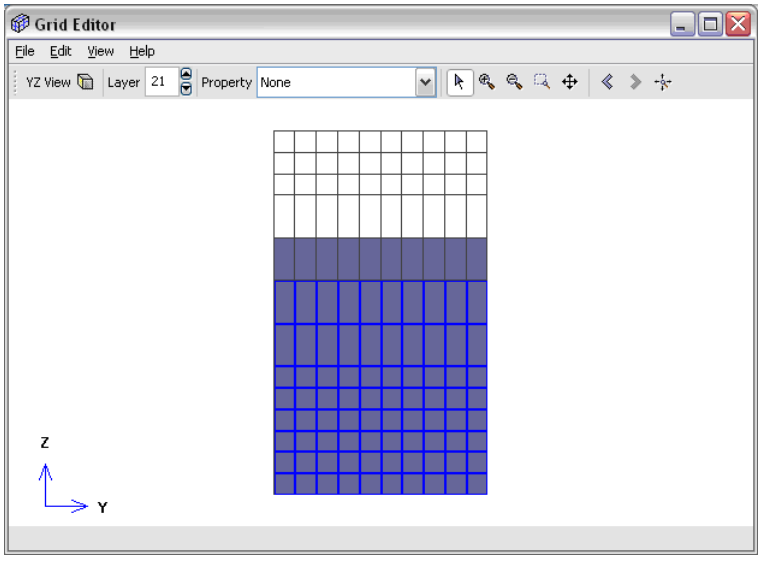

Figure 3.11. The remaining cells to disable

This leaves one line of cells that are still **Enabled** in **Layer 21**. We will define a fixed pressure for these cells.

1. Click and drag to select the cells shown in Figure 3.12.

2. Right-click on any of the selected cells and click **Properties**.

3. In the **Material** list, select **AQUIF**.

4. In the **Type** list, select **Fixed State**.

5. Click the **Initial Conditions** tab.

6. Click **Specify Initial Conditions by Cell**. The initial conditions for the individual cells override the global values.

7. In the **Pressure** box, type `3.5E6`. This corresponds to a hydrostatic pressure at 400 m depth. Since the AQUIF material has zero heat conductivity, the temperature of these cells will not affect heat flow, so we do not change it.

8. Click **OK** to close the **Edit Multi-Cell Data** dialog.

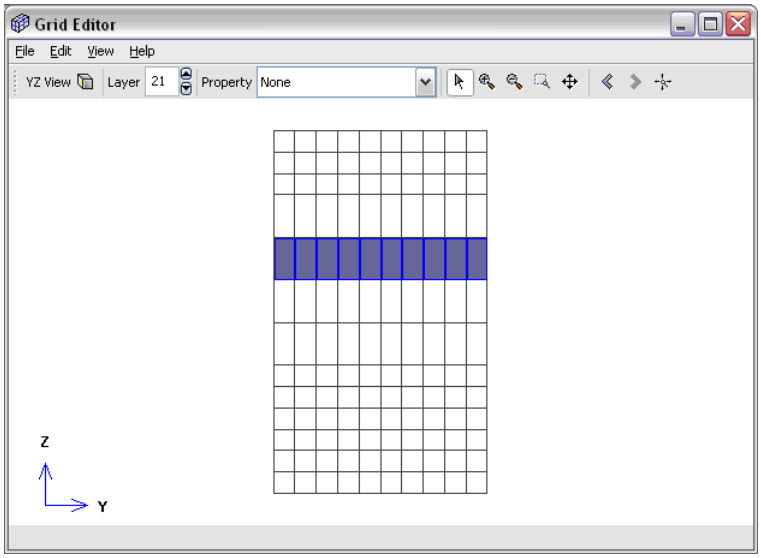

Figure 3.12. The remaining cells to be selected

Select Cells for Time History Output

We can select cells to print output more frequently than the frequency for the entire mesh.

1. In the **Grid Editor**, go to **Layer 1** in the **XY View**.

2. Right-click on a cell in the center of the heat source and click **Edit Properties...**.

3. In the **Name** box, type `Source`.

4. Click the **Print Options** tab.

5. Select the **Print Cell Time Dependent Data** check box.

6. Click **OK** to close the **Edit Cell Data** dialog.

Similarly, in **Layer 20** of the **YZ View**, select a cell near the outflow (approximate co-ordinates Y=450.0, Z=-400.0) for printing. Give it a **Name** of `Outflow` and select the **Print Cell Time Dependent Data** check box.

Close the grid editor.

Solution Controls

We will now define the solution options.

1. On the **Analysis** menu, click **Solution Controls...** (or click on the toolbar).
2. In the **End Time** box, type `6.308E11` sec (about 20,000 years).
3. In the **Time Step** list, ensure that `Single Value` is selected.
4. In the **Time Step** box, type `100`.
5. In the **Max Num Time Steps** box, type `500`.
6. Select **Enable Automatic Time Step Adjustment**.
7. Click **OK** to exit the **Solution Controls** dialog..

Output Controls

By default, the simulation will print output every 100 time steps. We can increase the frequency of the output in the **Output Controls** dialog.

1. On the **Analysis** menu, click **Output Controls...** (or click on the toolbar).
2. In the **Print and Plot Every # Steps** box, type `20`.
3. Click **OK** to exit the **Output Controls** dialog.

Save and Run

The input is complete and you can run the simulation. If you haven't already, you may want to save your model in a directory specifically intended for the simulation results. For example

1. On the **File** menu, click **Save** (or click on the toolbar).
2. Create a new folder named **Initial** and in the **File Name** box, type **initial.sim**.
3. Click **Save**.

To run the simulation, on the **Analysis** menu, click **Run TOUGH2** (or click on the toolbar).

During the solution, a graph will display the time step size. In this case, the time steps become very large near the end of the solution, which indicates that a steady state has been reached.

View 3D Results

To view the 3D results for a simulation, on the **Results** menu, click **3D Results** (or click on the toolbar). The data for the current simulation will be automatically loaded and displayed.

To show temperature contours for the last time step

1. In the **Time(s)** list, select the last entry (**6.308E11**).
2. In the **Scalar** list, select **T**.
3. Select the **Show Isosurfaces** checkbox.

To show water flow vectors

1. In the **Vectors** list, select **FLOF**.
2. Select the **Show Vectors** checkbox.

To add a slice plane on which contours will be displayed, click **Slice Planes...**. For this example we will show one slice plane. To configure the slice plane

1. In the **Axis** list, select **Y**.
2. In the **Coord** box, type `500.0`.
3. Select the **Scalar** check box.
4. Click **Close**.

The resulting contour and vector plot is shown in Figure 3.13. The heating upflow and the cooling downflow can be seen.

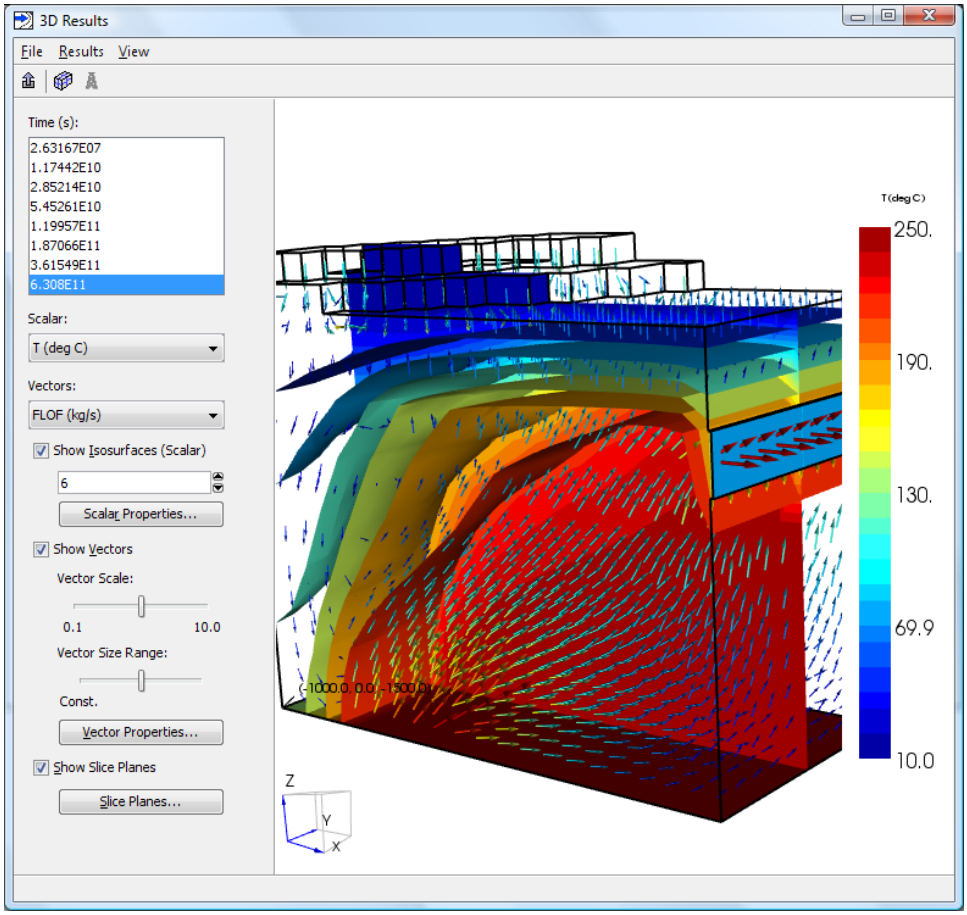

Figure 3.13. The resulting display of the simulation

Close the **3D Results** window.

View Cell History Plots

You can view time history plots with the Cell History dialog. On the **Results** menu, click **Cell History Plots....** (or click on the toolbar).

The **Cell History** dialog will be displayed. In this window, you can display time history data using a plotting parameter and a list of cells. For example, to view the temperature in the Outflow cell

1. In the **Variable** list, select **T**.

2. In the **Cell Name (Id#)** list, select **Outflow**.

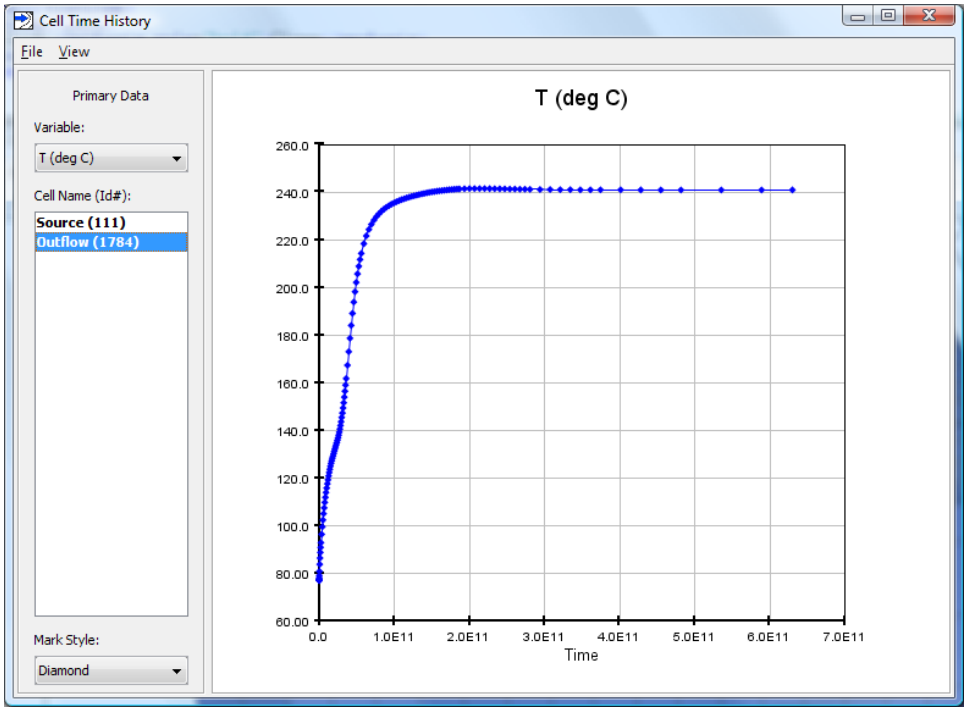

Figure 3.14. Time history plot at Outflow cell

In the **File** menu, click **Close** to close the Cell History window.

Production Analysis

We will now use the initial state results to perform a simplified production analysis. You will open the model file (initial.sim) that we previously saved and then save it to a new directory.

1. If the initial model is not already open, on the **File** menu, click **Open** (or click on the toolbar). In the **File Name** box, select the **initial.sim** file and click **Open**. This will open the existing model.

2. To save the production model, on the **File** menu, click **Save As...**.

3. Create a new folder named **Production** and in the **File Name** box, type **production.sim**.

4. Click **Save**.

Solution Controls for Production Run

This analysis will continue from the initial state analysis.

1. On the **Analysis** menu, click **Solution Controls...** (or click on the toolbar).

2. In the **End Time** box, type `6.307E8` sec (about 20 years).

3. Click **OK** to exit the **Solution Controls** dialog..

Load Initial Conditions

We will now perform a sample production analysis, using the previously calculated initial state results as initial conditions. We do this by reading the **SAVE** file that was output at the end of the initial state analysis. This file has the results for all the cells in the model. To read these initial conditions

1. On the **File** menu, click **Load Initial Conditions...** .

2. Browse to the **Initial**folder and select the **SAVE** file.

3. Click **Open**. This reads the saved data from the previous run and stores it as an initial condition for each cell in the current analysis.

To view the initial conditions, open the **Grid Editor**

1. On the **Model** menu, click **Edit Grid** (or click on the toolbar).

2. In the **Grid Editor**, click on the **View** icon to select the **XZ View**.

3. In the **Property** list, select **Temperature**.

4. The display will show the temperatures from the initial state analysis, Figure 3.15.

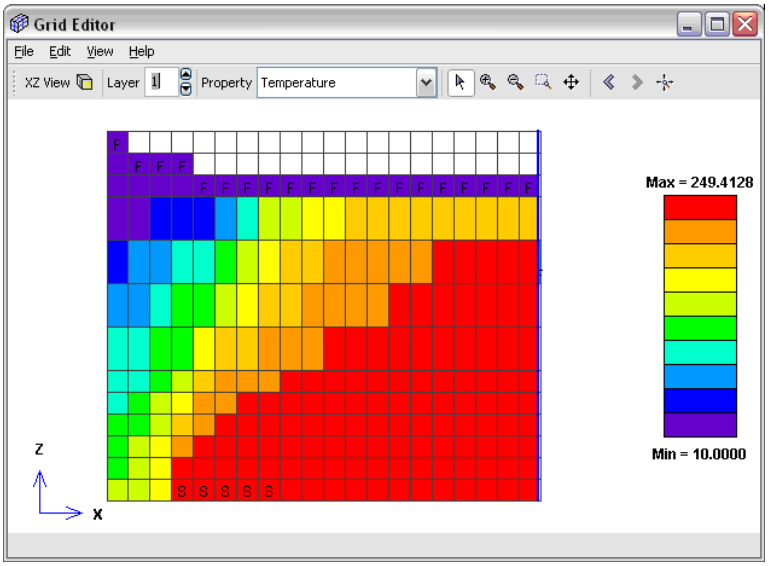

Figure 3.15. The grid editor with temperature as the display variable

Define Injection and Production

In the production run, we will produce from two wells and inject into one well. The injection and production data will be defined in a separate input file, but the data in the file uses names that must match cell names. To give the cell names

1. In the **Grid Editor**, click on the **View** icon to select the **XY View**.
2. In the **Layer** box, scroll to layer 3.
3. Right-click on the cell named **P1** as shown in Figure 3.16 and click **Properties**.
4. In the **Cell Name** box, enter **P1**.
5. Click **OK** to close the **Edit Cell Data** dialog..
6. Repeat, naming the **P2** and **I1** cells.

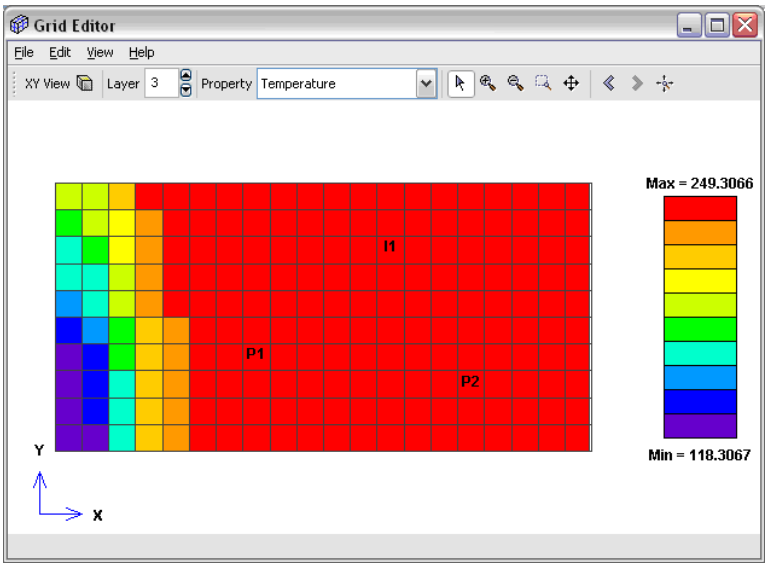

Figure 3.16. The cells to select and name

The well production and injection rates will be read from a file (download the welltable.dat file). The content of this file is shown below.

```
P1 P2 I1
MASS MASS COM1
     0.   10.   0.    0.   0.    0.       0.
3.154E7   10.   0.   10.   0.   15.   4.19E5
3.154E9   10.   0.   10.   0.   15.   4.19E5
```

The first line gives names of the wells. These names must also be defined as cell names in the Grid Editor. The second line gives the generation type (MASS for pro-

duction, COM1 for injection) for each well. The following lines each contain a time followed by pairs of flow rate and enthalpy for each well. Enthalpy is required, but not used, for production wells. In the above example, we produce from only P1 for one year, then begin producing from P2 and injecting in I1 after one year. This table input is provided so that the user could set up a spreadsheet with all well data. Note: The file MUST be in this format for it to load correctly.

To load the welltable file

1. Close the **Grid Editor**.
2. On the **File** menu, click **Load Well Flow Rates**.
3. In the **File Name** box, select the **welltable.dat** file that you downloaded.
4. Click **Open** to load the data.

If you now return to the **Grid Editor** and look at the **Source/Sink** data for the named cells, you will find that tables with the specified flow rates have been associated with each cell.

Save and Run Production Analysis

The input is complete and you can run the simulation. The model file will automatically be saved when you run the analysis.

To run the simulation, on the **Analysis** menu, click **Run TOUGH2** (or click on the toolbar).

View 3D Results for Production Run

To view the 3D results for a simulation, on the **Results** menu, click **3D Results** (or click on the toolbar). The data for the current simulation will be automatically loaded and displayed.

To show temperature contours for the last time step

1. In the **Time(s)** list, select the last entry (**6.308E8**).
2. In the **Scalar** list, select **T**.
3. Click to clear the **Show Isosurfaces** checkbox. The contours will be displayed on a slice plane.

To show water flow vectors

1. In the **Vectors** list, select **FLOF**.
2. Select the **Show Vectors** checkbox.

To add a slice plane on which contours will be displayed, click **Slice Planes...**. For this example we will show one slice plane. To configure the slice plane

1. In the **Axis** list, select **Y**.
2. In the **Coord** box, type `750.0`.
3. Select the **Scalar** check box.
4. Click **Close**.

The resulting contour and vector plot is shown in Figure 3.17. The cooling near the injection well and the flow of water from the injection wells can be seen.

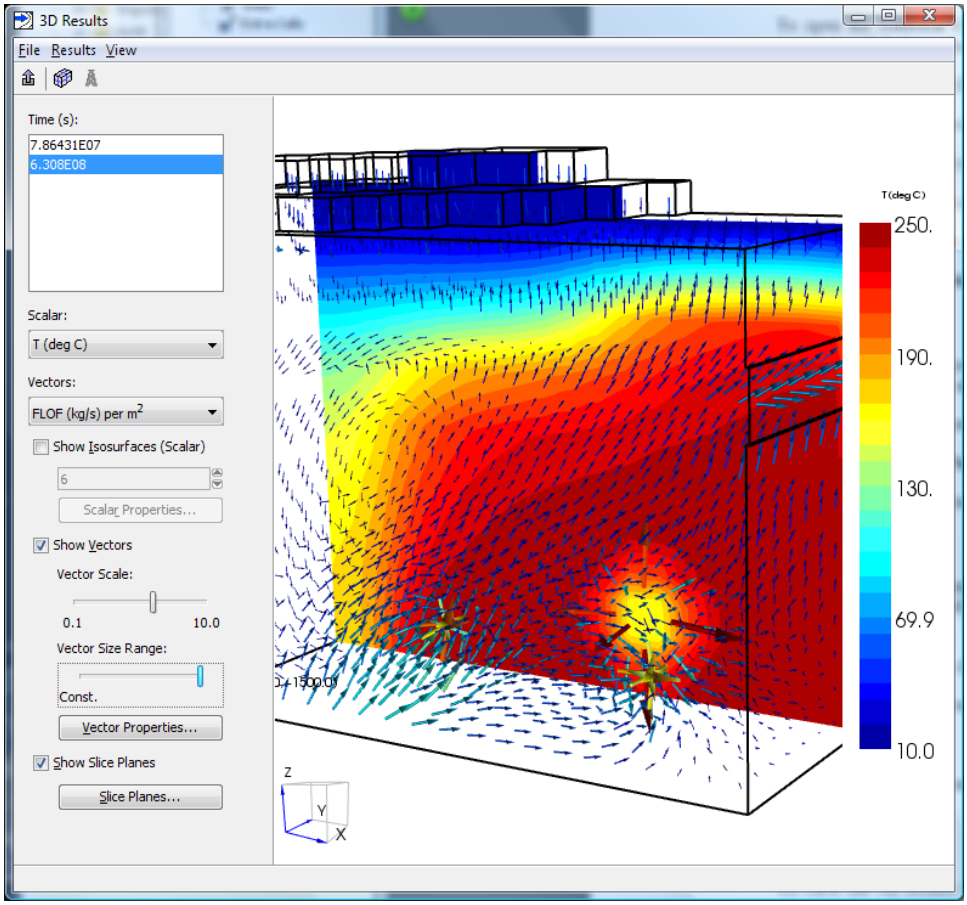

Figure 3.17. The final display

Close the **3D Results** window.

Summary

This analysis has given a simple example of an initial state run followed by a production run.

Reservoir simulation is typically carried out in three phases. The first is initial-state modeling, in which the pre-exploitation subsurface temperature and pressure conditions are simulated by assigning a set of hydrological and thermal properties to each grid block and matching the steady-state natural conditions after a simulated time of several thousand years. Matching of the observed and calculated initial conditions (such as temperature, pressure, enthalpy, heat flow, etc.) by trial and error provides the first round calibration of the model. This match is typically achieved by altering the distribution of hydrologic properties and the location and strengths of fluid sources and sinks until known or inferred conditions are reproduced by the model within a chosen tolerance.

The second phase is referred to as history matching, in which the historical behavior of production wells (rate, pressure, temperature and enthalpy) and injection wells (generally rate and injection pressure) are matched by trial and error using the model. Typically, the production history match is obtained by varying the hydrologic parameters used in the model, particularly storage-related parameters such as porosity, and often by refining the grid block arrangement in the vicinity of the production or injection wells and/or refining the relative permeability characteristics. After the history match is complete, the initial-state model is re-run to ensure that the changes made for history matching have not significantly affected the model's ability to again reproduce the initial state reservoir conditions.

The third stage is forecasting. Once the model has been calibrated by initial-state modeling and history matching, it can be considered fully calibrated and used to predict future well and reservoir behavior under various production and injection scenarios. Forecasting is the final stage of numerical modeling of geothermal reservoirs, and is an indispensable tool for optimizing resource recovery, project planning, mitigating potential development problems, and reservoir management.

Chapter 4. Heat Sweep in a Vertical Fracture (EOS1)

Description

This example is Problem 3 - Heat Sweep in a Vertical Fracture (EOS1) as described in the TOUGH2 User's Manual [Pruess, Oldenburg, and Moridis, 1999]. This problem models non-isothermal injection into and production from a single vertical fracture.

The geometry of the problem is given below. The fracture is bounded by semi-infinite half spaces of impermeable rock, which provide a conductive heat supply. Initial temperature is 300 C and initial average pressure is 10 MPa (100 bar). Water at 100 C is injected at a rate of 4 kg/s over the interval from -140 to -160 m on the left side and water is produced from -60 to -40 m on the right (origin of coordinate system on upper left corner of fracture). Only the fracture is meshed, a semi-analytical solution is used for the conduction in the confining layers.

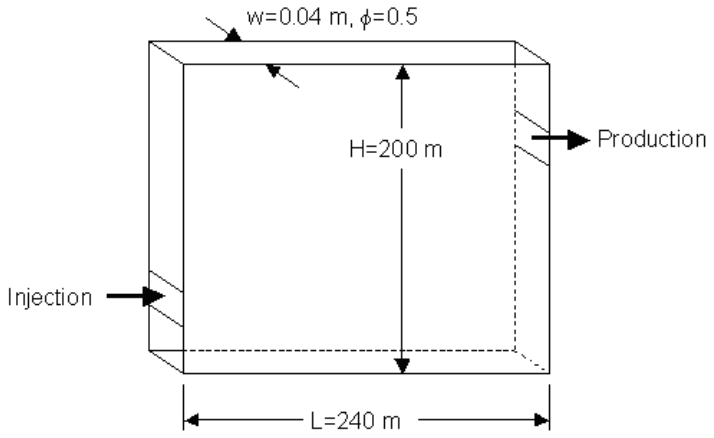

Figure 4.1. The injection-production system in the vertical fracture (after Pruess et al., 1999)

This analysis is run in two segments. The first segment is used to obtain an initial hydrostatic pressure profile. In the first segment, there is no heat transfer (isothermal). The initial conditions include a uniform temperature (300 C) and the average pressure for the fracture (10 MPa). Since there is no injection or production in this first segment, the solution will give a hydrostatic profile, with the largest pressure at the bottom of the fracture.

The second segment uses the hydrostatic profile as an initial condition. Injection and production is initiated in the model and the solution is continued for 1.57788E8 sec (1,826 days or 5 years). At the end of this time, there is significant cooling throughout the fracture, especially near the injection point.

Specify the Equation of State (EOS)

To ensure that PetraSim uses EOS1, edit your PetraSim preferences using the **Preferences** dialog.

1. On the **File** menu, click **Preferences...**
2. In the **Simulator Mode** list, select **TOUGH**.
3. In the **Default EOS** list, select **EOS1**.
4. Click **OK**.

Your preferences have now been updated, but you will need to create a new model or restart PetraSim before they become active. If you already have a model open, it will not be affected by the preference change.

On the **File** menu, click **New**.

Create the Model Boundary

To create the boundary for this model, use the **Define Model Boundary** dialog. The boundary parameters for this model are shown in Table 4.1.

Table 4.1. Model Boundary Dimensions

Axis	Min (m)	Max (m)
x	0.0	240.0
y	0.0	0.04
z	-200.0	0.0

To create the model boundary

1. On the **Model** menu, click **Define Boundary...** (or click on the toolbar).
2. Enter the values from Table 4.1.
3. Click **OK** to create the model boundary.
4. On the **View** menu, click **Front View** (or click on the toolbar).

Create the Grid

To create the grid

1. On the **Model** menu, click **Create Grid...** (or click on the toolbar).

2. In the **Division Method** box, select **Regular**.
3. In the **X Cells** box, type `12`.
4. In the **Y Cells** box, type `1`.
5. In the **Z Cells** box, type `10`.
6. Click **OK** to create the grid.

The solution grid is shown in Figure 4.2.

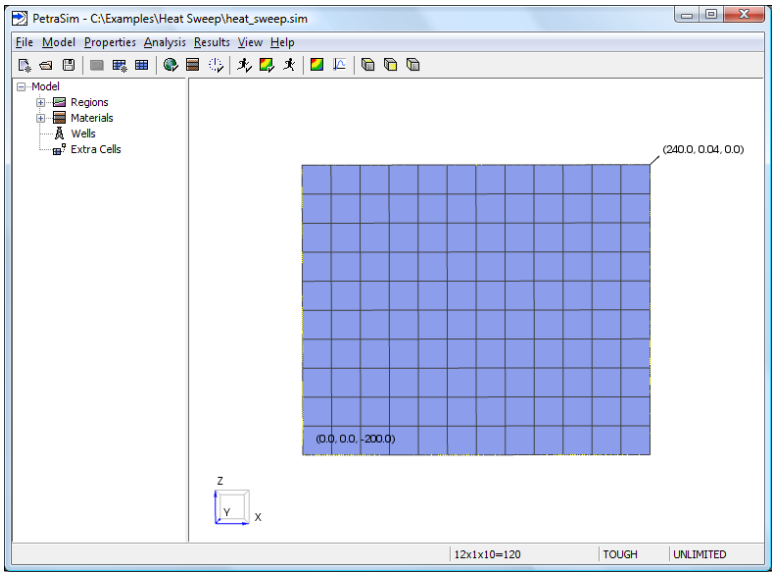

Figure 4.2. The solution grid

Global Properties

Global properties are those properties that apply to the entire model. In this example, we will only change the EOS mode. You can edit global properties with the **Global Properties** dialog.

On the **Properties** menu, click **Global Properties...** (or click on the toolbar).

1. In the **Global Properties** dialog, click the **EOS** tab.
2. Select **Single Phase, Isothermal**.
3. Click **OK** save your changes.

Material Properties

To specify the material properties, you can use the **Material Data** dialog. This example requires one material.

1. On the **Properties** menu, click **Materials** (or click on the toolbar).
2. In the **Name** box, type `FRACT`.
3. In the **Density** box, type `2650.0`.
4. In the **Porosity** box, type `0.5`.
5. In all three **Permeability** boxes (X, Y, and Z), type `200E-12`.
6. In the **Wet Heat Conductivity** box, type `0.0`.
7. In the **Specific Heat** box, type `1000.0`.
8. Click **OK** to save these changes.

Because this analysis is single phase liquid, we do not need to specify relative permeability or capillary pressure functions.

Initial Conditions

Correct specification of initial conditions is essential for proper convergence and obtaining a correct result. In general, the initial conditions need to physically meaningful. In this example, this requires an initial state analysis in which we will run a simulation to obtain initial equilibrium conditions before we run the heat sweep analysis.

To set the initial conditions for all cells

1. Select the **Single-Phase (P, T)** state option.
2. In the **Pressure** box, type `10.0E6`.
3. In the **Temperature** box, type `300.0`.
4. Click **OK**.

Solution Controls for Transient Analysis

For the transient analysis, we will specify the end time.

To open the **Solution Controls** dialog: on the **Analysis** menu, click **Solution Controls...** (or click on the toolbar).

To change the time step settings

1. In the **Solution Controls** dialog, click the **Times** tab.

2. In the **End Time** list, select `User Defined` and type `1.57788E8` in the box.

3. In the **Max Num Time Steps** box, type `500`.

Click **OK** to save your changes and exit the **Solution Controls** dialog.

Save and Run

The input is complete and you can run the simulation. The changes you have made will automatically be saved before execution.

To run the simulation, on the **Analysis** menu, click **Run TOUGH2** (or click on the toolbar).

View Transient Results

To view the 3D transient results

1. On the **Results** menu, click **3D Results** (or click on the toolbar). The data for the current simulation will be automatically loaded and displayed.

To show pressure contours for the last time step

1. In the **Time(s)** list, select the only entry (**1.3107E7**).

2. In the **Scalar** list, select **P (Pa)**.

3. Click to clear the **Show Isosurfaces** checkbox.

To view the fracture plane, on the **View** menu, click **Front View** (or click on the toolbar).

To add a slice plane on which contours will be displayed, click **Slice Planes...**. For this example we will show one slice plane. To configure the slice plane

1. In the **Axis** list, select **Y**.

2. In the **Coord** box, type `0.02`.

3. Select the **Scalar** check box.

4. Click **Close**.

The resulting contour plot is shown in Figure 4.3.

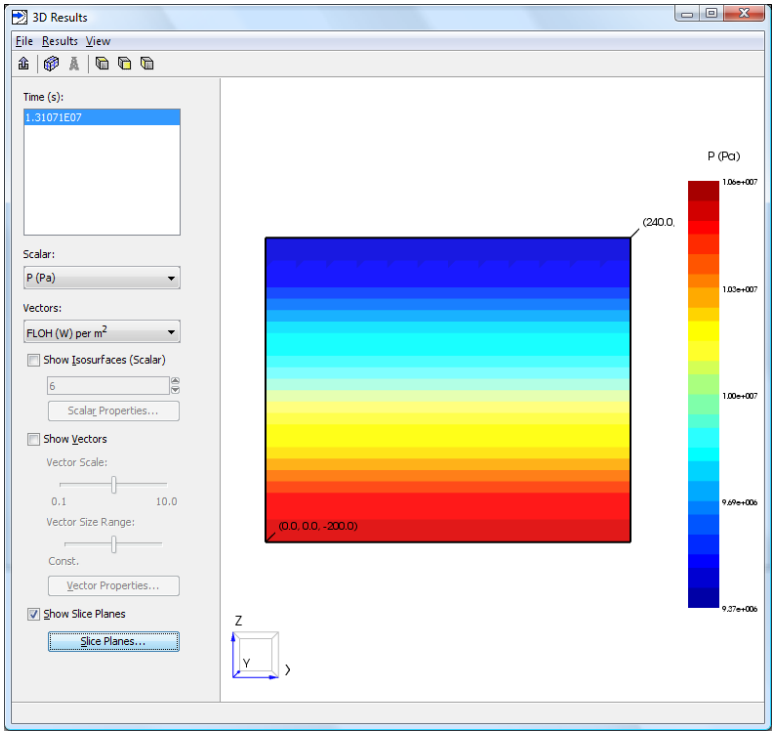

Figure 4.3. Pressure contours

Close the **3D Results** window.

Begin Transient Analysis

We are now ready to begin the second segement of the simulation. When running multi-part simulations it is best to save your PetraSim model to a different folder to prevent accidental overwriting of the data from earlier steps.

To save your model to a different folder

1. If the initial model is not already open, on the **File** menu, click **Open** (or click on the toolbar). In the **File Name** box, select the **heat_sweep.sim** file and click **Open**. This will open the existing model.

2. To save the transient model, on the **File** menu, click **Save As...**.

3. Create a new folder named **Transient** and in the **File Name** box, type **heat_sweep_transient.sim**.

4. Click **Save**.

Load Initial Conditions

We will now perform a transient analysis, using the previously calculated hydrostatic state results as initial conditions. We do this by reading the **SAVE** file that was output at the end of the hydrostatic analysis. This file has the results for all the cells in the model. To read these initial conditions

1. On the **File** menu, click **Load Initial Conditions...** .
2. Browse to the **Heat Sweep**folder and select the **SAVE** file.
3. Click **Open**. This reads the saved data from the previous run and stores it as an initial condition for each cell in the current analysis.

To view the initial conditions, open the **Grid Editor**

1. On the **Model** menu, click **Edit Grid** (or click on the toolbar).
2. In the **Grid Editor**, click on the **View** icon to select the **XZ View**.
3. In the **Property** list, select **Pressure**.
4. The display will show the pressures from the initial state analysis, Figure 4.4.

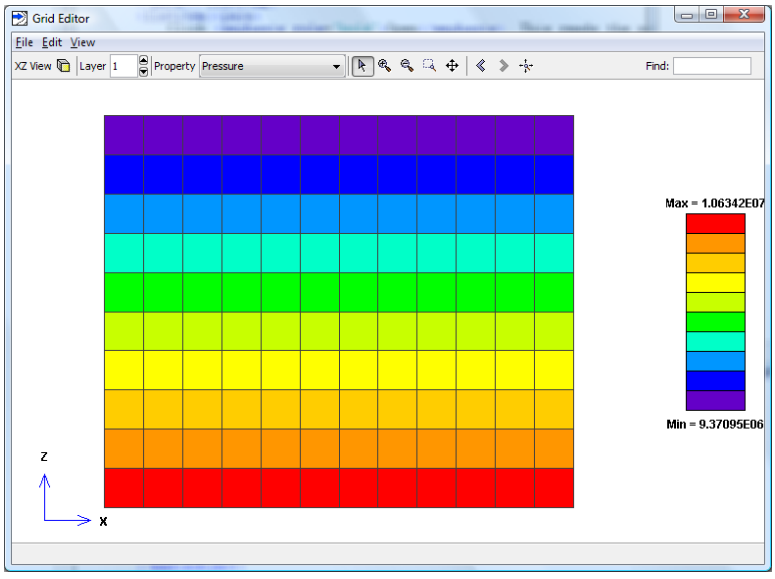

Figure 4.4. The grid editor with pressure as the display variable

Define Injection and Production

In the transient analysis, we will inject cold fluid and produce hot fluid from the fracture. We define the injection and production in the **Grid Editor**.

To define the injection

1. In the **Grid Editor**, click on the **View** icon to select the **XZ View**.
2. Right-click on the third cell up from the lower left corner and click **Edit Properties**. The **Cell ID** should be 25.
3. In the **Cell Name** box, enter `Injection`.
4. Click the **Sources/Sinks** tab.
5. In the **Injection** section, select the **Water/Steam** check box.
6. In the **Rate** box, type `4`.
7. In the **Enthalpy** box, type `4.2E5`.
8. Click the **Print Options** tab.
9. Select the **Print Cell Time Dependent Data** check box.
10. Click **OK** to close the **Edit Cell Data** dialog. You will see the name of the cell and an "S" to indicate a source and a "P" to indicate time history printing.

To define the production

1. Right-click on the third cell down from the upper right corner and click **Edit Properties**. The **Cell ID** should be 96.
2. In the **Cell Name** box, enter `Production`.
3. Click the **Sources/Sinks** tab.
4. In the **Production** section, select the **Well on Deliv.** check box.
5. In the **Productivity Index** box, type `4.0E-12`.
6. In the **Pressure** box, type `9.65E6`.
7. Click the **Print Options** tab.
8. Select the **Print Cell Time Dependent Data** check box.
9. Click **OK** to close the **Edit Cell Data** dialog. You will see the name of the cell and an "S" to indicate a source and a "P" to indicate time history printing.

Global Properties for Transient Analysis

The transient analysis is non-isothermal.

On the **Properties** menu, click **Global Properties...** (or click on the toolbar).

1. In the **Global Properties** dialog, click the **EOS** tab.
2. Select **Water, Non-Isothermal**.
3. Click **OK** save your changes.

Confining Bed Boundary Conditions for Transient Analysis

In the transient analysis, heat is conducted to the confining beds on either side of the fracture. To define this boundary condition, on the **Properties** menu, click **Boundary Conditions...**.

1. Select the **Enable Heat Exchange with Confining Beds** checkbox.
2. In the **Initial Temperature** box, type `300.0`.
3. In the **Specific Heat** box, type `1000`.
4. In the **Thermal Conductivity** box, type `2.1`.
5. In the **Density** box, type `2650.0`.
6. Click **OK** to save your changes.

Output Controls for Transient Analysis

By default, the simulation will print output every 100 time steps. We can increase the frequency of the output in the **Output Controls** dialog.

1. On the **Analysis** menu, click **Output Controls...** (or click on the toolbar).
2. In the **Print and Plot Every # Steps** box, type `10`.
3. Click **OK** to exit the **Output Controls** dialog.

Save and Run Transient Analysis

The input is complete and you can run the simulation. The model file will automatically be saved when you run the analysis.

To run the simulation, on the **Analysis** menu, click **Run TOUGH2** (or click on the toolbar).

View 3D Results for Transient Analysis

To view the 3D results, on the **Results** menu, click **3D Results** (or click on the toolbar). The data for the current simulation will be automatically loaded and displayed.

To show temperature contours for the last time step

1. In the **Time(s)** list, select the last entry (**1.578E8**).

2. In the **Scalar** list, select **T (deg C)**.

3. Click to clear the **Show Isosurfaces** checkbox. The contours will be displayed on a slice plane.

To show heat flow vectors

1. In the **Vectors** list, select **FLOH**.

2. Select the **Show Vectors** checkbox.

To add a slice plane on which contours will be displayed, click **Slice Planes...**. For this example we will show one slice plane. To configure the slice plane

1. In the **Axis** list, select **Y**.

2. In the **Coord** box, type `0.02`.

3. Select the **Scalar** check box.

4. Click **Close**.

The resulting contour and vector plot is shown in Figure 4.5. The cooling near the injection well and the flow of water from the injection well and to the production wells can be seen.

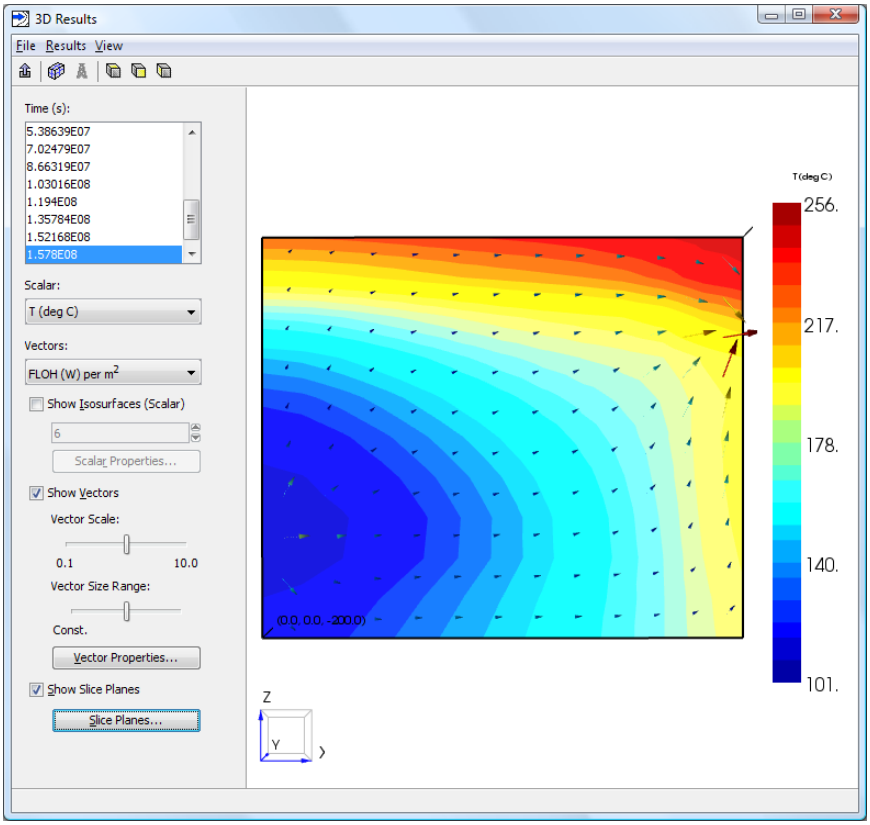

Figure 4.5. The final display

Close the **3D Results** window.

View Cell History Plots

You can view time history plots with the Cell History dialog. On the **Results** menu, click **Cell History Plots....** (or click on the toolbar).

The **Cell History** dialog will be displayed. In this window, you can display time history data using a plotting parameter and a list of cells. For example, to view the temperature in the **Production** cell

1. In the **Variable** list, select **T (deg C)**.

2. In the **Cell Name (Id#)** list, select **Production**.

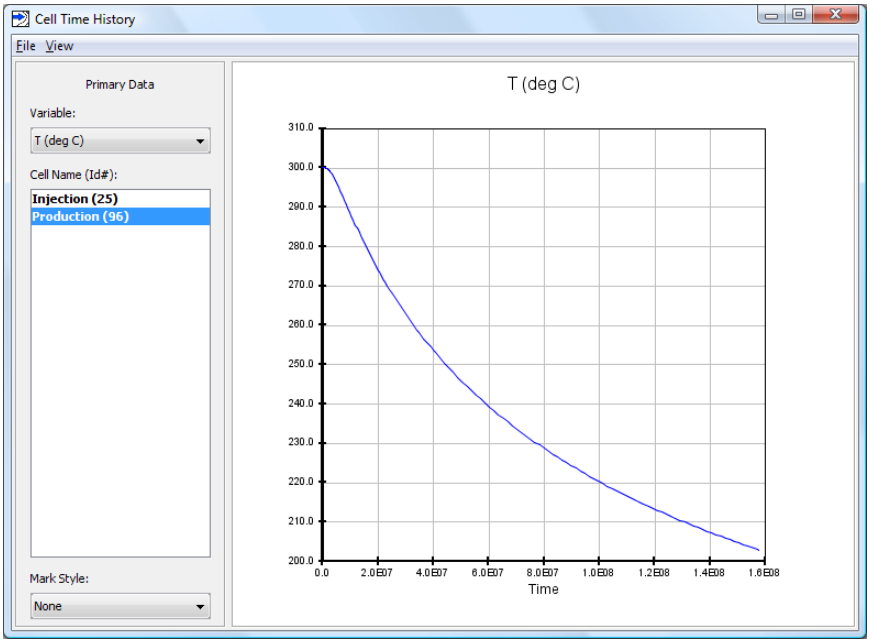

Figure 4.6. Time history plot at production cell

The user can also write this data to a file. On the **File** menu, click **Export Data.....** The data can then be imported in to another program for display. A plot of the same temperature data in Excel using a logarithmic X-axis is shown in Figure 4.7. This illustrates that the result is the same as reported in the TOUGH2 User's Manual.

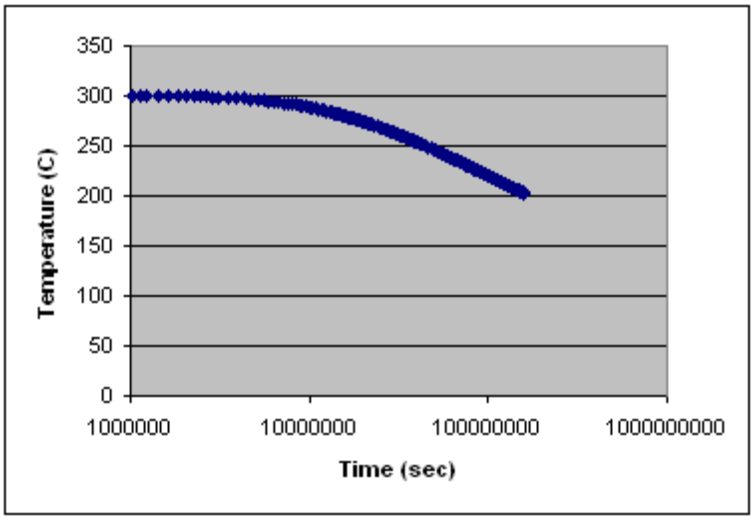

Figure 4.7. Excel graph of the temperature data

In the **File** menu, click **Close** to close the Cell History window.

Line Plots

PetraSim also supports line plots, where you define a line in 3D space and the data is interpolated along the line. To make a line plot

1. First open the 3D results view. On the **Results** menu, click **3D Results** (or click on the toolbar).

2. On the **File** menu, click **Line Plot....**

3. In the **Point 1** coordinate boxes (**X, Y, and Z**) type `240.0`, `0.02`, and `-200.0`, respectively.

4. In the **Point 2** coordinate boxes (**X, Y, and Z**) type `240.0`, `0.02`, and `0.0`, respectively.

5. Click **OK** to close the **Line Plot** dialog.

6. This will open a **Line Plot** window.

7. In the **Time** list, select **1.578E8** (the last time).

8. In the **Variable** list, select **T (Deg C)**.

The plot is shown in Figure 4.8. You can export this data to a comma separated value file for import into a spreadsheet.

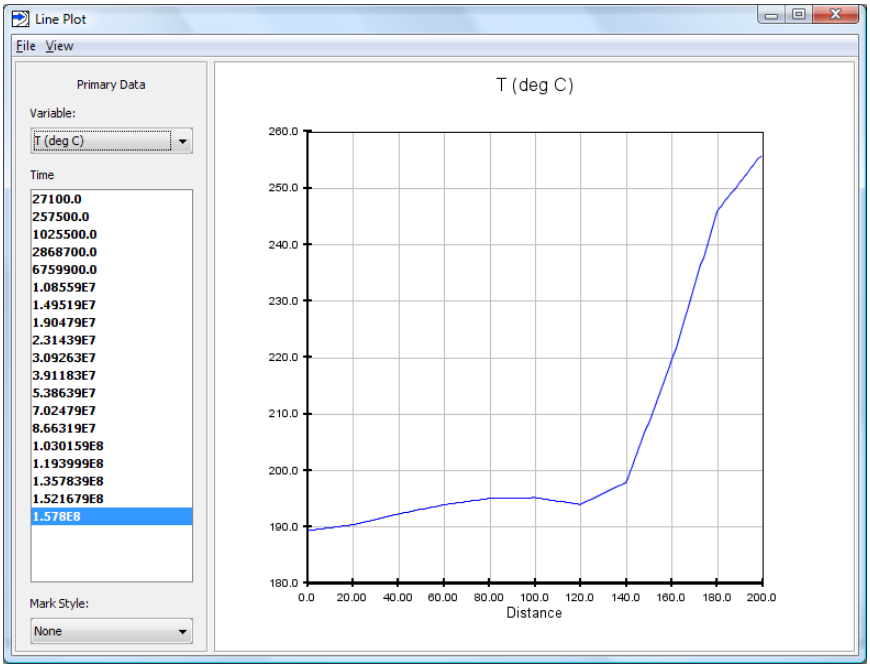

Figure 4.8. Time history plot at production cell

Close the **Line Plot** window.

Chapter 5. Heat Pipe in Cylindrical Geometry (EOS3)

Description

This example is Problem 2 - Heat Pipe in Cylindrical Geometry (EOS3, EOS4) described in the TOUGH2 User's Manual [Pruess, Oldenburg, and Moridis, 1999]. Heat pipes are systems in which an efficient heat transfer takes place by means of a liquid-vapor counterflow process, with vaporization and condensation occurring at the hot and cold ends. Heat pipe processes can occur in geothermal reservoirs and storage of heat-generating nuclear waste packages. This problem represents a simplified model of nuclear waste emplacement. A cylindrical heater with 0.3 m radius and 4.5 m height provides a constant heat input of 3 kW into a porous medium with uniform initial conditions of 18 C, 1 bar pressure (1E5 Pa), and 20% gas saturation.

The model uses a 1D radial grid of 200 elements extending to 10,000 m, so that boundary effects are not important. An alternate model, that gives essentially identical results, can be created using a radius of only 100 m, but with a fixed-state cell at the outer radius. This is because the solution only changes within a radius of about 50 m.

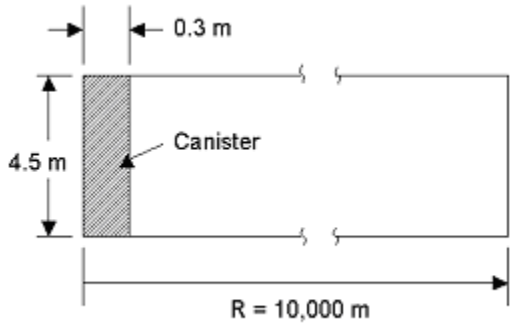

Figure 5.1. Heat Pipe in Cylindrical Geometry Model

EOS3 Specification

This example uses EOS3. The default EOS is EOS1. To change to EOS3

1. On the **File** menu, click **Preferences...** .
2. In the **Simulator Mode** list, select **TOUGH**.
3. In the **Default EOS** list, select **EOS3**.
4. Click **OK**.

Your preferences have now been updated, but you will need to create a new model or restart PetraSim before they become active. If you already have a model open, it will

not be affected by the preference change. On the **File** menu, click **New**.

Create the Model Boundary

To create the boundary, use the **Define Model Boundary** dialog. The boundary parameters for this model are shown in Table 5.1.

Table 5.1. Model boundary dimensions

Axis	Min (m)	Max (m)
x	0.0	10000.0
y	0.0	1.0
z	0.0	4.5

To create the model boundary

1. On the **Model** menu, click **Define Boundary...** (or click on the toolbar).
2. Enter the values from Table 5.1.
3. Click **OK** to create the model boundary.

Because this model has a very large radius, we will need to scale the dimension in the Z direction in order to manipulate the model. To do this

1. On the **View** menu, click **Scale Axis...**.
2. In the **Z Factor** box, type `1000`.
3. Click **OK** to close the **Scale Axis** dialog.

You can rotate, pan, and zoom the model using the mouse and **Shift** and **Alt** keys.

Create the Grid

To create the solution grid

1. On the **Model** menu, click **Create Grid...** (or click on the toolbar).
2. In the **Division Method** box, select **Regular**.
3. Click **Cells Above Top and Below Bottom are Inactive**.
4. Click **RZ Grid**. This creates a 2D cylindrical grid. It will be displayed as a plane,

but when the solution data is written, the volume and connections for the cells will be calculated in cylindrical coordinates.

5. In the **X Cells** box, type `200`.

6. In the **X Factor** box, type `1.0361057`. This value was calculated to give a cell size of 0.3 m for the first cell. See the PetraSim User Manual for instructions on how to do this calculation.

7. In the **Z Cells** box, type `1`.

8. In the **Z Factor** box, type `1.0`.

9. Click **OK** to create the grid.

The resulting mesh is displayed in Figure 5.2. Click on the model and spin it so that it is displayed as shown below.

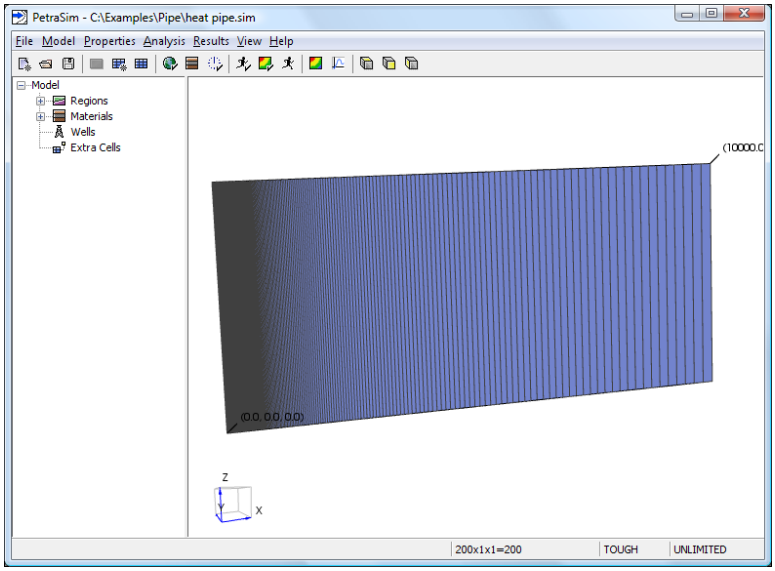

Figure 5.2. The resulting mesh

Global Properties

Global properties are those properties that apply to the entire model. We will make changes to some of the EOS options, including activating molecular diffusion. To edit global properties, you use the **Global Properties** dialog.

On the **Properties** menu, click **Global Properties...** (or click on the toolbar).

1. In the **Global Properties** dialog, select the **EOS** tab.

2. Select **Non-Isothermal**.
3. Select the **Molecular Diffusion** checkbox.
4. Click **Edit COEFs...**.
5. On the **Edit Coefficients** dialog, enter the values given in Table 5.2.
6. Click **OK** to close the **Edit Coefficients** dialog.
7. To be consistent with the TOUGH2 manual description, select **Tough Style** for the **Initialization** options.
8. Click **OK** to close the **Tough Global Data** dialog.

Table 5.2. Diffusion coefficients

	Gas	Liquid
Water	2.13E-5	0.0
Air	2.13E-5	0.0

Material Properties

To specify the material properties, you use the **Material Data** dialog. This example requires one material.

1. On the **Properties** menu, click **Materials** (or click on the toolbar).
2. In the **Name** box, type **POMED**.
3. In the **Density** box, type `2550.0`.
4. In the **Porosity** box, type `0.01`.
5. In all three **Permeability** boxes (X, Y, and Z), type `20.e-15`.
6. In the **Wet Heat Conductivity** box, type `2.0`.
7. In the **Specific Heat** box, type `800.0`.
8. Click **Apply** to save the changes.

In addition to the physical rock parameters, we also need to specify the relative permeability and capillary pressure functions for this material. These options can be found in the **Additional Material Data** dialog. To open this dialog, click the **Relative**

Perm... button.

To specify the relative permeability function

1. Select the **Relative Perm** tab.
2. In the **Relative Permeability** list, select **van Genuchten-Mualem Model**.
3. In the **Lambda** box, type `0.45`.
4. In the **Slr** box, type `9.6E-4`.
5. In the **Sls** box, type `1.0`.
6. In the **Sgr** box, type `0.0`.

To specify the capillary pressure function

1. Select the **Capillary Press** tab.
2. In the **Capillary Pressure** list, select **van Genuchten Function**.
3. In the **Lambda** box, type `0.45`.
4. In the **Slr** box, type `1.0E-3`.
5. In the **1/P0** box, type `8.0E-5`.
6. In the **Pmax** box, type `5.0E8`.
7. In the **Sls** box, type `1.0`.

To specify the tortuosity

1. Select the **Misc** tab.
2. In the **Tortuosity Factor** box, type `0.25`.

Click **OK** to exit the **Advanced Material Data** dialog.

Click **OK** again to save your settings and exit the **Material Data** dialog.

Initial Conditions

The initial state of each cell in the model must be defined. To specify global initial conditions that will be used as the default for all cells in the model, on the **Properties** menu, click **Initial Conditions...** (or click on the toolbar).

To set the initial conditions

1. Select the **Single-Phase (P, X, T)** state option.
2. In the **Pressure** box, type `1.0E5`.
3. In the **Temperature** box, type `18.0`.
4. In the **Air Mass Fraction** box, type `0.2`.
5. Click **OK**.

Define Heat Source

This model has a heat source at the center. This is defined in the **Grid Editor**.

To open the **Grid Editor**, on the **Model** menu, click **Edit Grid** (or click on the toolbar).

1. In the **Grid Editor**, click on the **View** icon to select the **XZ View**.
2. On the **View** menu, click **Scale Axis...**.
3. In the **Z Factor** box, type `1000`.
4. Using the **Zoom Box** tool, zoom in to the top left of the model until you can see the first cell.
5. Using the **Selection** tool, right-click on the first cell and click **Edit Properties...**, Figure 5.3.
6. In the **Cell Name** box, type `Heat Source`.
7. Click the **Sources/Sinks** tab.
8. In the **Heat** section, select the **Heat In** check box.
9. In the **Rate** box, type `3000`.
10. Click the **Print Options** tab.
11. Select the **Print Cell Time Dependent Data** check box.
12. Click **OK** to close the **Edit Cell Data** dialog.

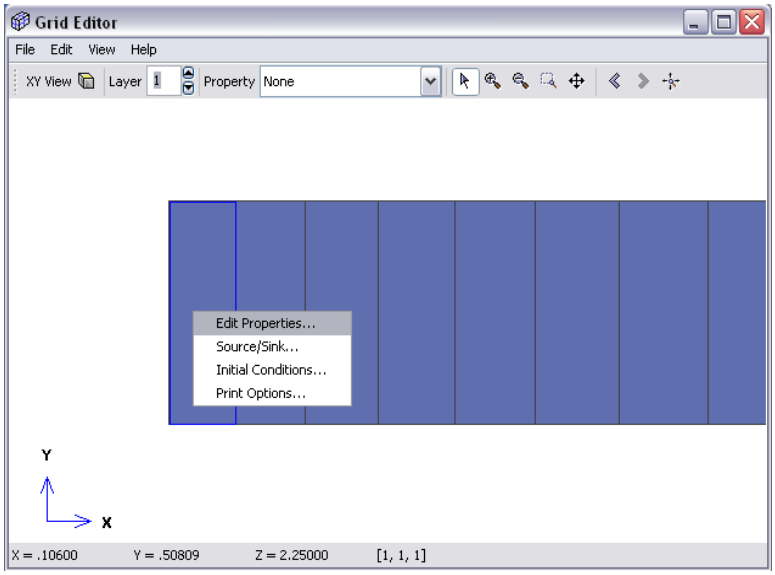

Figure 5.3. Select the left cell in the model

Close the **Grid Editor**.

Solution Controls

We will now define the solution control options.

1. On the **Analysis** menu, click **Solution Controls...** (or click on the toolbar).
2. In the **End Time** box, type `3.155E8`.
3. In the **Time Step** list, ensure that `Single Value` is selected.
4. In the **Time Step** box, type `100`. This is the initial time step.
5. In the **Max Num Time Steps** box, type `1000`.
6. Select **Enable Automatic Time Step Adjustment**.
7. Click **OK** to exit the **Solution Controls** dialog..

Output Controls

By default, the simulation will print output every 100 time steps. We can increase the frequency of the output in the **Output Controls** dialog.

1. On the **Analysis** menu, click **Output Controls...** (or click on the toolbar).
2. In the **Print and Plot Every # Steps** box, type `50`.

3. Click **OK** to exit the **Output Controls** dialog.

Save and Run

The input is complete and you can run the simulation. If you haven't already, you may want to save your model in a new directory. For example

1. On the **File** menu, click **Save** (or click on the toolbar).
2. Create a new folder named **Heat Pipe** and in the **File Name** box, type **heat_pipe.sim**.
3. Click **Save**.

To run the simulation, on the **Analysis** menu, click **Run TOUGH2** (or click on the toolbar).

During the solution, a graph will display the time step size. In this case, the time steps become very large near the end of the solution, which indicates that a steady state has been reached.

View 3D Results

To view the 3D results for a simulation, on the **Results** menu, click **3D Results** (or click on the toolbar). The data for the current simulation will be automatically loaded and displayed.

Since the model has a large radius relative to its height, we scale the Z coordinates.

1. On the **View** menu, click **Scale Axes...**.
2. In the **Z Factor** box, type `1000`.

To show temperature contours for the last time step

1. In the **Time(s)** list, select the last entry (**3.155E8**).
2. In the **Scalar** list, select **T**.
3. Click to clear the **Show Isosurfaces** checkbox.

To add a slice plane on which contours will be displayed, click **Slice Planes...**. For this example we will show one slice plane. To configure the slice plane

1. In the **Axis** list, select **Y**.
2. In the **Coord** box, type `0.5`.
3. Select the **Scalar** check box.

4. Click **Close**.

To turn on the mesh to help with distance orientation

1. On the **View** menu, click **Show Grid** .

After zooming in on the upper left corner of the model, the resulting contour plot is shown in Figure 5.4.

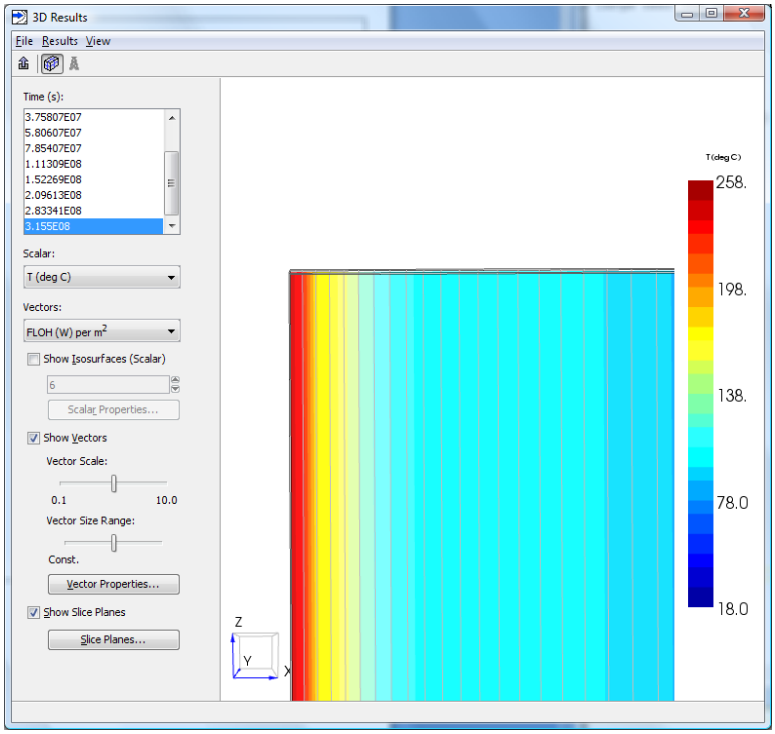

Figure 5.4. The resulting display

Close the **3D Results** window.

Time History Plots

You can view time history plots with the Cell History dialog. On the **Results** menu, click **Cell History Plots....** (or click on the toolbar).

The **Cell History** dialog will be displayed. In this window, you can display time history data using a plotting parameter and a list of cells. For example, to view the temperature in the Heat Source cell

1. In the **Variable** list, select **T**.

2. In the **Cell Name (Id#)** list, select **Heat Source**.

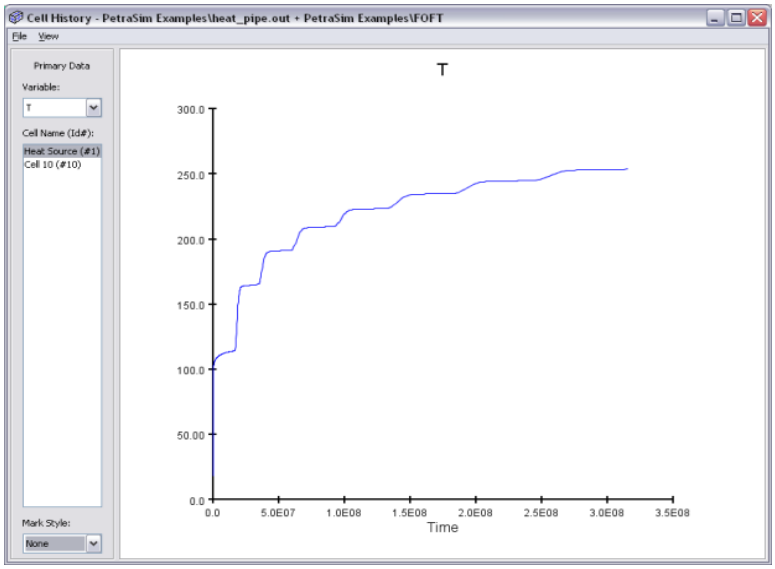

Figure 5.5. Cell history plot of temperature for cell #1

In the **File** menu, click **Close** to close the Cell History window.

Line Plots

PetraSim also supports line plots, where you define a line in 3D space and the data is interpolated along the line. To make a line plot

1. First open the 3D results view. On the **Results** menu, click **3D Results** (or click on the toolbar).

2. On the **File** menu, click **Line Plot....**

3. In the **Point 1** coordinate boxes (**X, Y, and Z**) type `0.0`, `0.5`, and `0.5`, respectively.

4. In the **Point 2** coordinate boxes (**X, Y, and Z**) type `100.0`, `0.5`, and `0.5`, respectively.

5. Click **OK** to close the **Line Plot** dialog.

6. This will open a **Line Plot** window.

7. In the **Variable** list, select **T (deg C)**.

8. In the **Time** list, select **3.155E8** (the last time).

The plot is shown in Figure 5.6. You can export this data to a comma separated value file for import into a spreadsheet.

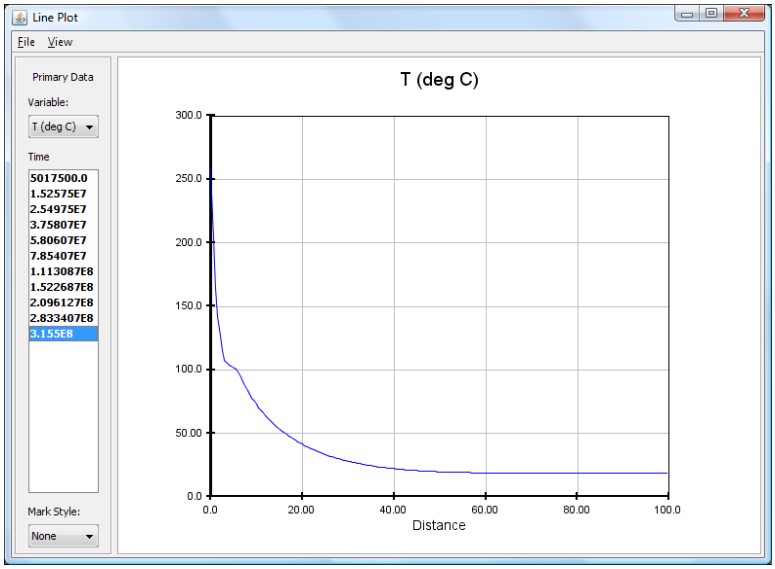

Figure 5.6. Line plot of temperature

Close the **Line Plot** window.

Figure 5.7. and Figure 5.8. display the results in a format that can be compared to the plot in the TOUGH2 User's Manual. These were made in Excel by exporting line plot data. Based on these displays, the present results are the same as given in the manual.

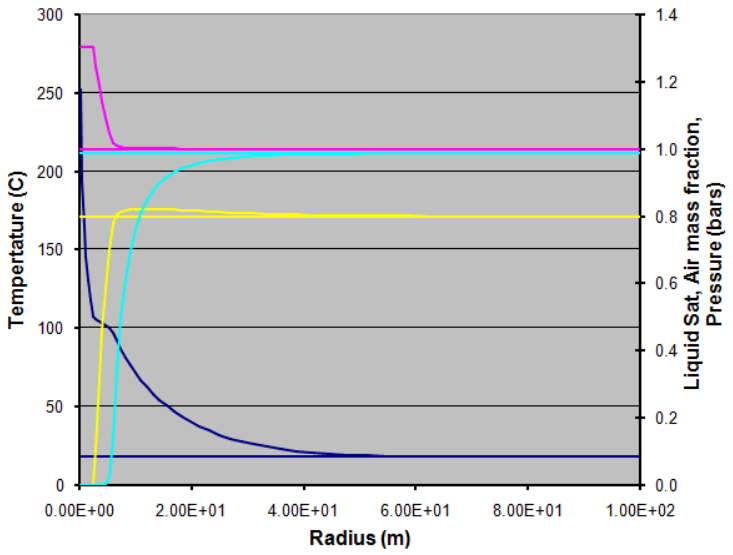

Figure 5.7. Results at the end time as a function of radius

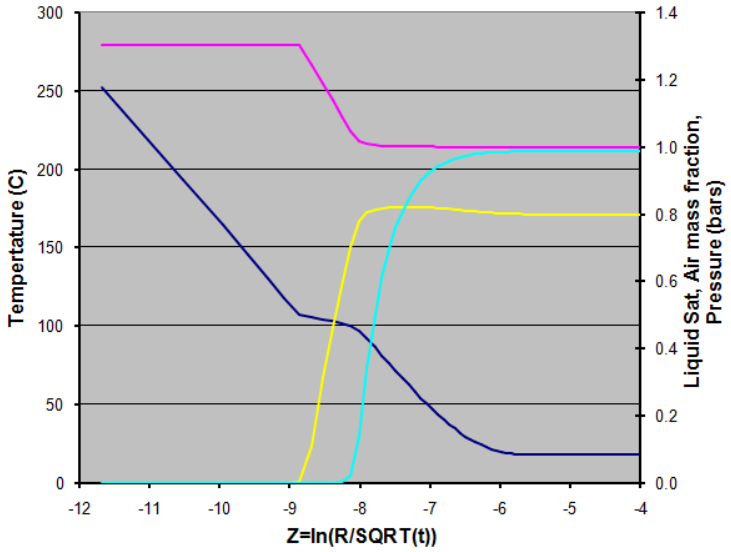

Figure 5.8. Results at the end time as a function of solution variable Z

Chapter 6. Production from a Geothermal Reservoir (EWASG)

Description

This example is Problem 12 - Production from a Geothermal Reservoir with Hypersaline Brine and CO2 (EWASG) described in the TOUGH2 User's Manual [Pruess, Oldenburg, and Moridis, 1999]. This problem examines production from a hypothetical geothermal reservoir with high salinity and CO2. Fluid withdrawal causes pressure to drop near the production well. Boiling of reservoir fluid gives rise to dilution of CO2 in the gas phase and to increased concentrations of dissolved NaCl, which begins to precipitate when the aqueous solubility limit is reached. As the boiling front receded from the well, solid precipitate fills approximately 10% of the original void space, causing permeability to decline to approximately 28% of its original value.

The mesh uses a 1D radial geometry.

EWASG Specification

This example uses EWASG. The default EOS is EOS1. To change to EWASG

1. On the **File** menu, click **Preferences...** .
2. In the **Simulator Mode** list, select **TOUGH**.
3. In the **Default EOS** list, select **EWASG**.
4. Click **OK**.

Your preferences have now been updated, but you will need to create a new model or restart PetraSim before they become active. If you already have a model open, it will not be affected by the preference change. On the **File** menu, click **New**.

Create the Model Boundary

To create the boundary for this model, use the **Define Model Boundary** dialog. The boundary parameters for this model are shown in Table 6.1.

Table 6.1. Model boundary dimensions

Axis	Min (m)	Max (m)
X	5.0	1000.0
Y	0.0	1.0
Z	-500.0	0.0

To create the model boundary

1. On the **Model** menu, click **Define Boundary...** (or click on the toolbar).
2. Enter the values from Table 6.1.
3. Click **OK** to create the model boundary.

You can rotate, pan, and zoom the model using the mouse and **Shift** and **Alt** keys.

Create the Grid

To create the solution grid

1. On the **Model** menu, click **Create Grid...** (or click on the toolbar).
2. In the **Division Method** box, select **Regular**.
3. Click **Cells Above Top and Below Bottom are Inactive**.
4. Click **RZ Grid**. This creates a grid a 2D cylindrical grid. It will be displayed as a plane, but when the solution data is written, the volume and connections for the cells will be calculated in cylindrical coordinates.
5. In the **X Cells** box, type `100`.
6. In the **X Factor** box, type `1.03705`.
7. In the **Z Cells** box, type `1`.
8. In the **Z Factor** box, type `1.0`.
9. Click **OK** to create the grid.

We have selected RZ Grid as the grid type. This means that a 2D cylindrical RZ grid will be created in which X corresponds to cylindrical R, Z corresponds to cylindrical Z, and the Y coordinate corresponds to cylindrical Theta (which is not used). 100 cells extend in the R direction, with an X Factor of 1.03705. This means that each cell is 1.03705 times the size of the previous cell in the R direction. These were chosen to give a first cell length of 2.0 m, which is the value used in the TOUGH2 example. See the PetraSim User Manual for instructions on how to calculate the appropriate factor.

The resulting mesh is displayed in Figure 6.1. Click on the model and spin it so that it is displayed as shown below.

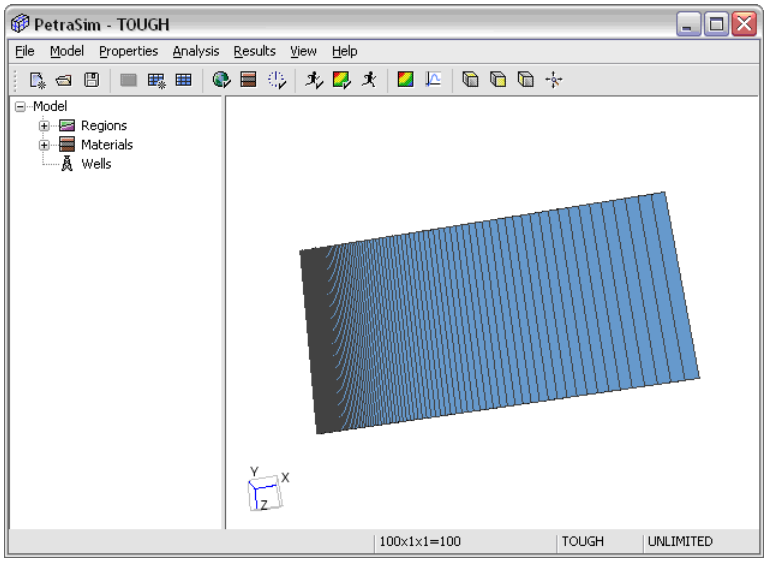

Figure 6.1. The resulting model

Global Properties

Global properties are those properties that apply to the entire model. We will make changes to some of the EOS options, including activating molecular diffusion. To edit global properties, you use the **Global Properties** dialog.

On the **Properties** menu, click **Global Properties...** (or click on the toolbar).

1. In the **Global Properties** dialog, select the **Analysis** tab.
2. In the **Name** box, type `Geothermal Production, Brine and CO2`.
1. In the **Global Properties** dialog, select the **EOS** tab.
2. Select **Non-Isothermal**.
3. In the **Type of NCG** list, select **CO2**.
4. Click **Tubes in Series**.
5. In the **phi** box, type `0.8`.
6. In the **G** box, type `0.8`.
7. In the **Property Dependence on Salinity** list, select **Full Dependence**.
8. In the **Brine Enthalpy Correcton** list, select **Michaelides**.
9. Select the **Include Vapor Pressure Lowering** checkbox.

10. Do NOT select **Molecular Diffusion**.

11. Click **OK** to close the **Global Properties** dialog.

Material Properties

To specify the material properties, use the **Material Data** dialog.

1. On the **Properties** menu, click **Materials** (or click on the toolbar).

2. In the **Name** box, type **POMED**.

3. In the **Density** box, type `2600.0`.

4. In the **Porosity** box, type `0.05`.

5. In all three **Permeability** boxes (X, Y, and Z), type `50e-15`.

6. In the **Wet Heat Conductivity** box, type `2.0`.

7. In the **Specific Heat** box, type `1000.0`.

8. Click **Apply** to save the changes.

In addition to the physical rock parameters, we also need to specify the relative permeability and capillary pressure functions for this material. These options can be found in the **Additional Material Data** dialog. To open this dialog, click the **Relative Perm...** button.

To specify the relative permeability function

1. Select the **Relative Perm** tab.

2. In the **Relative Permeability** list, select **Corey's Curves**.

3. In the **Slr** box, type `0.3`.

4. In the **Sgr** box, type `0.05`.

The default capillary pressure (none) is correct for this example.

Click **OK** to exit the **Advanced Material Data** dialog.

Click **OK** again to save your settings and exit the **Material Data** dialog.

Initial Conditions

The initial state of each cell in the model must be defined. To specify global initial conditions that will be used as the default for all cells in the model, on the **Properties**

menu, click **Initial Conditions...** (or click on the toolbar).

To set the initial conditions

1. Select the **Two Fluid Phases (P, Xsm, Sg, T)** state option.
2. In the **Pressure** box, type `6.0E6`.
3. In the **Temperature** box, type `275.55`.
4. In the **Gas Saturation** box, type `0.45`.
5. In the **Salt Mass Fraction** box, type `0.3`.
6. Click **OK** to close the **Default Initial Conditions** dialog.

Define Heat Source

In this model, fluid is produced from the inner cell. This is defined in the **Grid Editor**.

To open the **Grid Editor**, on the **Model** menu, click **Edit Grid** (or click on the toolbar).

1. In the **Grid Editor**, click on the **View** icon to select the **XZ View**.
2. Using the **Zoom Box** tool, zoom in to the top left of the model until you can see the first cell.
3. Using the **Selection** tool, right-click on the first cell and click **Edit Properties...**, Figure 6.2.
4. In the **Cell Name** box, type `Production`.
5. Click the **Sources/Sinks** tab.
6. In the **Production** section, select the **Mass Out** check box.
7. In the **Rate** box, type `65`.
8. Click the **Print Options** tab.
9. Select the **Print Cell Time Dependent Data** check box.
10. Click **OK** to close the **Edit Cell Data** dialog.

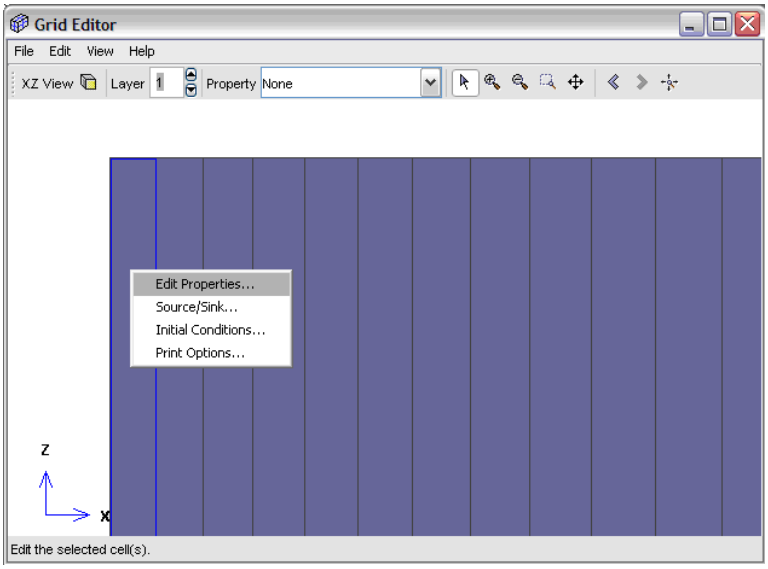

Figure 6.2. The cell to be selected

Close the **Grid Editor**.

Solution Controls

We will now define the solution control options.

1. On the **Analysis** menu, click **Solution Controls...** (or click on the toolbar).
2. In the **End Time** box, type `2.0E6` sec (approximately 23 days).
3. In the **Time Step** list, ensure that `Single Value` is selected.
4. In the **Time Step** box, type `1000`. This is the initial time step.
5. Select **Enable Automatic Time Step Adjustment**.
6. Click **OK** to exit the **Solution Controls** dialog..

Output Controls

By default, the simulation will print output every 100 time steps. We can increase the frequency of the output in the **Output Controls** dialog.

1. On the **Analysis** menu, click **Output Controls...** (or click on the toolbar).
2. In the **Print and Plot Every # Steps** box, type `10`.
3. Click **Edit**.

4. In the **Addtional Print Times** table, type `.50E5`. This will force a solution printout at this time.

5. Click **OK** to exit the **Additional Print Times** dialog.

6. Click **OK** to exit the **Output Controls** dialog.

Save and Run

The input is complete and you can run the simulation. If you haven't already, you may want to save your model in a new directory. For example

1. On the **File** menu, click **Save** (or click on the toolbar).

2. Create a new folder named **Geothermal** and in the **File Name** box, type **geothermal.sim**.

3. Click **Save**.

To run the simulation, on the **Analysis** menu, click **Run TOUGH2** (or click on the toolbar).

During the solution, a graph will display the time step size.

View 3D Results

To view the 3D results for a simulation, on the **Results** menu, click **3D Results** (or click on the toolbar). The data for the current simulation will be automatically loaded and displayed.

To show gas saturation contours for the last time step

1. In the **Time(s)** list, select the last entry (**2.0E6**).

2. In the **Scalar** list, select **SG**.

3. Click to clear the **Show Isosurfaces** checkbox.

To add a slice plane on which contours will be displayed, click **Slice Planes...**. For this example we will show one slice plane. To configure the slice plane

1. In the **Axis** list, select **Y**.

2. In the **Coord** box, type `0.5`.

3. Select the **Scalar** check box.

4. Click **Close**.

To turn on the mesh to help with distance orientation

1. On the **View** menu, click **Show Grid** .

After zooming in on the upper left corner of the model, the resulting contour plot is shown in Figure 6.3.

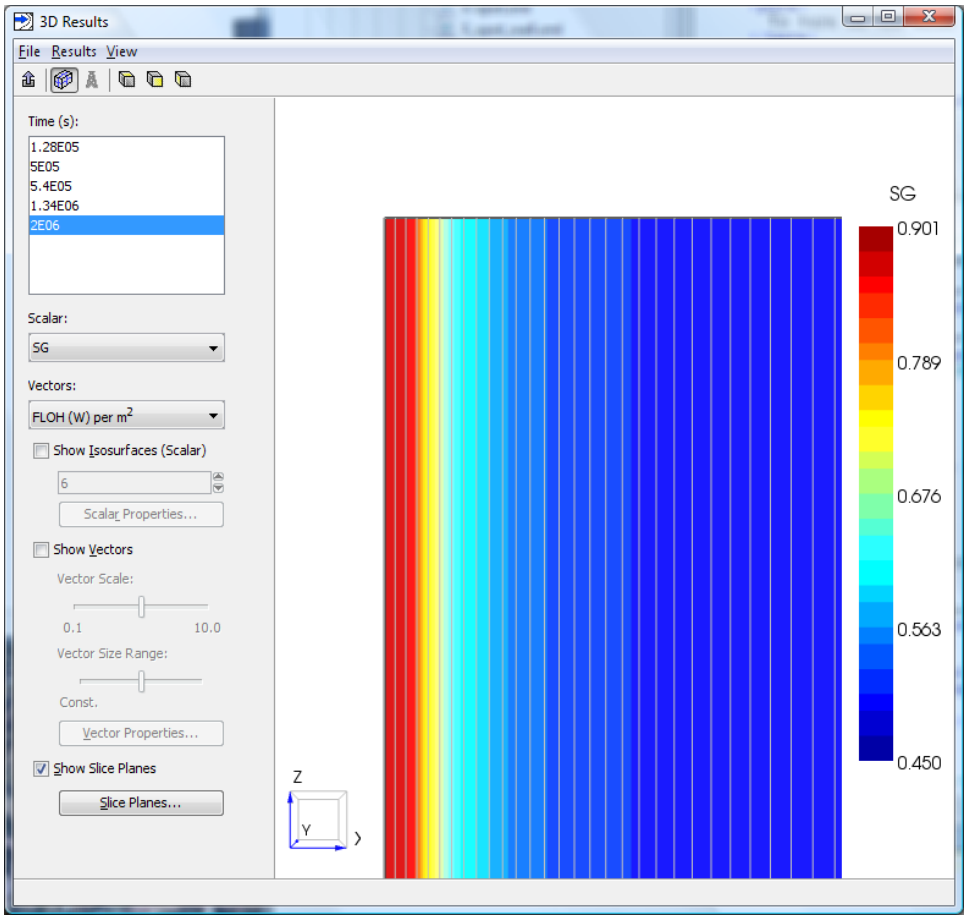

Figure 6.3. 3D representation of the saturation of gas

Close the **3D Results** window.

View Cell History Plots

You can view time history plots with the Cell History dialog. On the **Results** menu, click **Cell History Plots....** (or click on the toolbar).

The **Cell History** dialog will be displayed. In this window, you can display time history data using a plotting parameter and a list of cells. For example, to view the gas saturation in the Heat Source cell

1. In the **Variable** list, select **SG**.

2. In the **Cell Name** list, select **Production**.

Figure 6.4 shows the time history plot of SG at the production cell. The user can export this data for plotting in spreadsheets.

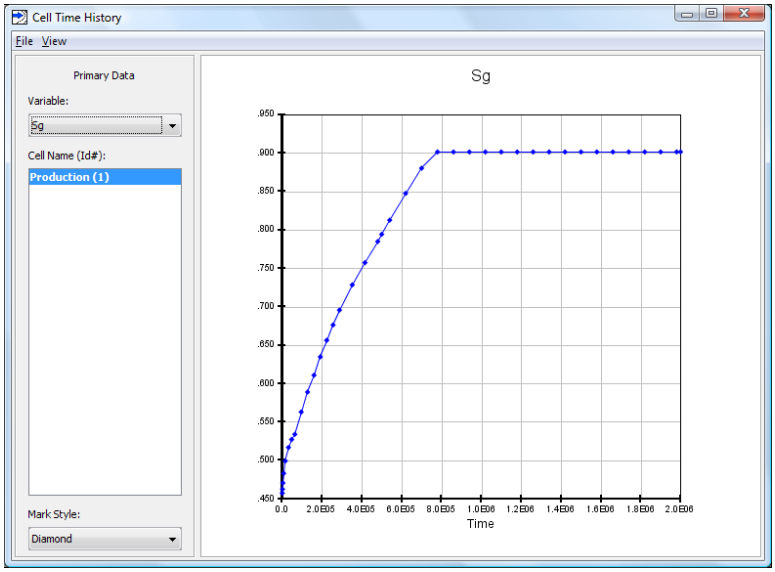

Figure 6.4. The cell history plot for gas saturation in the production cell

Close the **Cell History** window.

Line Plots

PetraSim also supports line plots, where you define a line in 3D space and the data is interpolated along the line. To make a line plot

1. First open the 3D results view. On the **Results** menu, click **3D Results** (or click on the toolbar).

2. On the **File** menu, click **Line Plot....**

3. In the **Point 1** coordinate boxes (**X, Y, and Z**) type `5.0`, `0.5`, and `-250.0`, respectively.

4. In the **Point 2** coordinate boxes (**X, Y, and Z**) type `1000.0`, `0.5`, and `-250.0`, respectively.

5. Click **OK** to close the **Line Plot** dialog.

6. This will open a **Line Plot** window.

7. In the **Variable** list, select **P (Pa)**.

8. In the **Time** list, select **2000000.** (the last time).

The plot is shown in Figure 6.5. You can export this data to a comma separated value file for import into a spreadsheet.

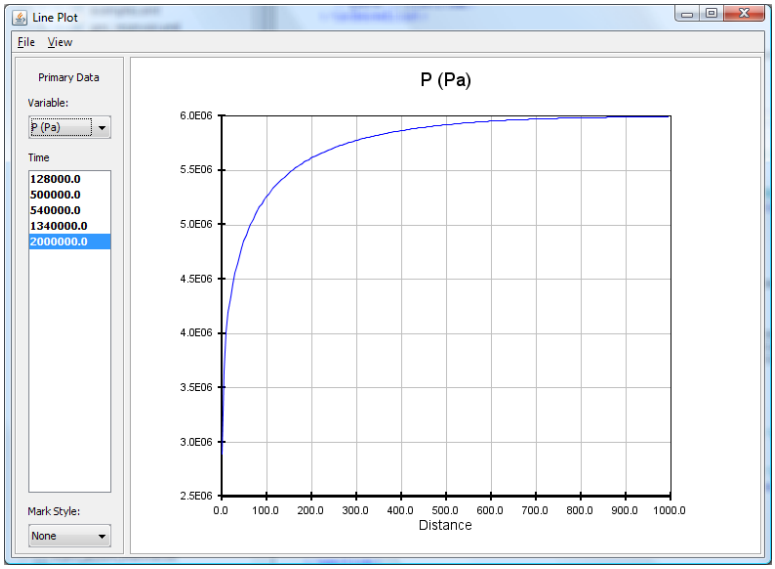

Figure 6.5. Line plot of pressure

Close the **Line Plot** window.

Data saved using the line plot are shown in the same format as in the TOUGH2 user's manual in Figure 6.6. The calculated results compare well with the manual results.

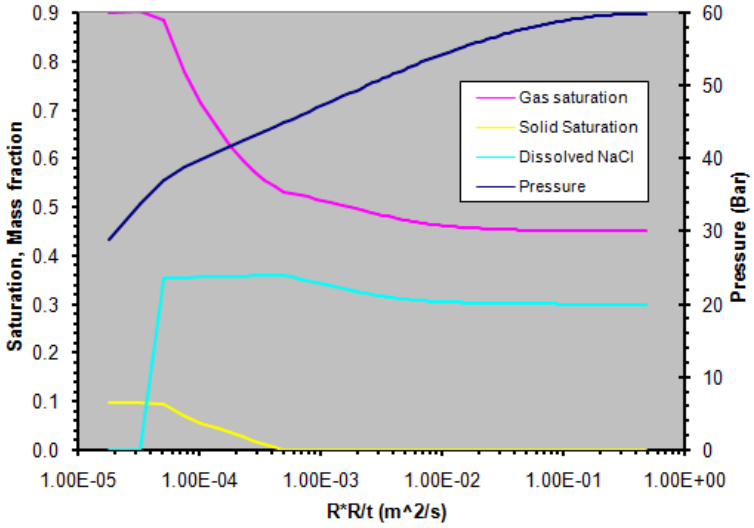
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
Saturation, Mass fraction
60
50
40
30
20
10
0
Pressure (Bar)
Gas saturation
Solid Saturation
Dissolved NaCl
Pressure
1.00E-05
1.00E-04
1.00E-03
1.00E-02
1.00E-01
1.00E+00
R*R/t (m^2/s)

Figure 6.6.

Chapter 7. VOC Contamination (TOUGH2 Problem 8)

Problem Description

This example uses EOS7R to simulate the diffusive and advective spreading of volatile organic contaminants (VOCs) in the vados zone, and their migration across the capillary fringe region into an underlying aquifer. Figure 7.1 shows a schematic of the system. The problem is run in two parts: first a solution is made to define the initial gravity/capillary equilibrium, then a transient solution is run with VOC diffusion.

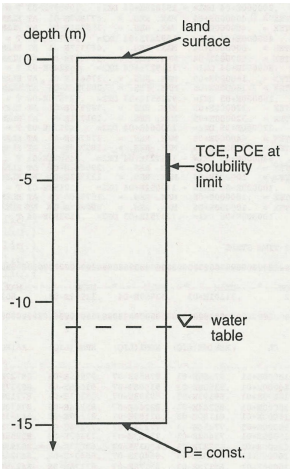

Figure 7.1. Model system for examining migration of VOC from the vados zone into an aquifer

This problem also demonstrates the use of "extra cells" to define cells that are created by editing a table and are not created as part of the geometric mesh.

This analysis uses the radionuclides in EOS7R to represent the two VOCs. The radionuclides are considered water-soluble as well as volatile, but are not allowed to form a separate non-aqueous phase. Volatile and water soluble organic chemicals are modeled by setting the half life to very large values.

Specify the Equation of State (EOS)

To ensure that PetraSim uses EOS7R, edit your PetraSim preferences using the **Preferences** dialog.

1. On the **File** menu, click **Preferences...** .
2. In the **Simulator Mode** list, select **TOUGH**.
3. In the **Default EOS** list, select **EOS7R**.
4. Click **OK**.

Your preferences have now been updated, but you will need to create a new model or restart PetraSim before they become active. If you already have a model open, it will not be affected by the preference change. On the **File** menu, click **New**.

Create the Model Boundary

To create the boundary, use the **Define Model Boundary** dialog. The boundary parameters for this model are shown in Table 3.1.

Table 7.1. Model boundary dimensions

Axis	Min (m)	Max (m)
x	0.0	1.0
y	0.0	1.0
z	-15.0	0.0

To create the model boundary, which extends 15.0 m below the surface

1. On the **Model** menu, click **Define Boundary...** (or click on the toolbar).
2. Enter the values from Table 7.1.
3. Click **OK** to create the model boundary.

You can rotate, pan, and zoom the model using the mouse and **Shift** and **Alt** keys.

Create the Grid

To create the solution grid

1. On the **Model** menu, click **Create Grid...** (or click on the toolbar).
2. In the **Division Method** box, select **Regular**.
3. Click **Cells Above Top and Below Bottom are Inactive**.
4. Click **XYZ Grid**.
5. In the **X Cells** box, type `1`.
6. In the **Y Cells** box, type `1`.
7. In the **Z Cells** box, type `15`.

8. Click **OK** to create the grid.

The resulting mesh is displayed in Figure 7.2. Click on the model and spin it so that it is displayed as shown below. Hold the **Shift** key and drag to pan; hold the **Alt** key and drag to zoom.

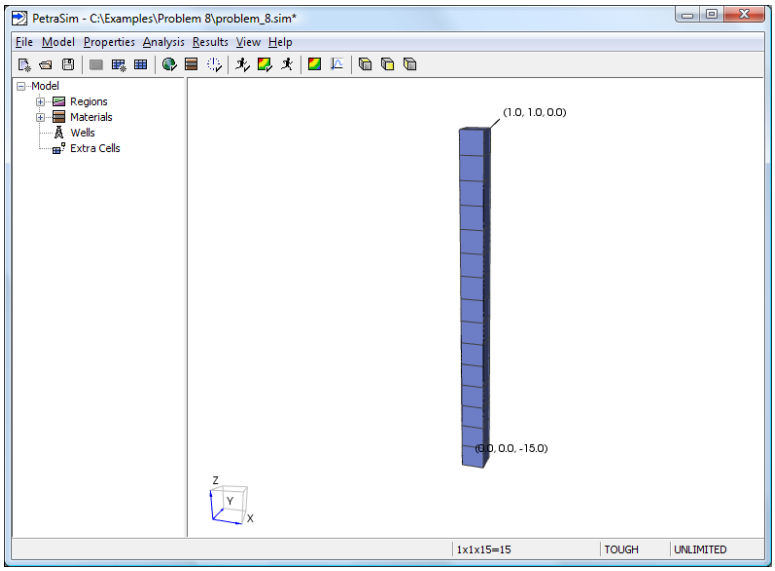

Figure 7.2. The geometric grid

Global Properties

Global properties are those properties that apply to the entire model. We will make changes to some of the EOS options, including activating molecular diffusion. To edit global properties, you use the **Global Properties** dialog.

On the **Properties** menu, click **Global Properties...** (or click on the toolbar).

1. In the **Global Properties** dialog, select the **EOS** tab.

2. Select **Isothermal**.

3. Select the **Molecular Diffusion** checkbox.

4. Click **Edit COEFs...**.

5. On the **Edit Coefficients** dialog, enter the values given in Table 7.2.

6. Click **OK** to close the **Edit Coefficients** dialog.

7. In the **Brine Data** list, select **Same as Water**.

8. In the **Radionuclide Data** box, click **Edit**.

9. To define properties for the **Parent Radionuclide Data**, enter the values given in Table 7.3.

10. To define properties for the **Daughter Radionuclide Data**, enter the values given in Table 7.4.

11. Click **OK** to close the **Radionuclide Properties** dialog.

12. Click **OK** to close the **Global Properties** dialog.

Table 7.2. Diffusion coefficients

Parameter	Gas	Liquid
Water	1.0E-6	1.0E-10
Brine	0.0	0.0
Radionuclide 1	1.0E-6	1.0E-10
Radionuclide 2	1.0E-6	1.0E-10
Air	1.0E-6	1.0E-10

Table 7.3. Parent Radionuclide Data

Parameter	Value
Half Life	1.0E50
Molecular Weight	131.389
Inverse Henry's Constant	2.0996E-8

Table 7.4. Daughter Radionuclide Data

Parameter	Value
Half Life	1.0E50
Molecular Weight	165.834
Inverse Henry's Constant	1.1816-8

Material Properties

To specify the material properties, you use the **Material Data** dialog. This problem uses three different materials: a material that represents the vadose zone (VADOS), a material that represents the atmosphere (ATMOS), and a material that allows only diffusion from the VOC source (TRAPP). We first define the vados material.

1. On the **Properties** menu, click **Materials** (or click on the toolbar).
2. In the **Name** box, type `VADOS`.
3. In the **Density** box, type `2600.0`.
4. In the **Porosity** box, type `0.35`.
5. In all three **Permeability** boxes (X, Y, and Z), type `1.0E-11`.
6. In the **Wet Heat Conductivity** box, type `2.51`.
7. In the **Specific Heat** box, type `920.0`.

We also need to specify the relative permeability and capillary pressure functions for this material. These options can be found in the **Additional Material Data** dialog. To open this dialog, click the **Relative Perm...** button.

To specify the relative permeability function

1. Select the **Relative Perm** tab.
2. In the **Relative Permeability** list, select **van Genuchten-Mualem Model**.
3. In the **Lambda** box, type `0.457`.
4. In the **Slr** box, type `0.15`.
5. In the **Sls** box, type `1.0`.
6. In the **Sgr** box, type `0.1`.

To specify the capillary pressure function

1. Select the **Capillary Press** tab.
2. In the **Capillary Pressure** list, select **van Genuchten Function**.
3. In the **Lambda** box, type `0.457`.
4. In the **Slr** box, type `0.0`.
5. In the **1/P0** box, type `5.105E-4`.

6. In the **Pmax** box, type `1.0E7`.

7. In the **Sls** box, type `1.0`.

To specify the tortuosity

1. Select the **Misc** tab.

2. In the **Tortuosity Factor** box, type `0.25`.

Click **OK** to exit the **Advanced Material Data** dialog. Click **Apply** to save the changes for the VADOS material.

We will now create a new cap rock material, based on VADOS

1. In the **Material Data** dialog, click **New**.

2. In the **Tough Name** box, type `TRAPP`.

3. In the **Description** box, type **VOC source**.

4. In the **Based On** list, select **VADOS**.

5. Click **OK** to create the new material.

The **TRAPP** will represent a material with zero permeability that is a source of VOC by diffusion only. Because it was based on the **VADOS** material, it has inherited all the properties we previously defined for that material. We will only set the permeabilities to zero. To modify the **TRAPP** material

1. On the **Materials** list, make sure that **TRAPP** is selected.

2. In all three **Permeability** boxes (X, Y, and Z), type `0.0`.

3. Click **Apply** to save the changes.

Finally, we will create one material to be used to represent the atmosphere. The atmosphere is modeled with zero capillary pressure.

1. In the **Material Data** dialog, click **New**.

2. In the **Tough Name** box, type `ATMOS`.

3. In the **Description** box, type **Atmosphere**.

4. In the **Based On** list, select **VADOS**.

5. Click **OK** to create the new material.

To modify the **ATMOS** material

1. On the **Materials** list, make sure that **ATMOS** is selected.
2. Click the **Relative Perm...** button to open the **Additional Material Data** dialog.
3. Click the **Capillary Press** tab.
4. In the **Capillary Pressure** list, select **No Capillary Pressure**.
5. Click the **Misc** tab.
6. In the **Tortuosity Factor** box, type `1.0`.
7. Click **OK** to exit the **Advanced Material Data** dialog.
8. Click **OK** to save the changes and close the **Material Data** dialog.

Initial Conditions

The initial state of each cell in the model must be defined. The default initial conditions represent an approximate starting state for the cells in the vadose zone above the water table. Default initial conditions are applied to all cells that do not have initial conditions specified individually. On the **Properties** menu, click **Initial Conditions...** (or click on the toolbar).

To set the default initial conditions

1. Select the **Two-Phase (Pg, Xb, Xrn1, Xrn2, Sg+10, T)** state option.
2. In the **Pressure** box, type `1.013E5`.
3. In the **Temperature** box, type `20.0`.
4. In the **Gas Saturation** box, type `0.5`.
5. In the **Brine Mass Fraction** box, type `0.0`.
6. In the **Parent Radionuclide Mass Fraction** box, type `0.0`.
7. In the **Daughter Radionuclide Mass Fraction** box, type `0.0`.
8. Click **OK**.

For the bottom four cells that are below the water table, the initial conditions are single phase liquid. To specify the initial conditions, we select the cells in the **Grid Editor**,. To open the **Grid Editor**, on the **Model** menu, click **Edit Grid** (or click on the toolbar).

1. Open the **Grid Editor**. On the **Model** menu, click **Edit Grid** (or click on the toolbar).

2. In the **Grid Editor**, click on the **View** icon to select the **YZ View**.

3. Using the **Selection** tool, select the four bottom cells of the model.

4. Right-click on the first cell and click **Initial Conditions...**, Figure 7.3.

5. Click **Specify Initial Conditions by Cell**. The initial conditions for the individual cells override the global values. Because these cells are below the water table, they are single phase liquid. There is a small amount of dissolved air in the water.

6. Select the **Single-Phase (P, Xb, Xrn1, Xrn2, X, T)** state option.

7. In the **Pressure** box, type `1.5E5`.

8. In the **Temperature** box, type `20.0`.

9. In the **Brine Mass Fraction** box, type `0.0`.

10. In the **Parent Radionuclide Mass Fraction** box, type `0.0`.

11. In the **Daughter Radionuclide Mass Fraction** box, type `0.0`.

12. In the **Air Mass Fraction** box, type `1.0E-12`.

13. Click **OK** to close the **Edit Multi-Cell Data** dialog.

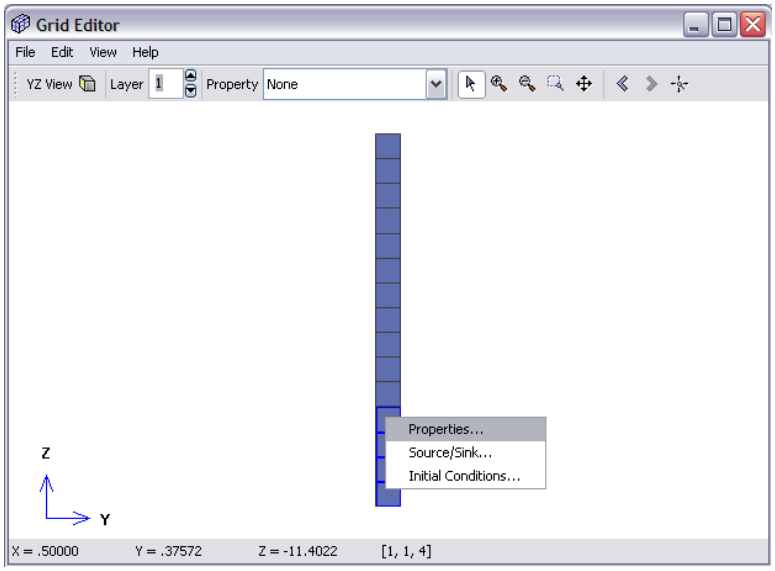

Figure 7.3. Selecting the bottom four cells.

The 5th cell from the bottom (Z=-10.5) will be the cell at the water table. During the gravity/capillary equilibrium solution, all other cells values will be calculated relative to this water table cell.

1. In the **Grid Editor**, click on the **View** icon to select the **YZ View**.

2. Using the **Selection** tool, right-click on the fifth cell from the bottom, and click **Edit Properties...**.

3. In the **Cell Name** box, type `Water Table`.

4. In the **Type** box, select `Fixed State`. This means that this cell will not change during the analysis, but will remain fixed at constant temperature, pressure, etc.

5. Click the **Initial Conditions** tab.

6. Click **Specify Initial Conditions by Cell**. The initial conditions for the individual cells override the global values.

7. Select the **Two-Phase (Pg, Xb, Xrn1, Xrn2, Sg+10, T)** state option.

8. In the **Pressure** box, type `1.013E5`.

9. In the **Temperature** box, type `20.0`.

10. In the **Gas Saturation** box, type `0.2`.

11. In the **Brine Mass Fraction** box, type `0.0`.

12. In the **Parent Radionuclide Mass Fraction** box, type `0.0`.

13. In the **Daughter Radionuclide Mass Fraction** box, type `0.0`.

14. Click the **Print Options** tab.

15. Select the **Print Cell Time Dependent Data** check box. This will output extra data for this cell every time step for later plotting.

16. Click **OK** to close the **Edit Cell Data** dialog.

Close the **Grid Editor**.

Add Extra Cells

Extra Cells are cells that are in addition to the geometric cells that define the solution grid. In this model, they will be used to define boundary conditions at the top and bottom. In the gravity/capillary equilibrium solution, these are **Enabled** and the state of the cells will be calculated. In the transient analysis, these cells will be **Fixed State** and they will define boundary conditions.

To add the **Extra Cells**

1. On the **Model** menu, click **Add Extra Cell...** .

2. Click the **Properties** tab.
3. In the **Cell Name** box, type `Top`.
4. In the **Volume** box, type `1.0`.
5. In the **Material** list, select **ATMOS**.
6. In the **Type** list, select **Enabled**.
7. Click the **Initial Conditions** tab.
8. Click **Specify Initial Conditions by Cell**.
9. Select the **Single-Phase (P, Xb, Xrn1, Xrn2, X, T)** state option.
10. In the **Pressure** box, type `1.013E5`.
11. In the **Temperature** box, type `20.0`.
12. In the **Brine Mass Fraction** box, type `0.0`.
13. In the **Parent Radionuclide Mass Fraction** box, type `0.0`.
14. In the **Daughter Radionuclide Mass Fraction** box, type `0.0`.
15. In the **Air Mass Fraction** box, type `0.99`.
16. Click the **Print Options** tab.
17. Select the **Print Cell Time Dependent Data** check box.
18. Click the **Connected Cells** tab. This table is used to input all the information that will connect this cell to the model. Enter the values from Table 7.5, which correspond to the input required by TOUGH2 for a CONNE connection record, Figure 7.4.
19. Click **OK** to close the **Edit Cell Data** dialog.

Table 7.5. Connection data for top extra cell

Parameter	Value
'To' Cell	15
Orientation	3
Dist 'This'	1.0E-9
Dist 'To'	0.5
Area	1.0

Parameter	Value
Gravita...	1.0
Rad. H...	0.0

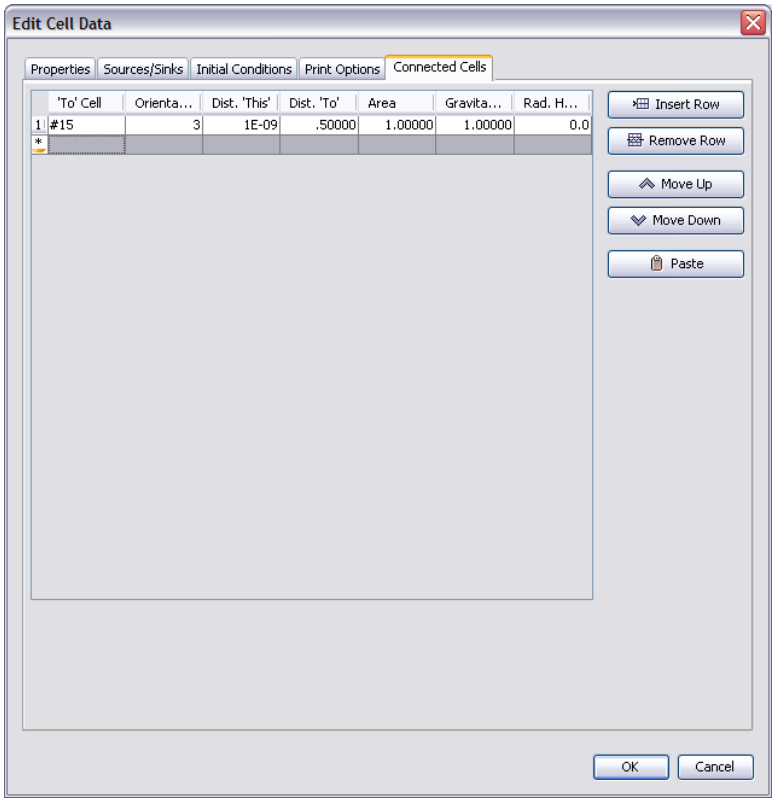

Figure 7.4. Top extra cell

Repeat these steps to add the bottom **Extra Cell**

1. On the **Model** menu, click **Add Extra Cell...** .
2. Click the **Properties** tab.
3. In the **Cell Name** box, type `Bot`.
4. In the **Volume** box, type `1.0`.
5. In the **Material** list, select **VADOS**.
6. In the **Type** list, select **Enabled**.
7. Click the **Initial Conditions** tab.

8. Click **Specify Initial Conditions by Cell**.
9. Select the **Single-Phase (P, Xb, Xrn1, Xrn2, X, T)** state option.
10. In the **Pressure** box, type `1.5E5`.
11. In the **Temperature** box, type `20.0`.
12. In the **Brine Mass Fraction** box, type `0.0`.
13. In the **Parent Radionuclide Mass Fraction** box, type `0.0`.
14. In the **Daughter Radionuclide Mass Fraction** box, type `0.0`.
15. In the **Air Mass Fraction** box, type `1.0E-12`.
16. Click the **Print Options** tab.
17. Select the **Print Cell Time Dependent Data** check box.
18. Click the **Connected Cells** tab. This table is used to input all the information that will connect this cell to the model. Enter the values from Table 7.6, which correspond to the input required by TOUGH2 for a CONNE connection record.
19. Click **OK** to close the **Edit Cell Data** dialog.

Table 7.6. Connection data for bottom extra cell

Parameter	Value
'To' Cell	1
Orientation	3
Dist 'This'	1.0E-9
Dist 'To'	0.5
Area	1.0
Gravita...	-1.0
Rad. H...	0.0

Select Cell for Time History Output

We can select cells to print output more frequently than the frequency for the entire mesh.

1. Open the **Grid Editor**. On the **Model** menu, click **Edit Grid** (or click  on the

toolbar).

2. In the **Grid Editor**, click on the **View** icon to select the **YZ View**.

3. Right-click on the 11th cell up from the bottom and click **Edit Properties...**. The **Z Center** should be at -4.5 m.

4. In the **Name** box, type `VOC Link`. This is the cell that will connect to the VOC source in the transient analysis.

5. Click the **Print Options** tab.

6. Select the **Print Cell Time Dependent Data** check box.

7. Click **OK** to close the **Edit Cell Data** dialog.

8. Close the **Grid Editor**.

Solution Controls

We will set the end time of the analysis.

1. On the **Analysis** menu, click **Solution Controls...** (or click on the toolbar).

2. In the **End Time** box, type `3.155E12` sec (about 100,000 years). This large time is needed to reach full equilibrium.

3. Click **OK** to exit the **Solution Controls** dialog..

Output Controls

By default, the simulation will print output every 100 time steps. We can increase the frequency of the output in the **Output Controls** dialog.

1. On the **Analysis** menu, click **Output Controls...** (or click on the toolbar).

2. In the **Print and Plot Every # Steps** box, type `2`.

3. Click **OK** to exit the **Output Controls** dialog.

Save and Run

The input is complete and you can run the simulation. If you haven't already, you may want to save your model in a directory specifically intended for the simulation results. For example

1. On the **File** menu, click **Save** (or click on the toolbar).

2. Create a new folder named **Equilibrium** and in the **File Name** box, type **equilib-**

rium.sim.

3. Click **Save**.

To run the simulation, on the **Analysis** menu, click **Run TOUGH2** (or click on the toolbar).

During the solution, a graph will display the time step size.

View 3D Results

To view the 3D results for a simulation, on the **Results** menu, click **3D Results** (or click on the toolbar). The data for the current simulation will be automatically loaded and displayed.

To show liquid saturation contours

1. In the **Time(s)** list, select the last entry (**3.155E12**).

2. In the **Scalar** list, select **SL**.

3. Click to clear the **Show Isosurfaces** checkbox.

To add a slice plane on which contours will be displayed, click **Slice Planes...**. For this example we will show one slice plane. To configure the slice plane

1. In the **Axis** list, select **Y**.

2. In the **Coord** box, type `0.5`.

3. Select the **Scalar** check box.

4. Click **Close**.

The resulting contour plot is shown in Figure 7.5. Below the water table, the soil is completely saturated, above it has a partial saturation of about 0.154.

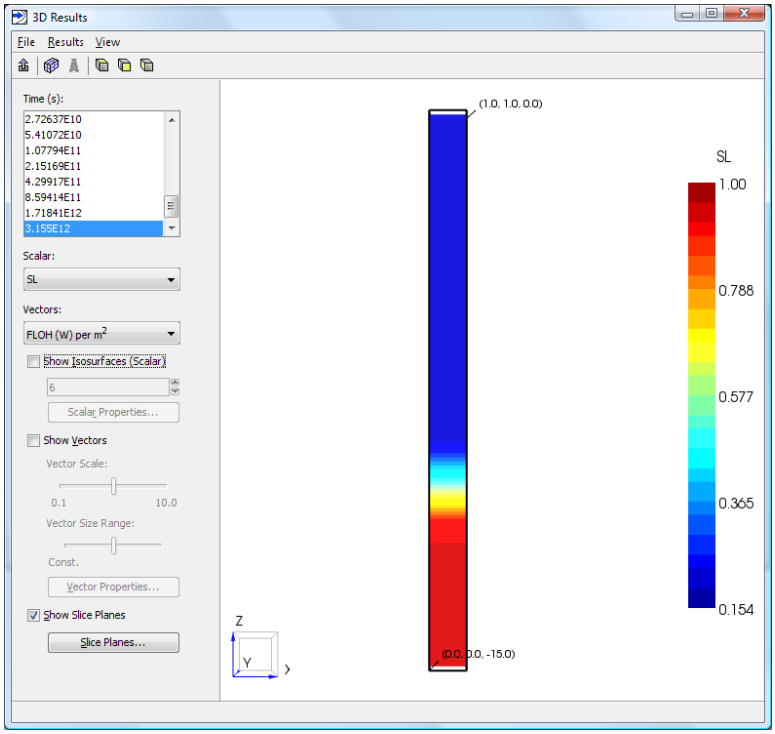

Figure 7.5. Contours of liquid saturation (SL).

Close the **3D Results** window.

View Cell History Plot

You can view time history plots with the Cell History dialog. On the **Results** menu, click **Cell History Plots....** (or click on the toolbar).

The **Cell History** dialog will be displayed. In this window, you can display time history data using a plotting parameter and a list of cells. For example, to view the temperature in the Outflow cell

1. In the **Variable** list, select **SL** (saturation of liquid).

2. In the **Cell Name (Id#)** list, select **VOC Link**.

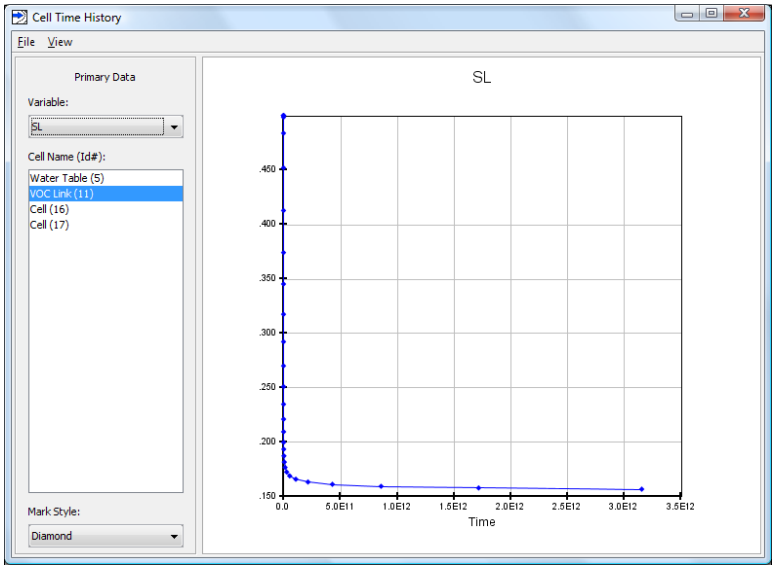

Figure 7.6. Time history of liquid saturation showing convergence to steady state.

Close the **Cell History** window.

Transient Analysis

We will now use the equilibrium state results as initial conditions for a transient analysis. You will open the model file (equilibrium.sim) that we previously saved and then save it to a new directory.

1. If the equilibrium analysis is not already open, on the **File** menu, click **Open** (or click on the toolbar). In the **File Name** box, select the **equilibrium.sim** file and click **Open**.

2. To save the transient model, on the **File** menu, click **Save As...**.

3. Create a new folder named **Transient** and in the **File Name** box, type **transient.sim**.

4. Click **Save**.

Load Initial Conditions

To load the previously calculated equilibrium results and use them as initial conditions for the transient analysis, we read the **SAVE** file that was output at the end of the equilibrium analysis. This file has the results for all the cells in the model. To read these initial conditions

1. On the **File** menu, click **Load Initial Conditions...** .

2. Browse to the **Equilibrium** folder and select the **SAVE** file.

3. Click **Open**. This reads the saved data from the previous run and stores it as an initial condition for each cell in the current analysis.

To view the initial conditions, open the **Grid Editor**

1. On the **Model** menu, click **Edit Grid** (or click on the toolbar).

2. In the **Grid Editor**, click on the **View** icon to select the **YZ View**.

3. In the **Property** list, select **Pressure**.

4. The display will show the pressures from the equilibrium analysis, Figure 7.7.

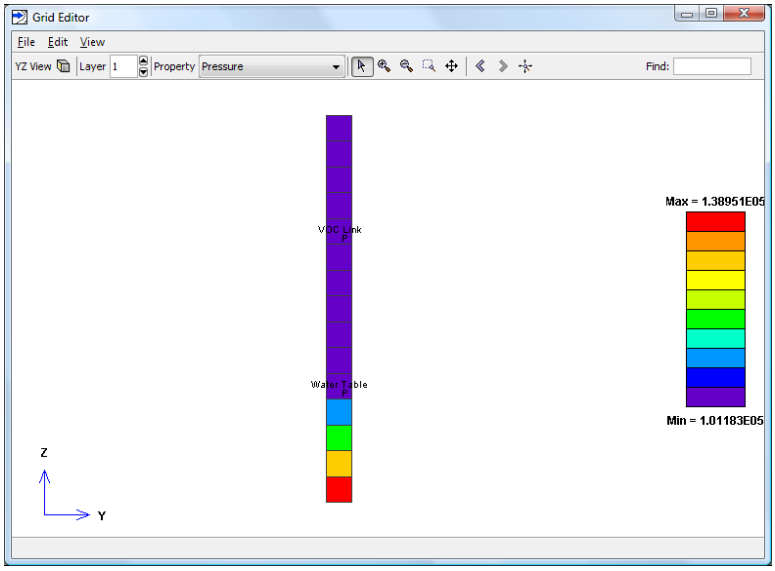

Figure 7.7. Default initial conditions.

Add VOC Source Cell

An **Extra Cell** is used to define the VOC source

1. On the **Model** menu, click **Add Extra Cell...** .

2. Click the **Properties** tab.

3. In the **Cell Name** box, type `Source`.

4. In the **Volume** box, type `1.0`.

5. In the **Material** list, select **TRAPP**.

6. In the **Type** list, select **Fixed State**.
7. Click the **Initial Conditions** tab.
8. Click **Specify Initial Conditions by Cell**.
9. Select the **Two-Phase (Pg, Xb, Xrn1, Xrn2, Sg, T)** state option.
10. In the **Pressure** box, type `1.0123E5`.
11. In the **Temperature** box, type `20.0`.
12. In the **Gas Saturation** box, type `0.84353`.
13. In the **Brine Mass Fraction** box, type `0.0`.
14. In the **Radionuclide 1** box, type `1.0998E-3`.
15. In the **Radionuclide 1** box, type `2.0063E-4`.
16. Click the **Print Options** tab.
17. Select the **Print Cell Time Dependent Data** check box.
18. Click the **Connected Cells** tab. This table is used to input all the information that will connect this cell to the model. Enter the values from Table 7.7, which correspond to the input required by TOUGH2 for a CONNE connection record.
19. Click **OK** to close the **Edit Cell Data** dialog.

Table 7.7. Connection data for source cell

Parameter	Value
'To' Cell	11
Orientation	1
Dist 'This'	1.0E-9
Dist 'To'	0.5
Area	0.1
Gravita...	0.0
Rad. H...	0.0

Change Fixed Cells

In the equilibrium analysis, we reached a steady state condition for gravity and capillary equilibrium. We will now use those values to define fixed top and bottom conditions for the model.

1. Open the **Grid Editor**. On the **Model** menu, click **Edit Grid** (or click on the toolbar).

2. In the **Grid Editor**, click on the **View** icon to select the **YZ View**.

3. Using the **Selection** tool, right-click on the fifth cell from the bottom, and click **Edit Properties...**.

4. In the **Type** box, select `Enabled`. This means that this cell is now part of the analysis.

5. Click **OK** to close the **Edit Cell Data** dialog.

6. Close the **Grid Editor** window.

We now change the extra cells to a fixed state to define the boundary conditions for the transient analysis.

1. In the **Tree View** (on the left of the display), expand the **Extra Cells** icon and double-click on the **Top** cell.

2. On the **Properties** tab, in the **Type** box, select `Fixed State`.

3. Click **OK** to close the **Edit Cell Data** dialog.

Repeat for the bottom (Bot) cell.

Solution Controls

We will now define the solution options.

1. On the **Analysis** menu, click **Solution Controls...** (or click on the toolbar).

2. In the **End Time** box, type `3.1557E9` sec (about 100 years).

3. Click **OK** to exit the **Solution Controls** dialog..

Output Controls

By default, the simulation will print output every 100 time steps. We can increase the frequency of the output in the **Output Controls** dialog.

1. On the **Analysis** menu, click **Output Controls...** (or click on the toolbar).

2. In the **Print and Plot Every # Steps** box, type `2`.

3. Click **Edit**.

4. In the **Additional Print Times** table, type `3.15576e7` (about 1 year). This will force a solution printout at this time.

5. Click **OK** to exit the **Additional Print Times** dialog.

6. Click **OK** to exit the **Output Controls** dialog.

Run Transient Analysis

To run the simulation, on the **Analysis** menu, click **Run TOUGH2** (or click on the toolbar). The model file will automatically be saved.

During the solution, a graph will display the time step size.

View Transient 3D Results

To view the 3D results for the transient simulation, on the **Results** menu, click **3D Results** (or click on the toolbar). The data for the current simulation will be automatically loaded and displayed.

To show the mass fraction of radionuclide in the gas

1. In the **Time(s)** list, select the **3.156E7** time.

2. In the **Scalar** list, select **XRN!(GAS)**.

3. Click to clear the **Show Isosurfaces** checkbox.

To add a slice plane on which contours will be displayed, click **Slice Planes...**. For this example we will show one slice plane. To configure the slice plane

1. In the **Axis** list, select **Y**.

2. In the **Coord** box, type `0.5`.

3. Select the **Scalar** check box.

4. Click **Close**.

The resulting contour plot is shown in Figure 7.8.

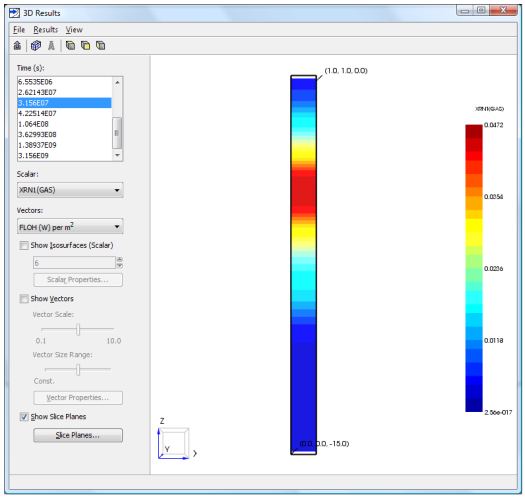

Figure 7.8. Contours of mass fraction of radionuclide 1 (TCE) in gas at one year.

Close the **3D Results** window.

View Cell History Plots

You can view time history plots with the Cell History dialog. On the **Results** menu, click **Cell History Plots....** (or click on the toolbar).

The **Cell History** dialog will be displayed. In this window, you can display time history data using a plotting parameter and a list of cells. For example, to view the temperature in the Outflow cell

1. In the **Variable** list, select **XRn1(gas)**.

2. In the **Cell Name (Id#)** list, select **Water Table**.

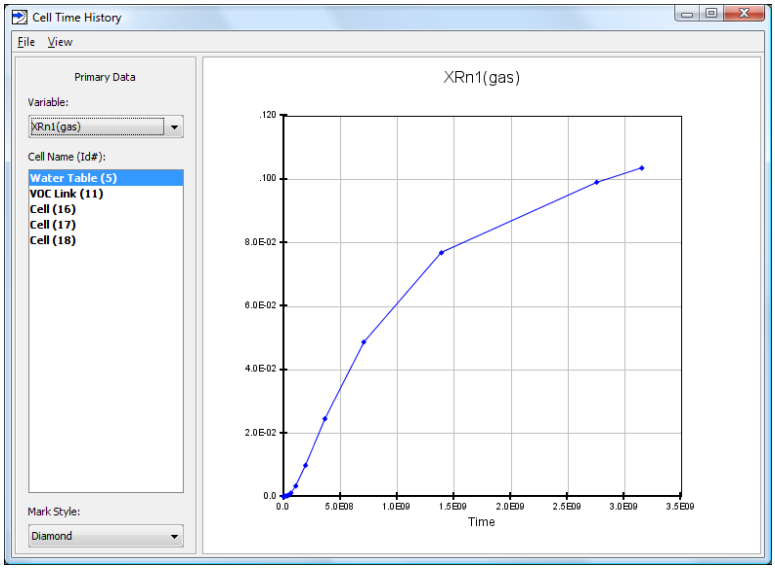

Figure 7.9. Time history of mass fraction of radionuclide 1 (TCE) in gas in Water Table cell.

Close the **Cell History** window.

Chapter 8. CO2 Injection (ECO2N)

Description

This example is Problem 2 "Radial Flow from a CO2 Injection Well" in the ECO2N module description, [Pruess, 2005]. This is a basic problem of CO2 injection into a saline aquifer, examining two-phase flow with CO2 displacing (saline) water under conditions that may be encountered in brine aquifers at a depth of the order of 1.2 km. A CO2 injection well fully penetrates a homogeneous, isotropic, infinite-acting aquifer of 100 m thickness (Fig. 13), at conditions of 120 bar pressure, 45 C temperature, and a salinity of 15% by weight. CO2 is injected uniformly at a constant rate of 100 kg/s. This problem had been included as test problem #3 in a recent code intercomparison project ([Pruess and Garcia, 2002] and [Pruess et al., 2002].

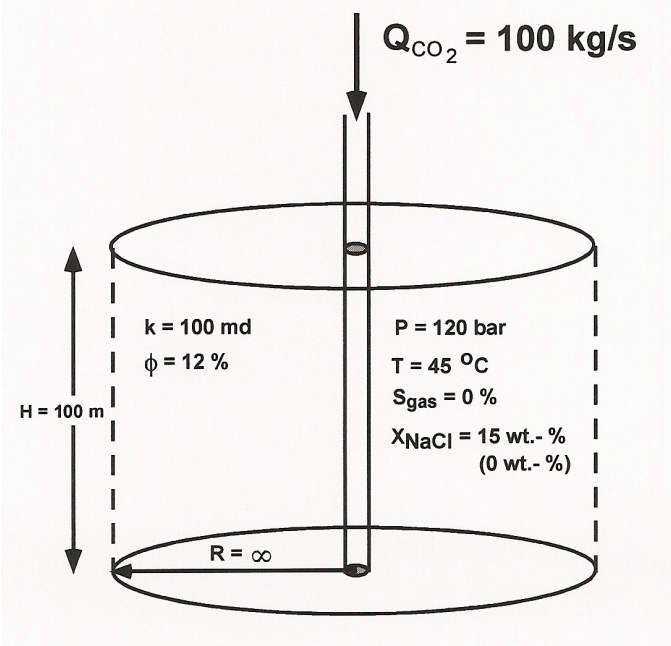

Figure 8.1. Schematic of problem

Specify the Equation of State (EOS)

To ensure that PetraSim uses ECO2N, edit your PetraSim preferences using the **Preferences** dialog.

1. On the **File** menu, click **Preferences...** .
2. In the **Simulator Mode** list, select **TOUGH**.
3. In the **Default EOS** list, select **ECO2N**.

4. Click **OK**.

Your preferences have now been updated, but you will need to create a new model or restart PetraSim before they become active. If you already have a model open, it will not be affected by the preference change. On the **File** menu, click **New**.

Create the Model Boundary

To create the boundary, use the **Define Model Boundary** dialog. The boundary parameters for this model are shown in Table 8.1.

Table 8.1. Model boundary dimensions

Axis	Min (m)	Max (m)
x	0.3	100000.0
y	0.0	1.0
z	0.0	100.0

To create the model boundary

1. On the **Model** menu, click **Define Boundary...** (or click on the toolbar).
2. Enter the values from Table 8.1.
3. Click **OK** to create the model boundary.

Because this model has a very large radius, we will need to scale the dimension in the Z direction in order to manipulate the model. To do this

1. On the **View** menu, click **Scale Axis...**.
2. In the **Z Factor** box, type `500`.
3. Click **OK** to close the **Scale Axis** dialog.

You can rotate, pan, and zoom the model using the mouse and **Shift** and **Alt** keys.

Create the Grid

To create the solution grid

1. On the **Model** menu, click **Create Grid...** (or click on the toolbar).
2. In the **Division Method** box, select **Regular**.

3. Click **Cells Above Top and Below Bottom are Inactive**.

4. Click **RZ Grid**. This creates a 2D cylindrical grid. It will be displayed as a plane, but when the solution data is written, the volume and connections for the cells will be calculated in cylindrical coordinates.

5. In the **X Cells** box, type `500`.

6. In the **X Factor** box, type `1.02`. This will exponentially increase the cell size in the X (radial) direction. See the PetraSim User Manual for instructions on how to calculate this factor.

7. In the **Z Cells** box, type `1`.

8. In the **Z Factor** box, type `1.0`.

9. Click **OK** to create the grid.

The resulting mesh is displayed in Figure 8.2. Click the **Front View** in the toolbar to display the model as shown below.

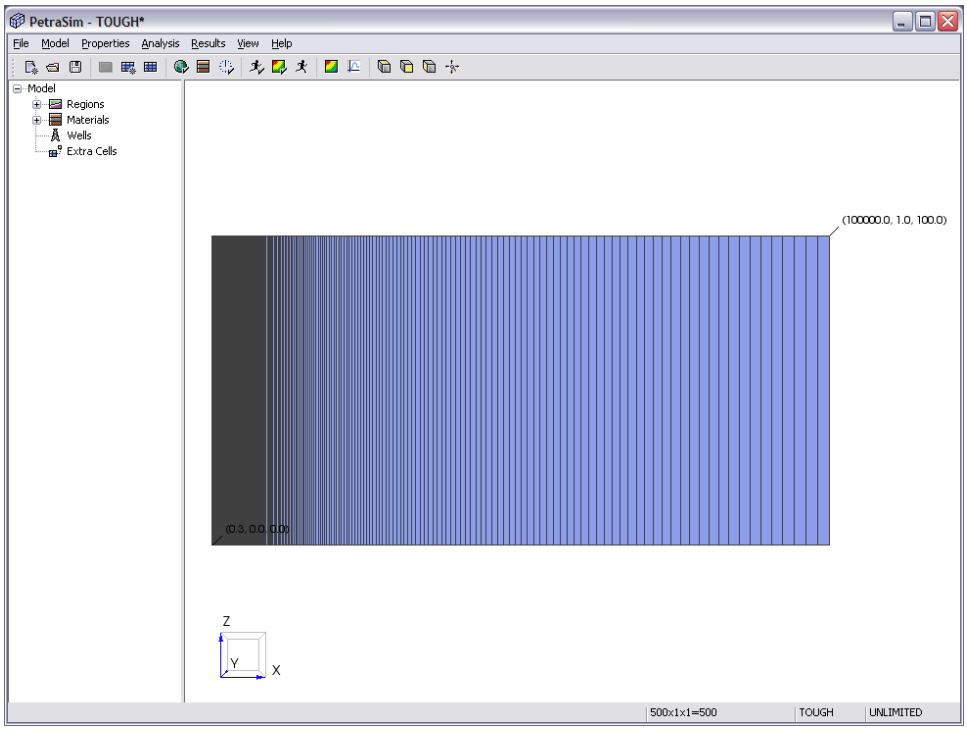

Figure 8.2. The resulting mesh

Global Properties

Global properties are those properties that apply to the entire model. We will make

changes to some of the EOS options, including activating molecular diffusion. To edit global properties, you use the **Global Properties** dialog.

On the **Properties** menu, click **Global Properties...** (or click on the toolbar).

1. Click the **Analysis** tab.
2. In the **Name** box, type `CO2 Injection`.
3. Click the **EOS** tab.
4. Select **Isothermal**.
5. Select **Tubes in Series**.
6. In the **phi** box, type `0.8`.
7. In the **G** box, type `0.8`.
8. Click **OK** to close the **Global Properties** dialog.

Material Properties

To specify the material properties, you use the **Material Data** dialog. This example requires one material.

1. On the **Properties** menu, click **Materials** (or click on the toolbar).
2. In the **Name** box, type `SAND`.
3. In the **Density** box, type `2600.0`.
4. In the **Porosity** box, type `0.12`.
5. In all three **Permeability** boxes (X, Y, and Z), type `1.0E-13`.
6. In the **Wet Heat Conductivity** box, type `2.51`.
7. In the **Specific Heat** box, type `920.0`.
8. Click **Apply** to save the changes.

In addition to the physical rock parameters, we also need to specify the relative permeability and capillary pressure functions for this material. These options can be found in the **Additional Material Data** dialog. To open this dialog, click the **Relative Perm...** button.

To specify the relative permeability function

1. Select the **Relative Perm** tab.
2. In the **Relative Permeability** list, select **van Genuchten-Mualem Model**.
3. In the **Lambda** box, type `0.457`.
4. In the **Slr** box, type `0.3`.
5. In the **Sls** box, type `1.0`.
6. In the **Sgr** box, type `0.05`.

To specify the capillary pressure function

1. Select the **Capillary Press** tab.
2. In the **Capillary Pressure** list, select **van Genuchten Function**.
3. In the **Lambda** box, type `0.457`.
4. In the **Slr** box, type `0.0`.
5. In the **1/P0** box, type `5.1E-5`.
6. In the **Pmax** box, type `1.0E7`.
7. In the **Sls** box, type `0.999`.

To specify the pore compressibility

1. Select the **Misc** tab.
2. In the **Pore Compressibility** box, type `4.5E-10`.

Click **OK** to exit the **Advanced Material Data** dialog.

Click **OK** again to save your settings and exit the **Material Data** dialog.

Initial Conditions

The initial state of each cell in the model must be defined. To specify global initial conditions that will be used as the default for all cells in the model

To set the initial conditions

1. On the **Properties** menu, click **Initial Conditions...** (or click on the toolbar).
2. Select the **Single-Phase (P, Xsm, Xncg, T)** state option.
3. In the **Pressure** box, type `120.0E5`.

4. In the **Temperature** box, type `45.0`.
5. In the **Salt Mass Fraction** box, type `0.15`.
6. In the **CO2 Mass Fraction** box, type `0.0`.
7. Click **OK** to close the **Default Initial Conditions** dialog.

Define CO2 Injection

This model has CO2 injected into the borehole. This is defined in the **Grid Editor**.

1. On the **Model** menu, click **Edit Grid** (or click on the toolbar).
2. In the **Grid Editor**, click on the **View** icon to select the **XZ View**.
3. On the **View** menu, click **Scale Axis...**.
4. In the **Z Factor** box, type `500`.
5. Using the **Zoom Box** tool, zoom in to the top left of the model until you can see the first cell.
6. Using the **Selection** tool, right-click on the first cell and click **Edit Properties...**, Figure 8.3.
7. In the **Cell Name** box, type `Injection`.
8. Click the **Sources/Sinks** tab.
9. In the **Injection** section, select the **CO2** check box.
10. In the **Rate** box, type `100`.
11. Click the **Print Options** tab.
12. Select the **Print Cell Time Dependent Data** check box.
13. Click **OK** to close the **Edit Cell Data** dialog.

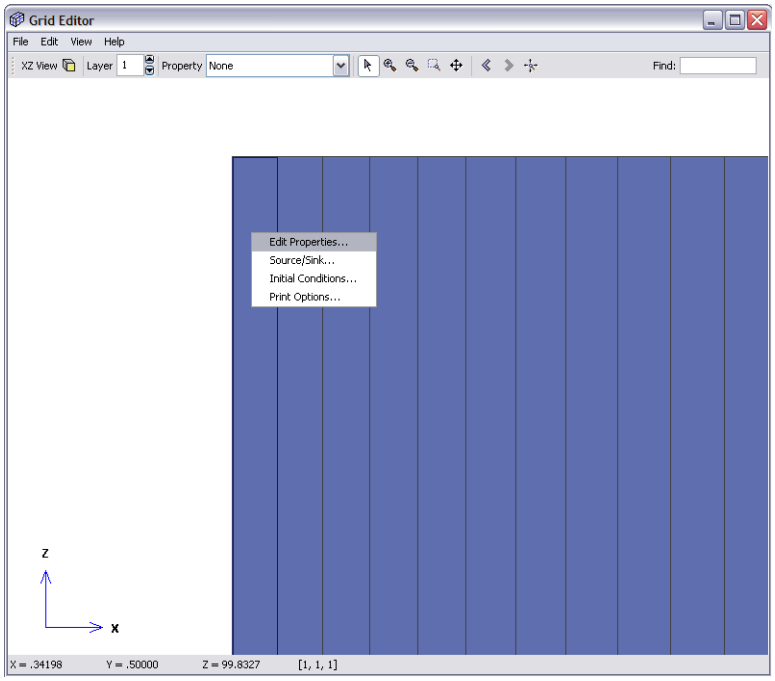

Figure 8.3. The cell to select

Select Additional Cell for Time History Output

We can select cells to print output more frequently than the frequency for the entire mesh.

1. On the **Model** menu, click **Edit Grid** (or click on the toolbar).
2. In the **Grid Editor**, click on the **View** icon to select the **XZ View**.
3. In the **Find** box, type `200`. This will select cell number 200, which is located at a radius of 255 m.
4. On the **Edit** menu, click **Properties**. This will open the properties of this cell for editing.
5. In the **Name** box, type `R=255`.
6. Click the **Print Options** tab.
7. Select the **Print Cell Time Dependent Data** check box.
8. Click **OK** to close the **Edit Cell Data** dialog.
9. Close the grid editor.

Solution Controls

We will now define the solution control options.

1. On the **Analysis** menu, click **Solution Controls...** (or click on the toolbar).
2. In the **End Time** box, type `8.64E8`.
3. In the **Time Step** list, ensure that `Single Value` is selected.
4. In the **Time Step** box, type `1.0`. This is the initial time step.
5. In the **Max Num Time Steps** box, type `2000`.
6. Select **Enable Automatic Time Step Adjustment**.
7. Click the **Solver** tab.
8. Select **Stabilized Bi-Conjugate Gradient**.
9. Click **OK** to exit the **Solution Controls** dialog..

Output Controls

By default, the simulation will print output every 100 time steps. We can increase the frequency of the output in the **Output Controls** dialog.

1. On the **Analysis** menu, click **Output Controls...** (or click on the toolbar).
2. In the **Print and Plot Every # Steps** box, type `50`.
3. Click **OK** to exit the **Output Controls** dialog.

Save and Run

The input is complete and you can run the simulation. If you haven't already, you may want to save your model in a new directory. For example

1. On the **File** menu, click **Save** (or click on the toolbar).
2. Create a new folder named **ECO2N** and in the **File Name** box, type **eco2n.sim**.
3. Click **Save**.

To run the simulation, on the **Analysis** menu, click **Run TOUGH2** (or click on the toolbar).

During the solution, a graph will display the time step size.

View 3D Results

To view the 3D results for a simulation

1. On the **Results** menu, click **3D Results** (or click on the toolbar). The data for the current simulation will be automatically loaded and displayed.

Since the model has a large radius relative to its height, we scale the Z coordinates.

1. On the **View** menu, click **Scale Axes...**.
2. In the **Z Factor** box, type `500`.
3. On the **View** menu, click **Front View** (or click on the toolbar).

To show pressure contours for the last time step

1. In the **Time(s)** list, select the last entry (**8.64E8**).
2. In the **Scalar** list, select **P (Pa)**.
3. Click to clear the **Show Isosurfaces** checkbox.

To add a slice plane on which contours will be displayed, click **Slice Planes...**. For this example we will show one slice plane. To configure the slice plane

1. In the **Axis** list, select **Y**.
2. In the **Coord** box, type `0.5`.
3. Select the **Scalar** check box.
4. Click **Close**.

After zooming in to the left side of the model, the resulting contour plot is shown in Figure 8.4.

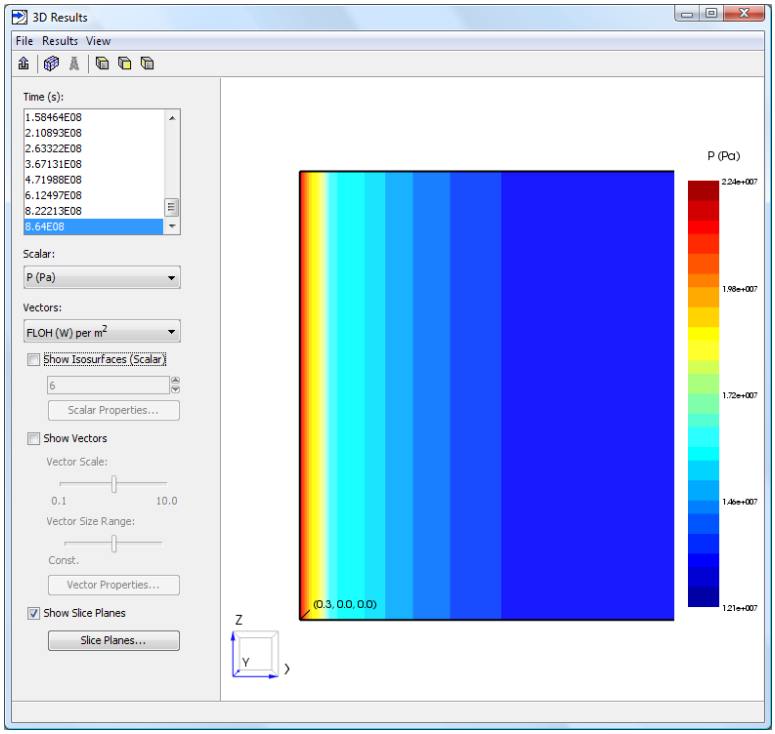

Figure 8.4. Pressure contours

Close the **3D Results** window.

Time History Plots

You can view time history plots with the Cell History dialog. On the **Results** menu, click **Cell History Plots....** (or click on the toolbar).

The **Cell History** dialog will be displayed. In this window, you can display time history data using a plotting parameter and a list of cells. For example, to view the temperature in the Heat Source cell

1. In the **Variable** list, select **Sg** (gas saturation).

2. In the **Cell Name (Id#)** list, select **R=255**.

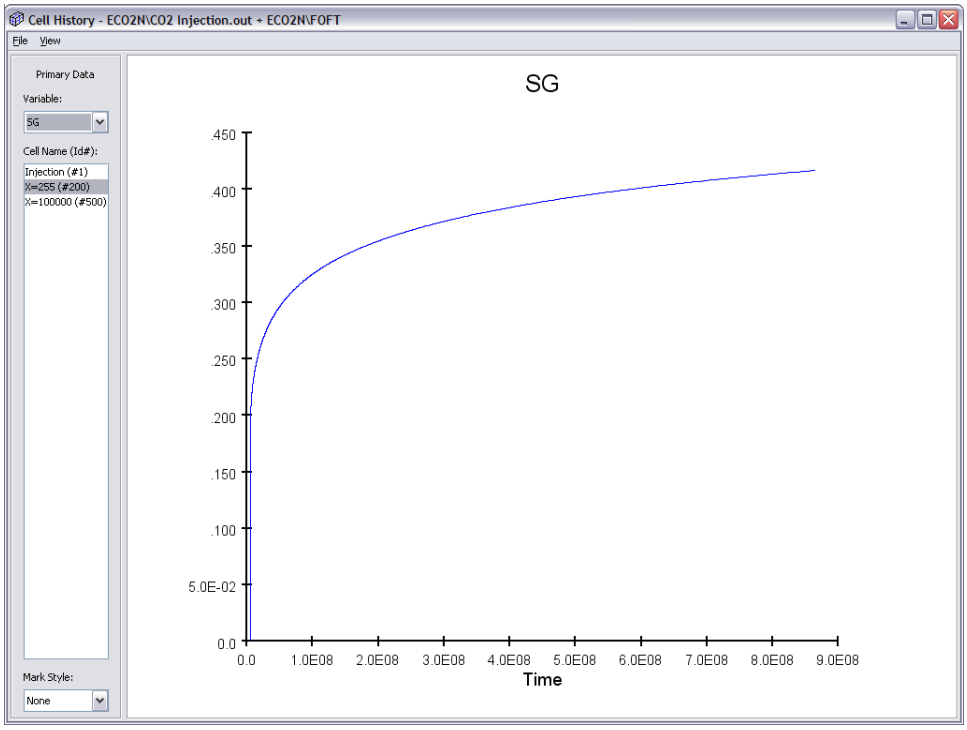

Figure 8.5. Cell history plot of gas saturation for the cell at 255 m

Close the Cell History window.

Line Plots

PetraSim also supports line plots, where you define a line in 3D space and the data is interpolated along the line. To make a line plot

1. On the **Results** menu, click **3D Results** (or click on the toolbar).
2. On the **File** menu, click **Line Plot....**
3. In the **Point 1** coordinate boxes (**X, Y, and Z**) type `0.3`, `0.5`, and `50.0`, respectively.
4. In the **Point 2** coordinate boxes (**X, Y, and Z**) type `1000.0`, `0.5`, and `50.0`, respectively.
5. Click **OK** to close the **Line Plot** dialog.
6. This will open a **Line Plot** window.
7. In the **Variable** list, select **P (Pa)**.
8. In the **Time** list, select **8.64E8** (the last time).

The plot is shown in Figure 8.6. You can export this data to a comma separated value file for import into a spreadsheet.

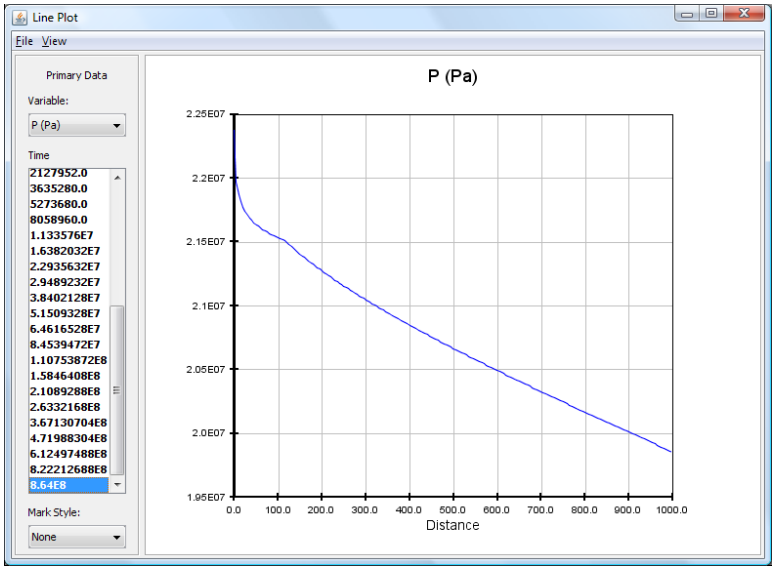

Figure 8.6. Line plot of pressure

Close the **Line Plot** window.

Figure 8.7 displays the results in a format that can be compared to the plot in the ECO2N User's Manual. These were made in Excel by importing the saved line plot data. The present results are the same as given in the manual.

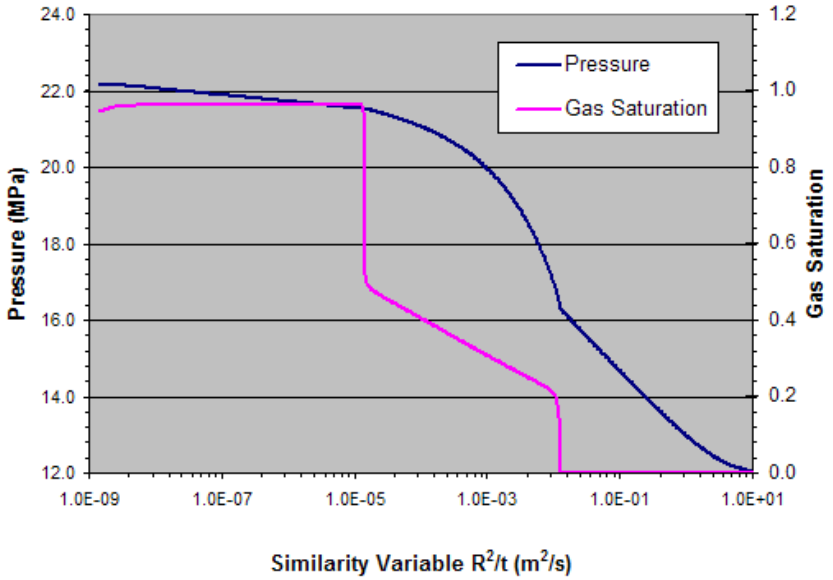

Figure 8.7. Results at time 8.64E7 s (for comparison with ECO2N manual)

Chapter 9. T2VOC Example Problem 1

Description

This example demonstrates one dimensional gas diffusion of an organic chemical with phase partitioning - as described in the T2VOC User's Guide (Ralta, Pruess, Finsterle, and Battistelli, LBL-36400, 1995).

A horizontal column has an initial temperature of 10 C and an initial pressure of 101325 Pa. The left cell has a fixed thermodynamic state and acts as a source of chlorobenzene. The geometry of the problem is shown in Figure 9.1.

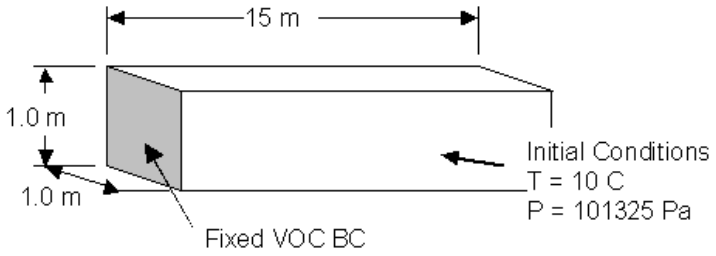

Figure 9.1. Example Problem Overview

We will use a mesh with 150 cells in the horizontal direction.

Specify the T2VOC Simulator

To ensure that PetraSim uses T2VOC as the simulator for this problem, you may need to edit your PetraSim preferences. To edit preferences, you can use the **PetraSim Preferences** dialog.

1. On the **File** menu, click **Preferences...**.
2. In the **Simulator Mode** list, select **TOUGH**.
3. In the **Default EOS** list, select **T2VOC**.
4. Click **OK**.

Your preferences have now been updated, but you will need to create a new model or restart PetraSim before they become active. If you already have a model open, it will be unaffected by the preferences change.

On the **File** menu, click **New**

Create the Model Boundary

To create the boundary for this model, you can use the **Define Model Boundary** dialog. This example will use the x-axis as the horizontal direction. The boundary parameters for this model are shown in Table 9.1.

Table 9.1. Model boundary dimensions

Axis	Min (m)	Max (m)
x	0.0	15.0
y	0.0	1.0
z	0.0	1.0

To create the model boundary:

1. On the **Model** menu, click **Define Boundary...** (or click on the toolbar).
2. Enter the values from Table 9.1.
3. Click **OK** to create the model boundary.

You can rotate, pan, and zoom the model using the mouse and **Shift** and **Alt** keys. The resulting boundary is shown in Figure 9.2. PetraSim will automatically add labels for the min point and max point of the boundary.

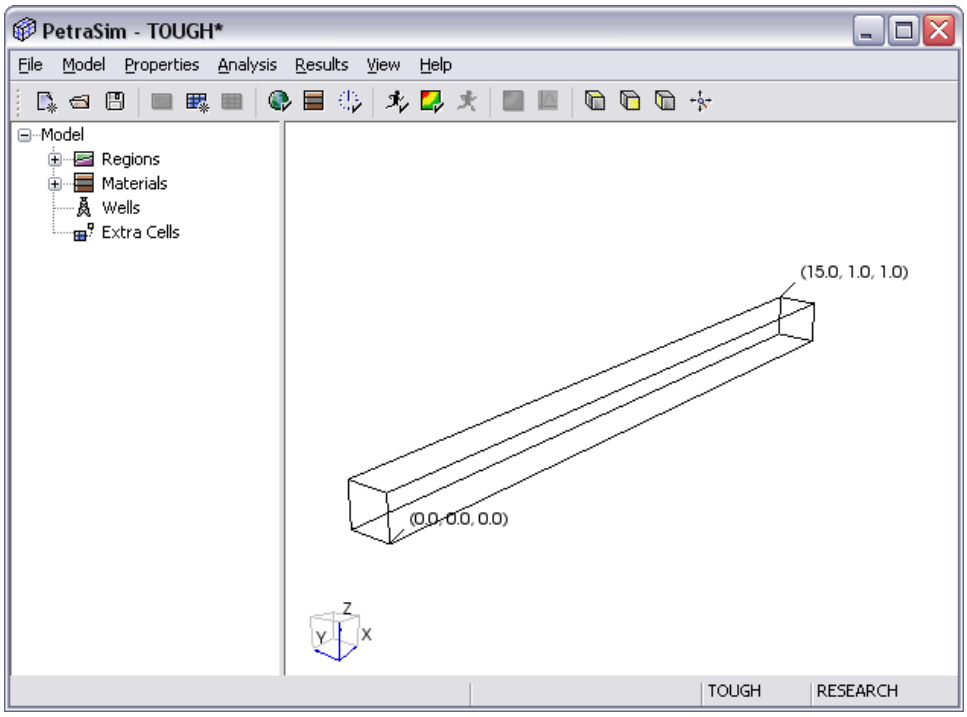

Figure 9.2. The Model Boundary

Create the Grid

To create the grid:

1. On the **Model** menu, click **Create Grid...** (or click on the toolbar).
2. In the **Division Method** box, select **Regular**.
3. In the **X Cells** box, type `150`.
4. In the **Y Cells** box, type `1`.
5. In the **Z Cells** box, type `1`.
6. Click **OK** to create the grid.

Global Properties

Global properties are those properties that apply to the entire model. In this example we will set the simulation name and configure the simulation VOC. To edit global properties, you can use the **Global Properties** dialog.

On the **Properties** menu, click **Global Properties...** (or click on the toolbar).

Simulation Name

1. In the **Global Properties** dialog, select the **Analysis** tab.
2. In the **Name** box, type `T2VOC Problem 1`.

EOS Data

The EOS (Equation of State) tab displays options for the T2VOC simulator. In this example, we will perform an isothermal (no heat flow) analysis. We will also specify a variant of chlorobenzene as the simulation VOC and specify the Air-Vapor diffusion constant.

In the **Global Properties** dialog, select the **EOS** tab

By default, the simulator will run in isothermal mode. Nothing needs to be changed.

To specify the VOC, you will need to create a variant of chlorobenzene using the **Edit VOC Data** dialog.

1. Click **Edit VOC Data...**.

2. Click **New**.

3. In the **Name** box, type `Chlorobenzene Ex 1`

4. In the **Based On** list, select **Chlorobenzene (STD)**.

5. Click **OK**. This creates a new VOC.

6. Update the values for **CHEMP.4**, **CHEMP.6**, and **CHEMP.7** according to the values shown in Table 9.2, Table 9.3, and Table 9.4.

7. Click **OK** and ensure that the selected **Simulation VOC** is **Chlorobenzene Ex 1**

8. This simulation will use gas diffusion. You can enable gas diffusion by setting the **Air-Vapor Diffusion** to a non-zero value. In the **Air-Vapor Diffusion** box, type `2.13e-5`.

9. Click **OK** to close the **Global Properties** dialog.

Table 9.2. Chlorobenzene Ex 1 (CHEMP.4)

Field	Value
Ref NAPL	1106.0
Ref Temp for NAPL	293
Ref Binary Diffusivity in Air	8.0e-6
Ref Temp for Gas Diffusivity	283.15
Chem Diffusivity Exponent	1.0

Table 9.3. Chlorobenzene Ex 1 (CHEMP.6)

Field	Value
SOLA	7.996e-5
SOLB	0.0
SOLC	0.0
SOLD	0.0

Table 9.4. Chlorobenzene Ex 1 (CHEMP.7)

Field	Value
Chem Organic Carbon Partition Coef	0.15
Default Fraction of Organic Carbon	0.005
VOC Biodegradation Decay Constant	0.0

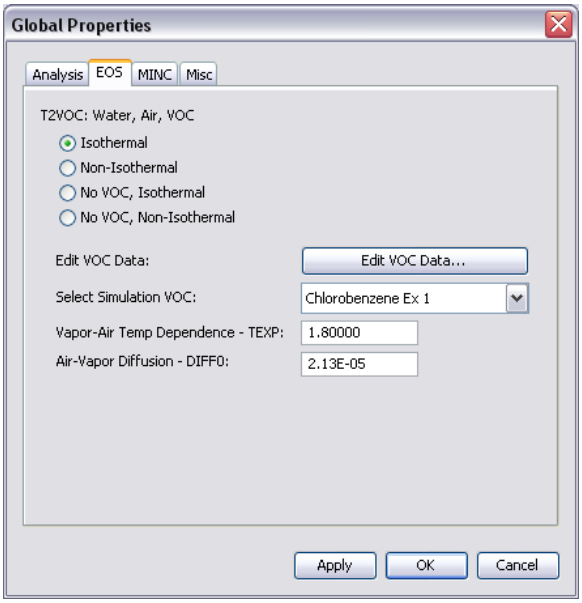

Figure 9.3. T2VOC Simulation Parameters

Material Properties

To specify the material properties, you can use the **Material Data** dialog.

1. On the **Properties** menu, click **Materials** (or click on the toolbar).
2. In the **Name** box, type **DIRT1**
3. In the **Density** box, type `2650.0`
4. In the **Porosity** box, type `0.4`
5. In all three **Permeability** boxes, type `1e-14`
6. In the **Wet Heat Conductivity** box, type `3.1`
7. In the **Specific Heat** box, type `1000.0`
8. Click **Apply** to save the changes

We still need to specify the relative permeability function and fraction of organic carbon for this material. These options can be found in the **Advanced Material Data** dialog. To open this dialog, click the **Relative Perm...** button.

To specify the relative permeability function:

1. Select the **Relative Perm** tab
2. In the **Relative Permeability** list, select **Stone's 3-Phase**
3. In the **Swr** box, type `0.4`
4. In the **Snr** boxes, type `0.1`
5. In the **Sgr** box, type `1.0e-3`
6. In the **n** box, type `1.0`

The default capillary pressure (none) is correct for this example.

To specify the fraction of organic carbon:

1. Select the **Misc** tab
2. In the **Fraction of Organic Carbon** box, type `0.005`

Click **OK** to exit the **Additional Material Data** dialog.

Click **OK** again to save your settings and exit the **Material Data** dialog.

Initial Conditions

You can control the initial state of the primary variables using initial conditions. Primary variable selection will depend on several factors including EOS selection, simulator mode, and the initial state of the simulation. You can edit initial conditions globally and on a cell-by-cell basis.

To edit global initial conditions: on the **Properties** menu, click **Initial Conditions...**

For this example, we will initialize all cells to a two-phase water and air state. There is no initial chlorobenzene saturation. To set the initial conditions:

1. Select the **Two-Phase Water/Air** state option
2. In the **Pressure** box, type `101325.0`
3. In the **Temperature** box, type `10.0`
4. In the **Water Saturation** box, type `0.25`

5. In the **VOC Mole Fraction in Air** box, type `0.0`

6. Click **OK**

Boundary Conditions

We will inject chlorobenzene into the model using a cell-specific initial condition. Then we will force the state of that cell to remain constant. To edit individual cells, you can use the **Grid Editor**.

To open the **Grid Editor**: on the **Model** menu, click **Edit Grid** (or click on the toolbar).

Every cell in the model has a unique ID number. You can find and select cells based on their ID number using the **Find** field in the upper-right corner of the **Grid Editor**. In this example, cell 1 will be the chlorobenzene source. To find and select cell 1:

1. In the **Find** box, type `1`

2. Press `ENTER`. The cell should be selected and shown in the center of the grid editor.

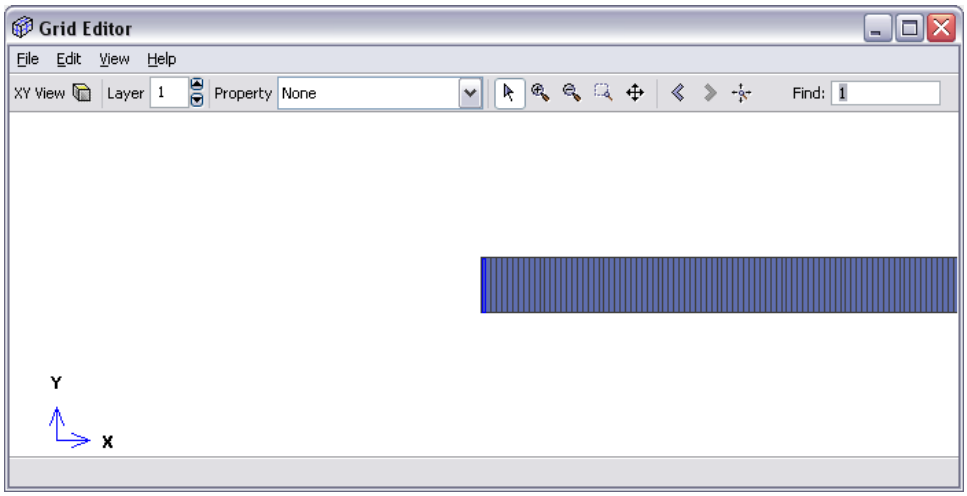

Figure 9.4. Finding a Cell in the Grid Editor

You can now edit the properties of cell 1. Ensure cell 1 is selected. On the **Edit** menu, click **Properties...**

To force the state of this cell to remain constant throughout the simulation, you can adjust its type. Select the **Properties** tab. Then, in the **Type** list, select **Fixed State**.

Now you can give the cell a custom initial condition that will remain constant throughout the simulation. Select the **Initial Conditions** tab. To enter the custom ini-

tial conditions:

1. Select **Specify Initial Conditions by Cell**
2. Select the **Three-Phase Water/Air/NAPL** state
3. In the **Water Saturation** box, type `0.2`

Notice that we did not explicitly specify a NAPL saturation. With the gas saturation at `0.75` and the water saturation at `0.2` the NAPL saturation will be `0.05`. T2VOC will perform this calculation during the simulation.

Click **OK** to close the **Edit Cell Data** dialog

On the **File** menu, click **Close** to exit the grid editor.

Solution Controls

We will now adjust the time step T2VOC will use while executing the simulation. Options relating the time step and other simulation options can be found in the **Solution Controls** dialog.

To open the **Solution Controls** dialog: on the **Analysis** menu, click **Solution Controls...** (or click  on the toolbar).

For this example, we will adjust the end time, increase the maximum number of time steps, and limit the size of the maximum time step.

1. In the **End Time** box, type `3.1558e7`
2. In the **Max Num Time Steps** box, type `350`
3. In the **Max Time Step** list, select **User Defined**
4. In the **Max Time Step** box, type `4.32e5`

Click **OK** to exit the **Solution Controls** dialog.

Output Controls

By default, T2VOC will print output every 100 time steps. We can increase the resolution of the output with the **Output Controls** dialog.

1. On the **Analysis** menu, click **Output Controls...** (or click  on the toolbar).
2. In the **Print and Plot Every # Steps** box, type `5`
3. Click **OK** to exit the **Output Controls** dialog.

Save and Run

The input is complete and you can now run the simulation. Bear in mind that T2VOC generates many output files and they will overwrite the output from any previous simulations in a directory. If you haven't already, you may want to save your model in a directory specifically intended for the simulation results. For example:

1. On the **File** menu, click **Save** (or click on the toolbar).

2. Create a new folder named **T2VOC Problem 1** and in the **File Name** box, type **t2voc_prob1.sim**.

3. Click **Save**.

To run the simulation, on the **Analysis** menu, click **Run TOUGH2** (or click on the toolbar).

During the solution, a graph will display the time step size. In this case, the time steps increase until they remain constant at the specified maximum.

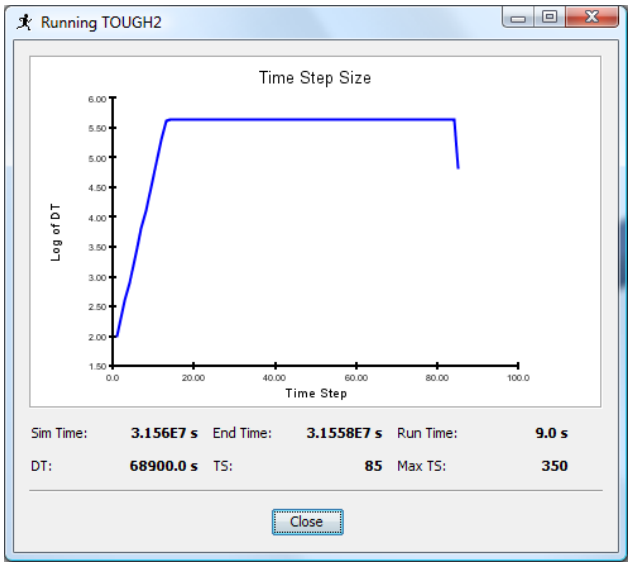

Figure 9.5. Running T2VOC

View 3D Results

To view the 3D results for a simulation

1. On the **Results** menu, click **3D Results** (or click on the toolbar). The data for the current simulation will be automatically loaded and displayed.

To view the VOC concentration for the last time step

1. In the **Time(s)** list, select the last entry (**3.156E7**).

2. In the **Scalar** list, select **CVOCGAS**.

3. Click to clear the **Show Isosurfaces** checkbox.

To add a slice plane on which contours will be displayed, click **Slice Planes...**. For this example we will show one slice plane. To configure the slice plane

1. In the **Axis** list, select **Z**.

2. In the **Coord** box, type `0.5`.

3. Ensure that the **Scalar** check box is checked.

4. Click **Close**.

Your results should now look similar to the screenshot in Figure 9.6. You can now see the gas-phase VOC concentration emanating from the left side of the model.

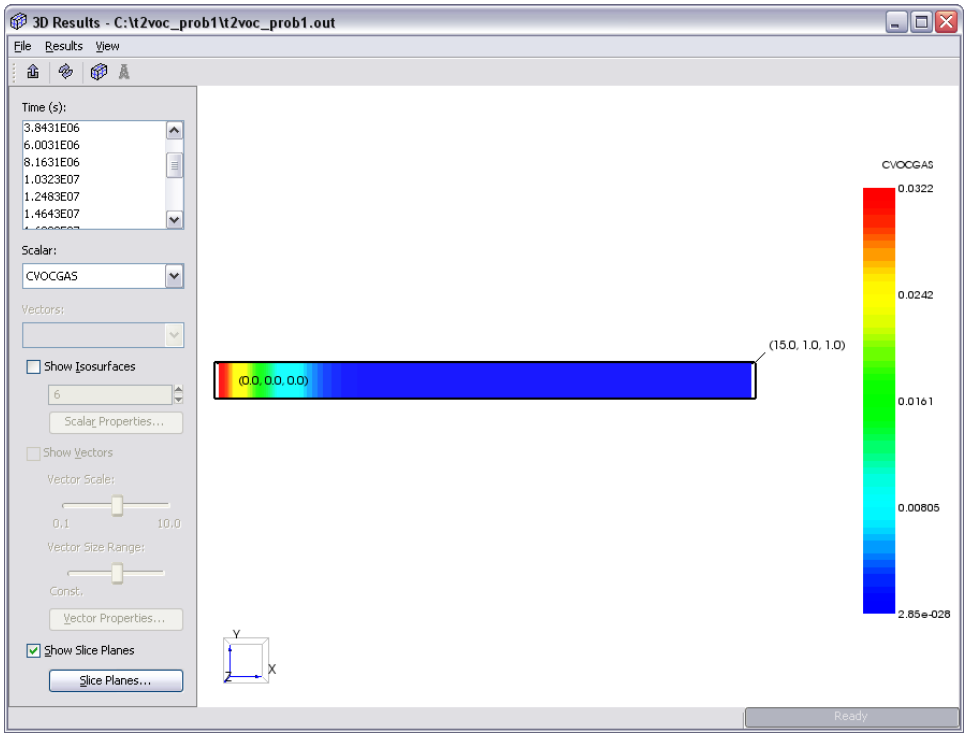

Figure 9.6. T2VOC 3D Results

Close the **3D Results** window.

References

[Pruess, Oldenburg, and Moridis, 1999] Karsten Pruess, Curt Oldenburg, and George Moridis. *TOUGH2 User's Guide, Version 2.0*. November, 1999. Earth Sciences Division, Lawrence Berkeley National Laboratory. Berkeley CA USA . LBNL-43134.

[Pruess and Garcia, 2002] Karsten Pruess and J. Garcia. *Solutions of Test Problems for Disposal of CO2 in Saline Aquifers*. December, 2002. Earth Sciences Division, Lawrence Berkeley National Laboratory. Berkeley CA USA . LBNL-51812.

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[Xu, Sonnenthal, Spycher, and Pruess, 2004] Tianfu Xu, Eric Sonnenthal, Nicolas Spycher, and Karsten Pruess. *TOUGHREACT User's Guide: A Simulation Program for Non-isothermal Multiphase Reactive Geochemical Transport in Variably Saturated Geologic Media*. September, 2004. Earth Sciences Division, Lawrence Berkeley National Laboratory. Berkeley CA USA . LBNL-55460.