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# User Manual

## PetraSim 2022

# PetraSim User Manual

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# Disclaimer

RockWare makes no warranty, expressed or implied, to users of PetraSim, and accepts no responsibility for its use. Users of PetraSim assume sole responsibility under Federal law for determining the appropriateness of its use in any particular application; for any conclusions drawn from the results of its use; and for any actions taken or not taken as a result of analyses performed using these tools.

Users are warned that PetraSim is intended for use only by those competent in the field of multi-phase, multi-component fluid flow in porous and fractured media. PetraSim is intended only to supplement the informed judgment of the qualified user. The software package is a computer model that may or may not have predictive capability when applied to a specific set of factual circumstances. Lack of accurate predictions by the model could lead to erroneous conclusions. All results should be evaluated by an informed user.

Throughout this document, the mention of computer hardware or commercial software does not constitute endorsement by RockWare, nor does it indicate that the products are necessarily those best suited for the intended purpose.

# 1. Getting Started

## Welcome

PetraSim is an interactive pre-processor and post-processor for the TOUGH family of codes. It helps users rapidly develop models and view results for these general-purpose simulators which model nonisothermal flows of multicomponent, multiphase fluids in porous and fractured media. The T2VOC and TMVOC simulators include three-phase flows of water, air, and volatile organic chemicals. The TOUGHREACT simulator adds chemical reactions.

## Installation

A PetraSim installer can be obtained at http://www.rockware.com/ by searching for "PetraSim".

You must install PetraSim with administrator privileges. If your current account is not an administrator account, use the Run as Administrator option on the right-click menu.

## Included and Third-Party Simulators

PetraSim includes the capability to run TOUGH2, TMVOC, and TOUGHREACT v1.2 simulations without installing any additional software.

For other simulator modes, including TOUGH2-MP, TOUGH v2.1, TOUGH3, TOUGHREACT v2.0, and TOUGHREACT v3.32, the corresponding simulator EXE must be purchased separately though Lawrence Berkeley National Labs. This simulator EXE can then be copied into a specific folder, where it will be used by the Run action in PetraSim. The locations where PetraSim expects to find simulator EXEs are listed in Appendix B. Alternately, PetraSim can be used to generate the necessary input files and custom simulators can be run manually through a command line. TOUGH3 simulations must be run from a command line.

## Software Registration

When you purchase a license, you will receive a key that activates the software. You must enter this key in the **Licensing and Activation** dialog. To activate your license using Online Activation:

1. Start PetraSim. If the installation of PetraSim is not currently licensed, the **Licensing and Activation** dialog will automatically appear and you can skip to step 3.
2. On the **Help** menu, click **License…**
3. Select the **License File** option.
4. Click the **Online** button.
5. Enter your **Activation key** into the **Key** box shown in Figure 1-1.
6. Click the **Activate** button.

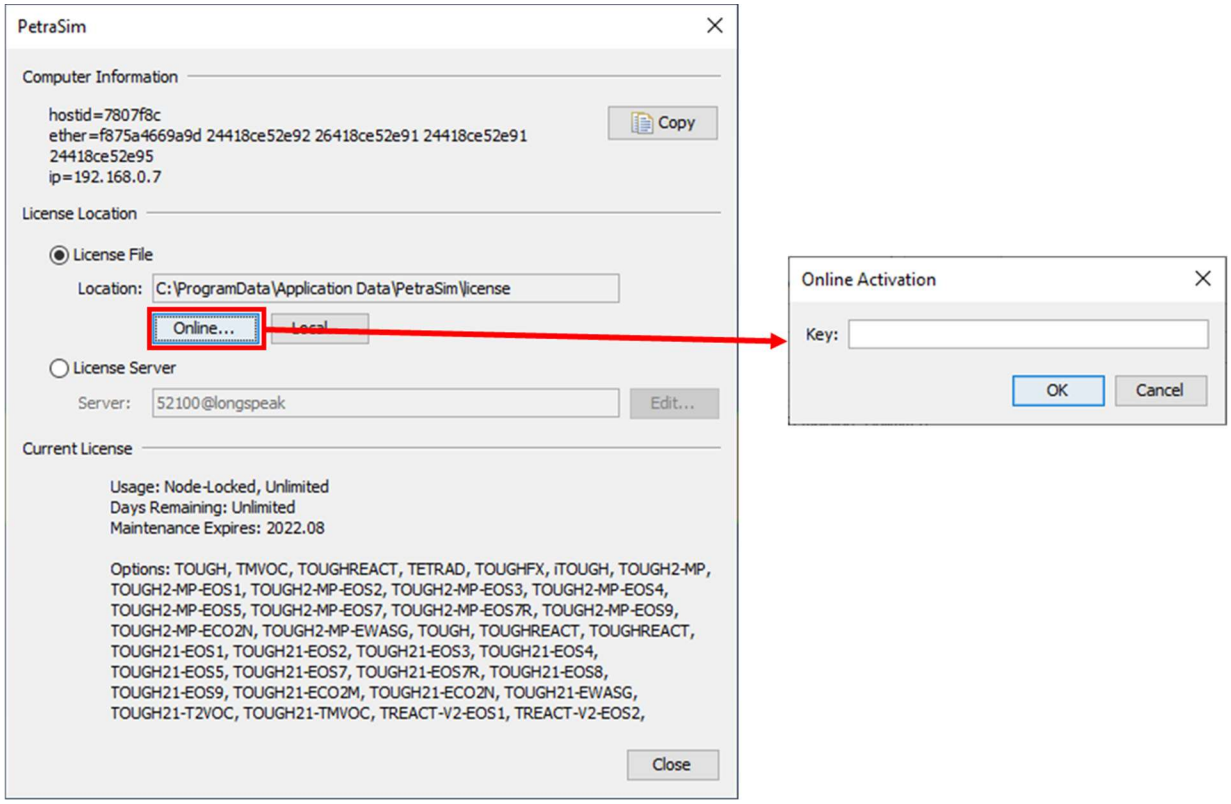


**Figure 1-1: Licensing and Activation dialog**

## Additional TOUGH Documentation

In preparing this manual, we have liberally used descriptions from the user manuals for the TOUGH family of codes. Links to download the TOUGH manuals are given at https://www.rockware.com/petrasim-documentation/. More information about the TOUGH family of codes can be found at: https://tough.lbl.gov/.

## System Requirements

PetraSim will run well on any newer computer. At a minimum, the processor should be at least as fast as a 1 GHz Pentium III, with at least 512 MB RAM. A graphics card that supports OpenGL 1.1 or later with 64 MB of graphics memory is recommended.

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# 2. Background

## Flow in Porous Media

This section will provide only the briefest overview of the basic assumptions used in the TOUGH family of codes. The reader is referred to the TOUGH User's Guide (1), the T2VOC User's Guide (2), the TMVOC User's Guide (3), the TOUGHREACT User's Guides (4) and (20), and the TOUGH3 User's Guide (5) for detailed information on the TOUGH codes.

A good fundamental reference on flow in porous media is *The Physics of Flow Through Porous Media* (6).

### Darcy's Law for Single Phase Flow

The TOUGH family of codes (and thus PetraSim) simulates flow in porous media. A basic assumption is that the flow is described by Darcy's law,

$$\boldsymbol{u} = -\frac{k}{\mu}(\nabla p - \rho \boldsymbol{g})$$

where $\boldsymbol{u}$ is the seepage velocity vector, $k$ is the total permeability, $\mu$ the viscosity, $p$ the pressure, $\rho$ the density, and $\boldsymbol{g}$ is the gravity vector.

### Multi-Phase Flow

As described by Scheidegger (6), when two (or more) immiscible fluids or phases exist simultaneously in a porous medium one phase will generally wet the solid. There are in general three saturation regimes:

- Saturation regime: The porous medium is completely saturated with one phase.
- Pendular regime: The porous medium has the lowest possible saturation with one phase. This phase occurs in the form of pendular bodies throughout the porous medium. These pendular bodies do not touch each other so that there is no possibility of flow for that phase; see Figure 2-1 (a).
- Fenicular regime: The porous medium exhibits an intermediate saturation with both phases. If the pendular bodies of the pendular regime expand through addition of the corresponding fluid, they eventually become so large that they touch each other and merge. The result is a continuous network of both phases across the porous medium. It is thus possible that simultaneous flow of both phases occurs along tortuous paths; see Figure 2-1 (b).

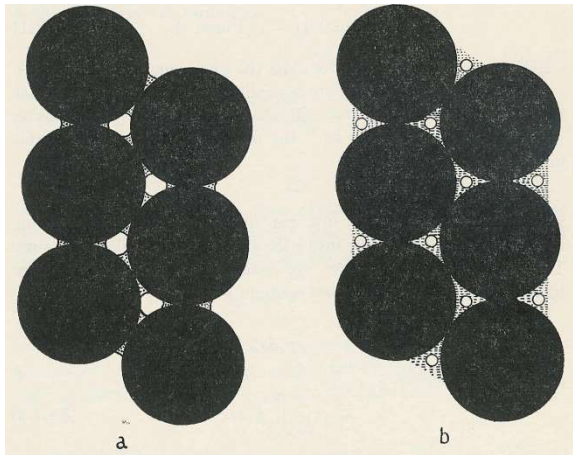



**Figure 2-1: Illustration of pendular (a) and funicular (b) saturation regime in the case of an idealized porous medium consisting of packed spheres (7)**

For multi-phase flow, Darcy's law is modified to introduce the concept of relative permeability:

$$\boldsymbol{u}_\beta = -k\frac{k_{\gamma\beta}}{\mu_\beta}\left(\nabla p_\beta - \rho_\beta \boldsymbol{g}\right)$$

where $\beta$ indicates the phase, $k_{\gamma\beta}$ is the relative permeability (between 0 and 1) for the phase, and

$$p_\beta = p + p_{c\beta}$$

is the fluid pressure in the phase, which is the sum of the pressure in a reference phase (usually the gas phase) and the capillary pressure $p_{c\beta}$ (capillary pressure is negative).

### *Relative Permeability*

The TOUGH codes provide several options for relative permeability. A typical option is the use of Corey's curves (8) as illustrated in Figure 2-2. At low liquid saturation, the gas relative permeability is 1.0 and the liquid permeability is very low. Conversely, at high liquid saturation the gas relative permeability is very low and the liquid permeability is 1.0. This is consistent with the flow regimes as described above.

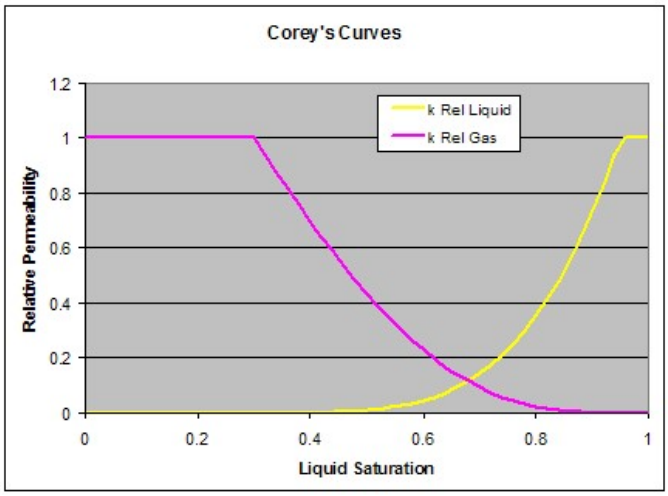



**Figure 2-2: Capillary Pressure**

### *Capillary Pressure*

The TOUGH codes also provide several options for capillary pressure. A typical option is the van Genuchten function (9) as illustrated in Figure 2-3. At low liquid saturation, the capillary pressure is large, but rapidly becomes smaller as liquid saturation increases.

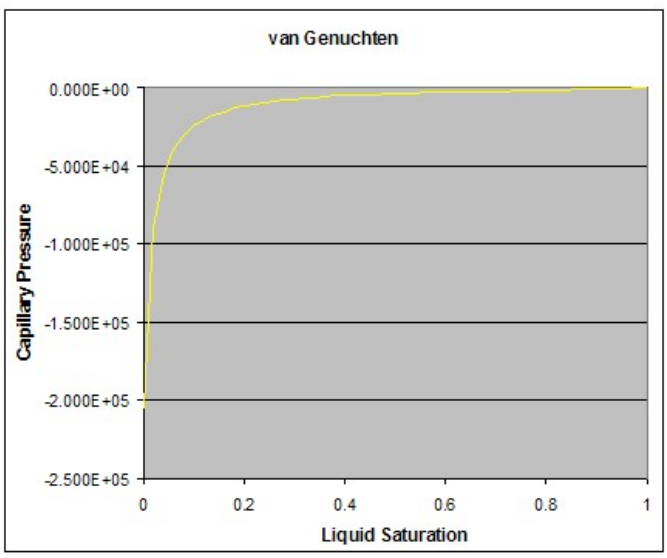



**Figure 2-3: Capillary pressure using van Genuchten function**

# TOUGH Concepts

## Components and Phases

A clear understanding of the terms **component** and **phase** is necessary when using the TOUGH codes. Consider a system consisting of water and air (implemented as EOS3 in TOUGH2). This system consists of two components (water and air) and will have two phases (liquid and gas).

Importantly, the two components (water and air) can be present in both phases. The liquid phase can consist of liquid water **and** dissolved air. Similarly, the gaseous phase can be comprised of gaseous air **and** water vapor.

For single phase conditions, the thermodynamic state is defined by pressure, temperature, and air mass fraction. If the single phase is liquid, then the air mass fraction will be the air dissolved in the water, which is a small value. An example of a valid initial condition specification for single phase liquid is shown in Figure 2-4, with pressure of 1.0E5 Pa, temperature of 20 C, and a small air mass fraction of 1.0E-5. This small amount of air will be dissolved in the water.

If the single phase is gas, the gas can consist of both water vapor and air. The air mass fraction can be as large as 1. A valid initial condition specification for single phase gas is given in Figure 2-5 with pressure of 1.0E5 Pa, temperature of 20 C, and air mass fraction of 0.999. This means that a small amount of the gas will consist of water vapor.

For two phase conditions, the thermodynamic state is defined by gas phase pressure, gas saturation, and temperature. An example of a two-phase initial condition is given in Figure 2-6, with pressure of 1.0E5 Pa, temperature of 20 C, and gas saturation of 0.5.

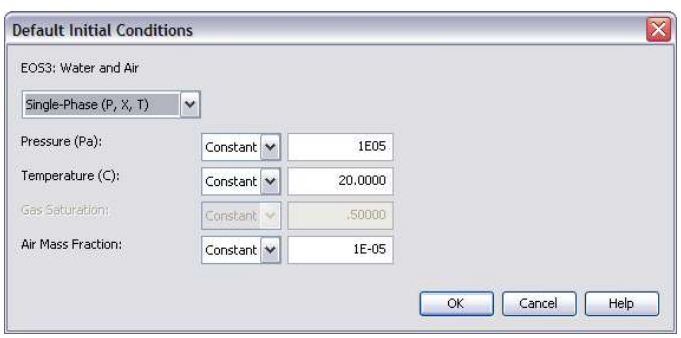



**Figure 2-4: Single phase liquid initial conditions for EOS3**

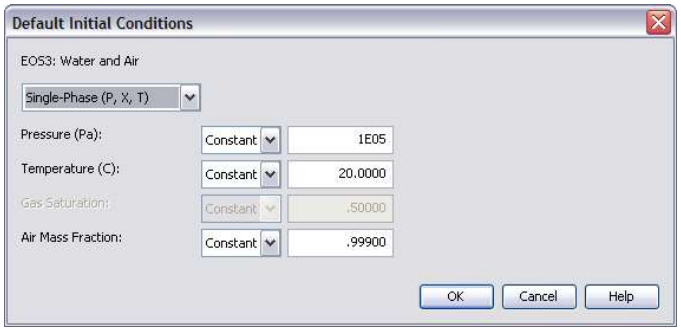



**Figure 2-5: Single phase gas initial conditions for EOS3**

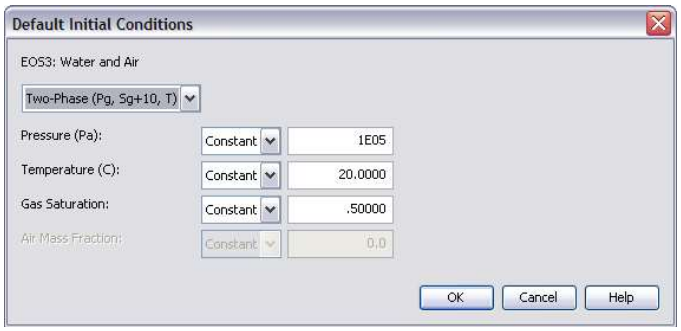



**Figure 2-6: Two phase initial conditions for EOS3**

As an example, a single element with a volume of 1 cubic meter and 0.1 porosity was run using the initial conditions given above. The resulting solution and mass fractions for each component are given below, in Figure 2-7 and Figure 2-8. The two-phase solution is of particular interest since this case provides the saturation conditions for water vapor in the gas phase and dissolved air in the liquid phase. The reader is encouraged to use single element problems when starting to use a new equation of state (EOS).

| State | P (Pa) | T (C) | Gas Saturation | Liquid Saturation | Mass Frac. Air in Gas | Mass Frac. Air in Liq. | Perm. Modifier | Density Gas | Density Liquid |
|---|---|---|---|---|---|---|---|---|---|
| Single Phase Liquid | 1.000E+05 | 20.000 | 0.000 | 1.000 | 0.000 | 0.000 | 1.000 | 0.000 | 998.320 |
| Single Phase Gas | 1.000E+05 | 20.000 | 1.000 | 0.000 | 0.999 | 1.605E-05 | 1.000 | 1.187 | 0.000 |
| Two Phase | 1.000E+05 | 20.000 | 0.500 | 0.500 | 0.985 | 1.570E-05 | 1.000 | 1.177 | 998.300 |

**Figure 2-7: States corresponding to the three initial condition options**

| State | Phase Volumes in Place ($m^3$) | | Mass in Place (kg) | | | | |
|---|---|---|---|---|---|---|---|
| | Gas | Liquid | Gas | Liquid | Air | Vapor | Liquid Water |
| Single Phase Liquid | 0.000 | 0.100 | 0.000E+00 | 9.983E+01 | 9.983E-04 | 0.000E+00 | 9.983E+01 |
| Single Phase Gas | 0.100 | 0.000 | 1.187E-01 | 0.000E+00 | 1.186E-01 | 1.187E-04 | 0.000E+00 |
| Two Phase | 0.050 | 0.050 | 5.888E-02 | 4.992E+01 | 5.880E-02 | 8.645E-04 | 4.992E+01 |

**Figure 2-8: States corresponding to the three initial condition options**

In TOUGH2, water properties are represented by the steam table equations as given by the International Formulation Committee (10) and IAPWS-IF97. Air is approximated as an ideal gas, and addititivity is assumed for air and vapor partial pressures in the gas phase. The viscosity of air-vapor mixtures is computed from a formulation given by Hirshfelder et al. (11). The solubility of air in liquid water is represented by Henry's law.

Because of the detailed physics that are included in the TOUGH codes, setting of multi-phase initial conditions requires detailed understanding of the problem. For help in setting mixture conditions, the user may refer to a thermodynamics text, such as (12).

### Mass and Energy Balance

As described in the TOUGH2 manual, the basic mass and energy balance equations solved by TOUGH2 can be written in the general form:

$$\frac{d}{dt}\int_{V_n} M^K dV_n = \int_{\Gamma_n} \boldsymbol{F}^K \bullet \boldsymbol{n} d\Gamma_n + \int_{V_n} q^K d\, V_n$$

The integration is over an arbitrary subdomain $V_n$ of the flow system under study, which is bounded by the closed surface $\Gamma_n$. The quantity $M$ appearing in the accumulation term (left hand side) represents mass or energy per volume, with $K$ labeling the mass components and an extra heat "component" if the analysis is nonisothermal. $\boldsymbol{F}$ denotes mass or heat flux and $q$ denotes sinks and sources. $\boldsymbol{n}$ is a normal vector on surface element $d\Gamma_n$, pointing inward to $V_n$.

The user should consult Appendix A of the TOUGH2 User's Guide (1) for a further discussion of this topic.

### Spatial Discretization

As described in the TOUGH2 User's Manual, the continuum equations are discretized in space using the integral finite difference method (IFD), (13) and (14). Introducing appropriate volume averages, we have

$$\int_{V_n} M dV = V_n M_n$$

where $M$ is a volume-normalized extensive quantity, and $M_n$ is the average value of $M$ over $V_n$. Surface integrals are approximated as a discrete sum of averages over surface segments $A_{nm}$:

$$\int_{\Gamma_n} \boldsymbol{F}^K \bullet \boldsymbol{n} d\Gamma_n = \sum_m A_{nm} F_{nm}$$

Here $F_{nm}$ is the average value of the (inward) normal component of $F$ over the surface segment $A_{nm}$ between volume elements $V_n$ and $V_m$. The discretization approach used in the integral finite difference method and the definition of the geometric parameters are illustrated in Figure 2-9.

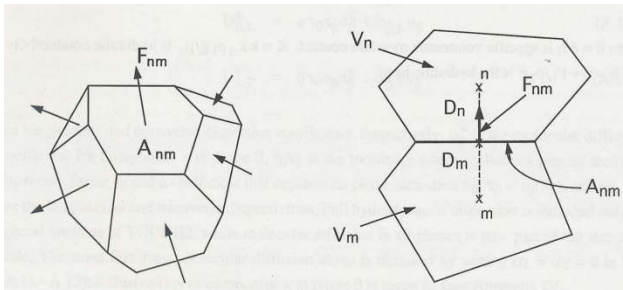



**Figure 2-9: Space discretization and geometry data in the integral finite difference method (from TOUGH2 User's Guide)**

The discretized flux is expressed in terms of averages over parameters for elements $V_n$ and $V_m$. For the basic Darcy flux term, we have

$$F_{\beta nm} = -k_{nm}\left[\frac{k_{r\beta}\rho_\beta}{\mu_\beta}\right]_{nm}\left[\frac{P_{\beta,n} - P_{\beta,m}}{D_{nm}} - \rho_{\beta,nm}g_{nm}\right]$$

Where the subscripts $(nm)$ denote a suitable averaging at the interface between grid blocks $n$ and $m$ (interpolation, harmonic weighting, upstream weighting). $D_{nm} = D_n + D_m$ is the distance between the nodal points $n$ and $m$, and $g_{nm}$ is the component of gravitational acceleration in the direction from $m$ to $n$.

The user should consult Appendix B of the TOUGH2 User's Guide (1) for a further discussion of this topic.

### Temporal Discretization

Substituting the volume averaged quantities and surface integral approximations into the mass and energy balance, a set of first-order ordinary differential equations in time is obtained.

$$\frac{dM_n^K}{dt} = \frac{1}{V_n}\sum_m A_{nm}F_{nm}^K + q_n^K$$

Time is discretized as a first order finite difference, and the flux and sink and source terms on the right-hand side are evaluated at the new time, to obtain the numerical stability needed for an efficient calculation of multiphase flow.

The user should consult Appendix B of the TOUGH2 User's Guide (1) for a further discussion of this topic.

## Equations of State

As described in the TOUGH2 User's Guide, the thermophysical properties of fluid mixtures needed for assembling the governing mass- and energy-balance equations are provided by "equation-of-state" (EOS) modules. Each EOS uses a different set of primary variables (such as pressure, temperature, and mass fractions) to define each possible phase condition.

PetraSim supports the following EOS options in TOUGH2 and TOUGH3 (Figure 2-10). PetraSim also supports TOUGHREACT and TMVOC.

| EOS | Description |
|---|---|
| 1 | Water, water with tracer |
| 2 | Water and CO2 |
| 3 | Water and air |
| 4 | Water and air with vapor pressure lowering |
| 5 | Water and hydrogen |
| 7 | Water, brine and air |
| 7C* | Water, brine, $CO_2$ (or $N_2$), gas tracer, $CH_4$ |
| 7R | Water, brine, two radionuclides and air |
| 8 | Water, "dead" oil, non-condensible gas |
| 9 | Saturated-unsaturated flow (used for vadose zone) |
| EWASG | Water, NaCl, non-condensible gas |
| ECO2N | Water, brine, and CO2 for sequestration studies |
| ECO2M* | Water, NaCl, CO2, including transitions between super- and sub-critical conditions, and phase change between liquid and gaseous CO2 |
| *Requires ownership of TOUGH v2.1 or TOUGH3 | |

**Figure 2-10: States corresponding to the three initial condition options**

## Selecting an EOS

There can be only one EOS in an analysis at a time. The EOS can be specified when creating a new model or changed while working on the model.

To specify the EOS when creating a new model, select **File->New…**. The **New Model** dialog will appear, as shown in Figure 2-11. First select the desired simulator mode on the left. Depending on the mode chosen, different EOS options will be enabled on the right. Select the desired EOS on the right and then click **OK** to create the new model with the chosen EOS.

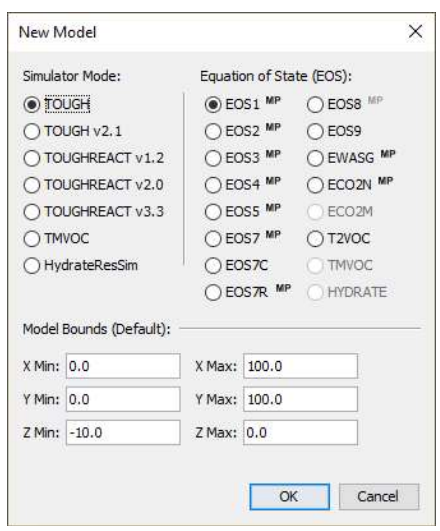



**Figure 2-11: New Model dialog**

To change the EOS while working on a model, from the **Properties** menu choose **Global Properties**. Click **Change EOS…** as shown in Figure 2-12.

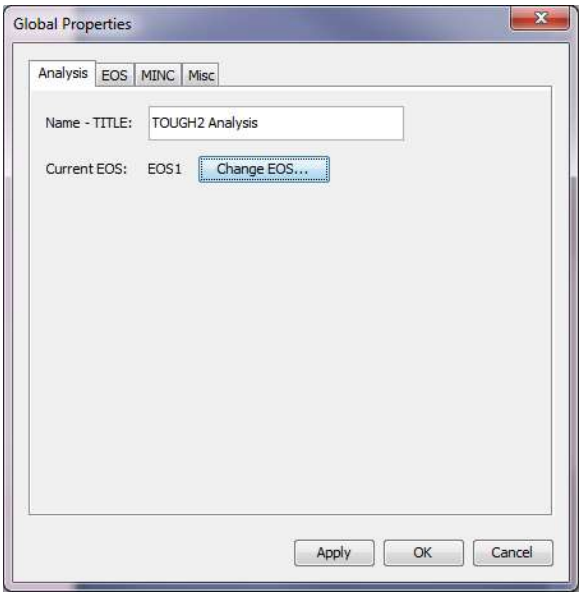



**Figure 2-12: Global Properties dialog**

*NOTE:* While it is possible to change the EOS while working on a model, this is discouraged. PetraSim does not have a reliable way to re-interpret state variable information. For example, consider a model where you are using EOS1 and have set the default initial condition to be two-phase (Pg, Sg, X), then you change EOS to EOS7R [which contains more state variables, e.g. single-phase (P, Xb, Xrn1, Xrn2, Xair, T)].

Rather than attempt to guess the user's intent, PetraSim behaves defensively. Initial conditions will be set to single-phase mode and some primary variable values will be carried over. In this case gas-phase pressure will be copied into the value for pressure and the tracer mass fraction will be copied over to the brine mass fraction. All other values will be the defaults. With the exception of pressure and temperature, this mapping is entirely dependent on the internal numbering of the state variables and does not necessarily follow a particular pattern. After changing EOS, you should always re-check any EOS-related settings.

## Global Properties

Each EOS has different options that define the assumptions used in the analysis. For EOS3, this includes whether to include heat transfer (isothermal or non-isothermal) and whether to include molecular diffusion. These options are selected by selecting **Properties->Global Preferences...** or on the toolbar. On the **EOS** tab all available options will be displayed.

## Details for Each EOS

The user is referred to the TOUGH2 User's Guide (1) or TOUGH3 User's Guide (5) for detailed descriptions of the options available for each EOS.

# 3. PetraSim at a Glance

## Main Window

The main window contains a 3D design view of the model (3D Model View) which can be used to visualize and edit simulator input.

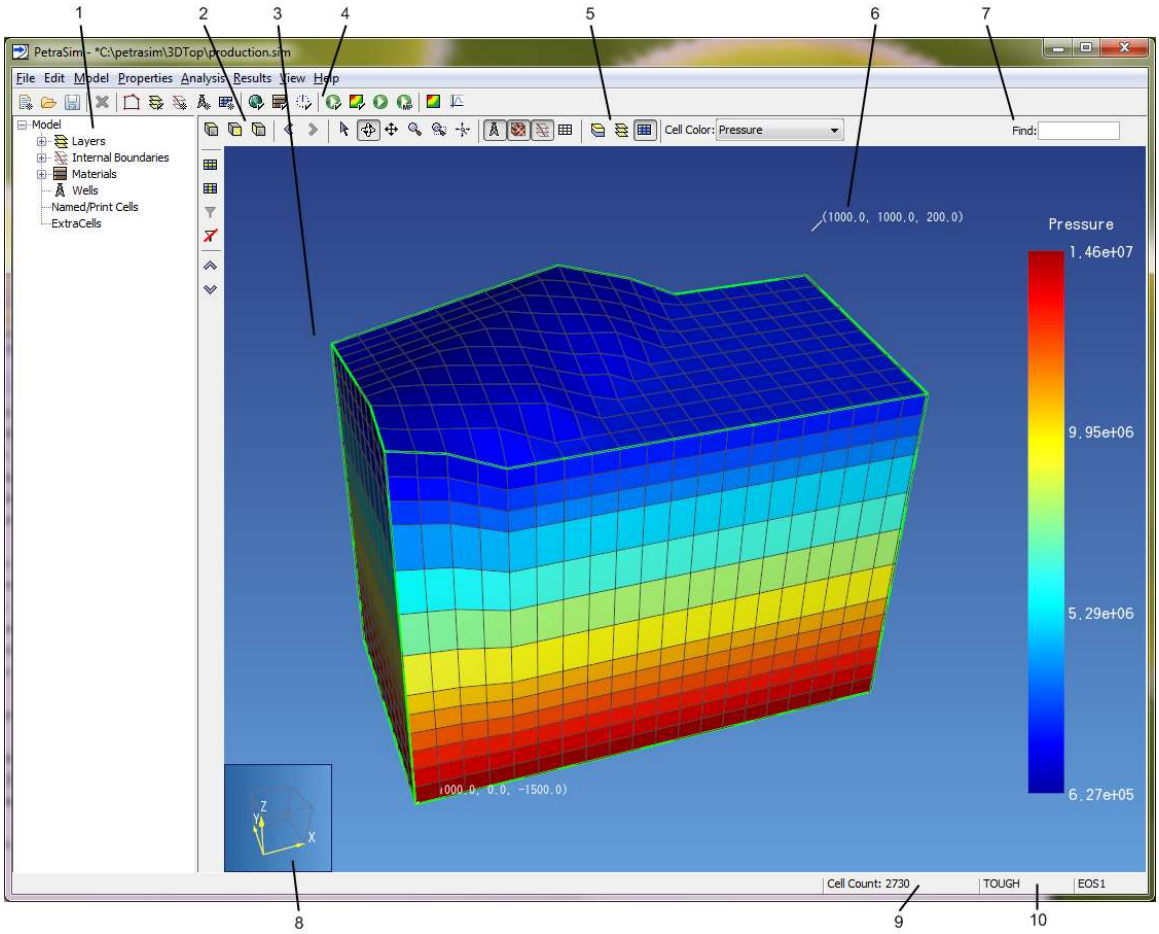



**Figure 3-1: Main Window**

1. **Navigation Tree** – Use this to quickly identify and manage items in your model.
2. **View** - Click to reset the 3D Model View to top, front, or side views.
3. **3D Model View** – Use this to visualize and interact with the structure of your model in 3D. This view is also used to edit mesh cells.
4. **Toolbar** – The toolbar provides quick access to the steps required to define, run, and post-process an analysis.
5. **View Mode** – Use this to switch between viewing the conceptual model with layer sides on or off or viewing the solution mesh. This is also used to color regions or cells by different properties.
6. **3D Labels** - Add 3D labels to help keep track of model features. Labels are added automatically when you add wells and when you create a model.

7. **Find** – Use this to find cells by name or id.
8. **Axis Legend** – To ensure that you never become disoriented, the axis legend rotates with your model and always displays the x, y, and z axes.
9. **Cell Count** – Use the cell count display to see how many cells are in your model.
10. **Simulator** – Display the current simulator and EOS.

## 3D Results View

You can use the 3D Results View to visualize properties of your model as they evolved over time.

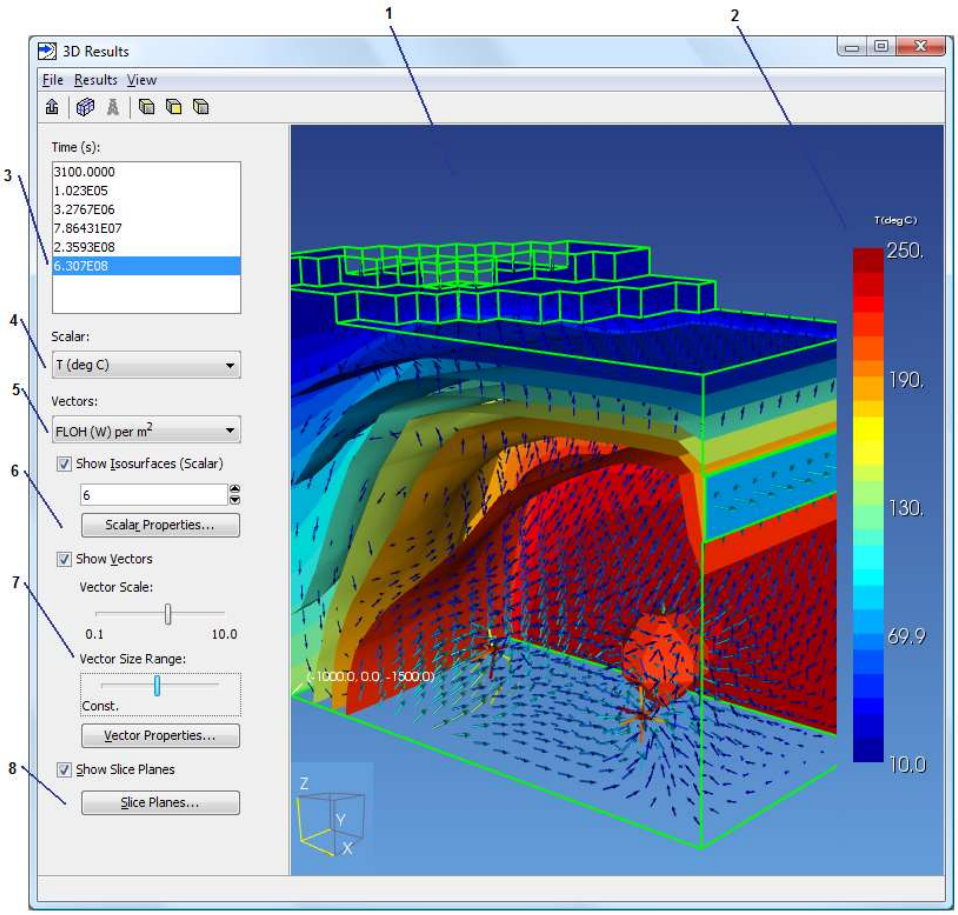



**Figure 3-2: 3D Results View**

1. **3D Results Display** – Contours, vectors, and slice planes are shown against an outline of your model. You can also make high-resolution screen shots for publications or presentation graphics.
2. **Scalar Legend** – The scalar legend shows what colors were used to display scalar quantities. You can also double-click the legend to define the range and number of colors.
3. **Time List** – Click a time step to view the results data at that time during the simulation.
4. **Scalar Property** – Select a scalar property, such as temperature or pressure) to display from this list. All slice planes and contours will be updated show the new property.

5. **Vector Property** – Select a vector property (such as water flow rate) to display from this list. All vectors will be updated to show the new property.
6. **Isosurface Controls** – Change the number of isosurfaces and and other scalar display properties.
7. **Vector Controls** – Use sliders to scale the vectors in the 3D view.
8. **Slice Planes** – Click this to add 2D slice planes to the 3D view.

## Time History Results

You can make time history plots of individual cell data and export the data in a format for import into spreadsheets.

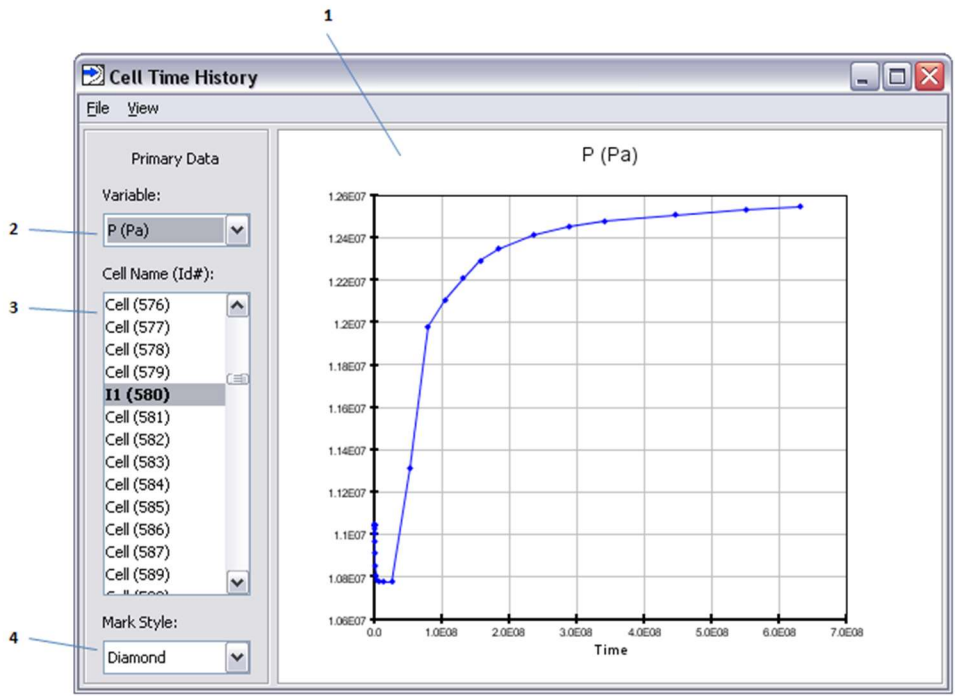



**Figure 3-3: Time History Results**

1. **Time History Results** – You can plot output data for any cell.
2. **Output Variable** – Select the output variable for plotting.
3. **Cell Selection** – Plots can be made for any cell. Named cells display the name and the cell number.
4. **Line Style** – Select the style for the graph.

## Example Problems

Examples problems for loading in PetraSim can be downloaded from the web at https://www.rockware.com/petrasim-documentation/.

# PetraSim Tour (Five Spot)

This section is a (very) quick walkthrough for one of the sample problems included with TOUGH2. The problem specification is not discussed. You can just load the data, run the simulator, and look at the results. When you are ready, follow the steps below.

## Load the EOS1 *five_spot* sample model

1. Download the resources.zip file containing five_spot.sim from https://www.rockware.com/petrasim-documentation/.
2. Extract the zip file to the desired directory.
3. Start PetraSim.
4. Under the **File** menu, click **Open…**.
5. Choose *five_spot.sim* from the extracted location, and then click **Open**.

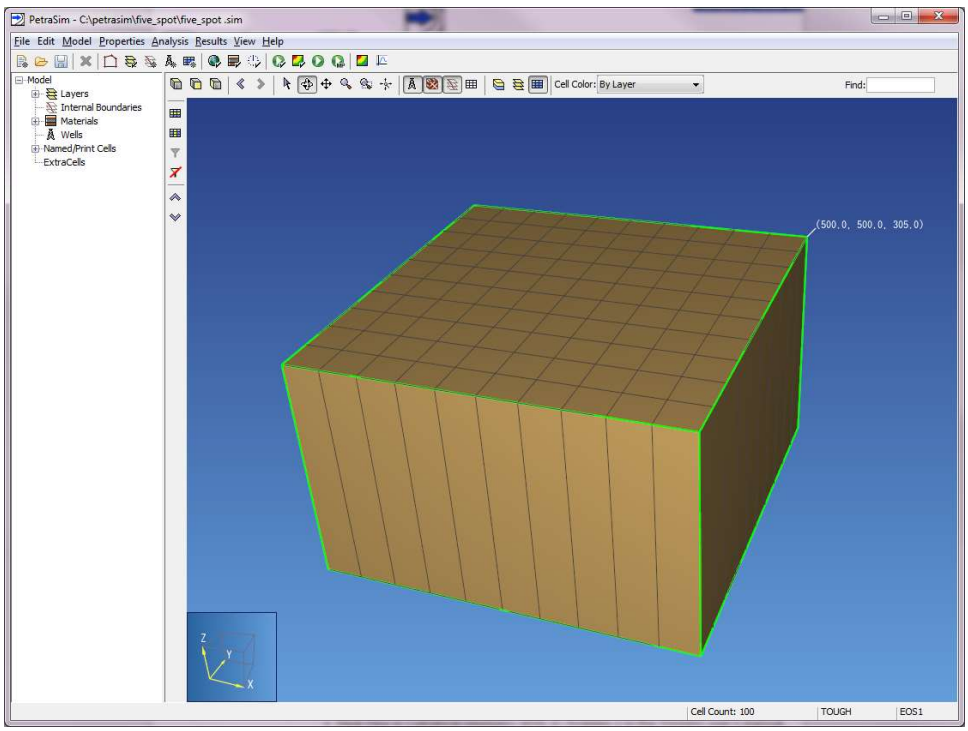



**Figure 3-4: Opening the five spot model**

## Enable flux output

1. On the **Analysis** menu, click **Output Controls…**
2. Click to select **Fluxes and Velocities**
3. Click **OK**

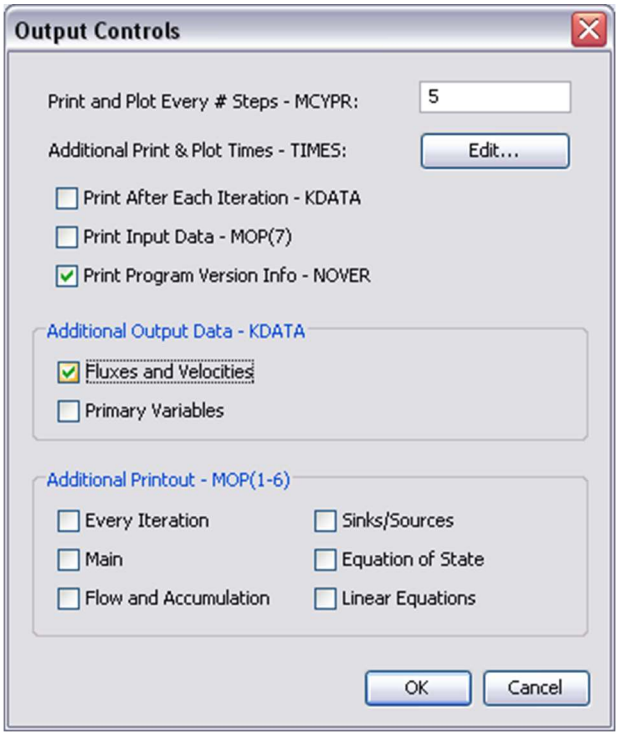



**Figure 3-5: Select fluxes and velocities output**

## Run the simulation

To run the simulation: On the **Analysis** menu, click **Run TOUGH2**.

The Running TOUGH2 dialog will open and show how the simulation is progressing. The graph displays simulation time steps on the X-axis and the log10 of the time step on the Y-axis. As a rule of thumb, an increasing Y value is a good sign of simulation progress. If your time steps start to become smaller, it may indicate that the simulator is having a difficult time converging.

When the simulation finishes (approx 10 seconds), a message will be displayed and the Cancel button will turn into a Close button. Click the **Close** button.

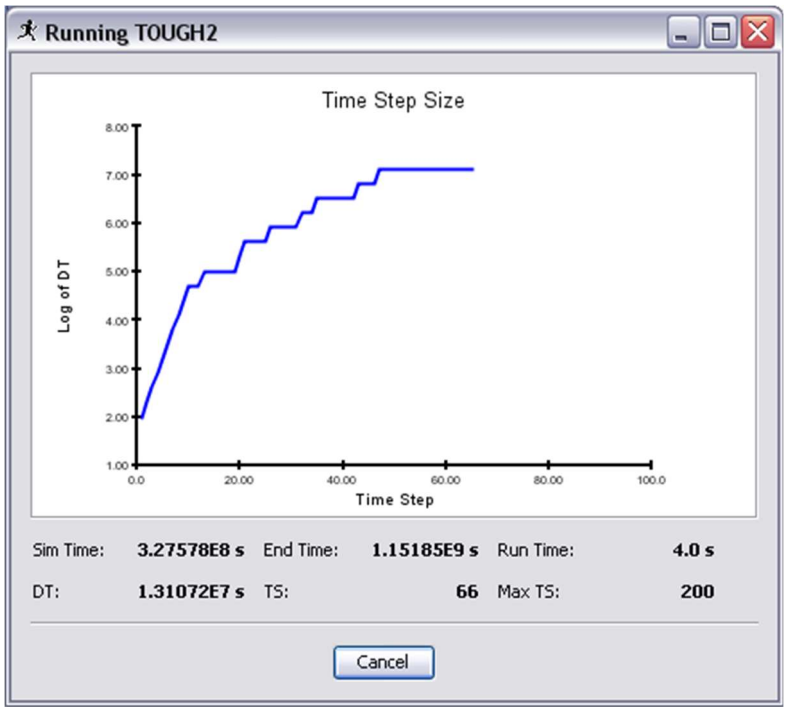



**Figure 3-6: Time step graph during simulation**

## View 3D simulation results

To view 3D simulation results: On the **Results** menu, click **3D Results...**.

Since this example problem is a 2D problem, it might be useful to add a scaling factor to the Z-axis. To scale an axis in the 3D Results:

1. On the **View** menu, click **Scale…**
2. In the **Z-Factor** box, type **0.01**
3. Click **OK**

The image below shows contour data for temperature and vectors for heat flow at the end of the simulation. When you are finished looking at the 3D results, close the 3D Results dialog and return to the PetraSim main window.

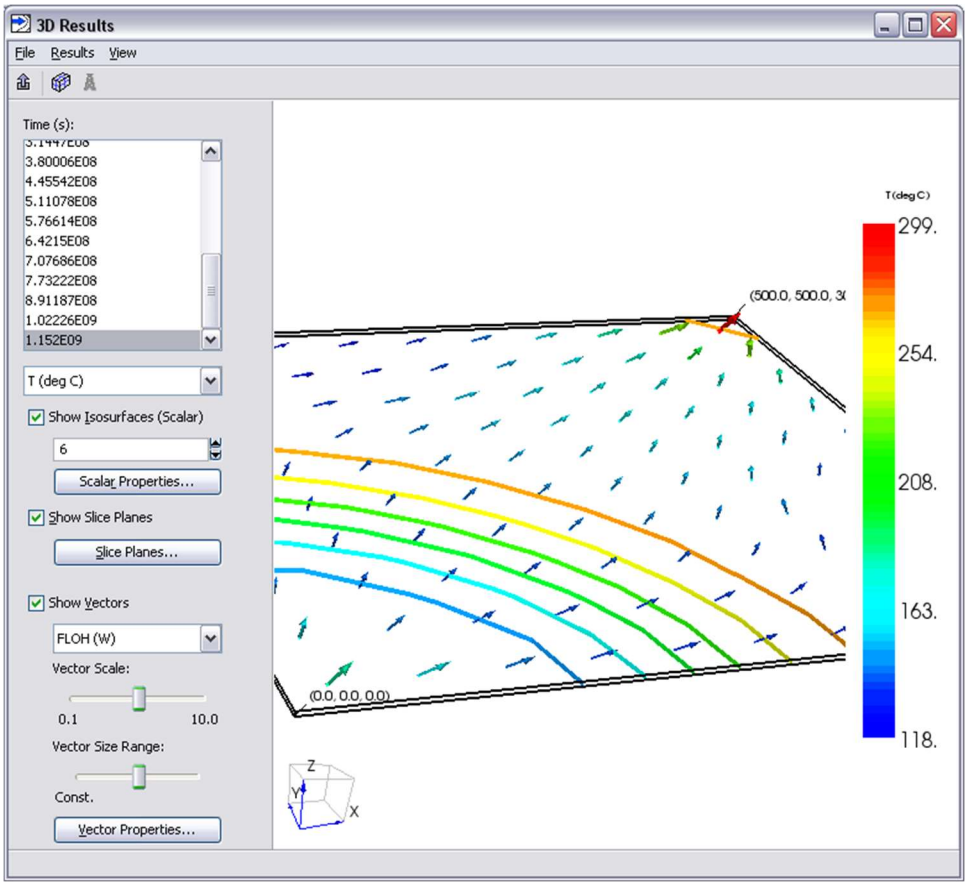



**Figure 3-7: Temperature contours and flow vectors**

## View cell time history data

To open the cell time history view: On the **Results** menu, click **Cell History Plots**.

If you ask for additional time history data for some of your cells, they will appear in bold in the cell list. In this example, the injection and production cells were marked for additional output. These cells will have a data point for each time step of the simulation. You can view the time history of the rest of your cells by selecting the **Show All** option in the **View** menu.

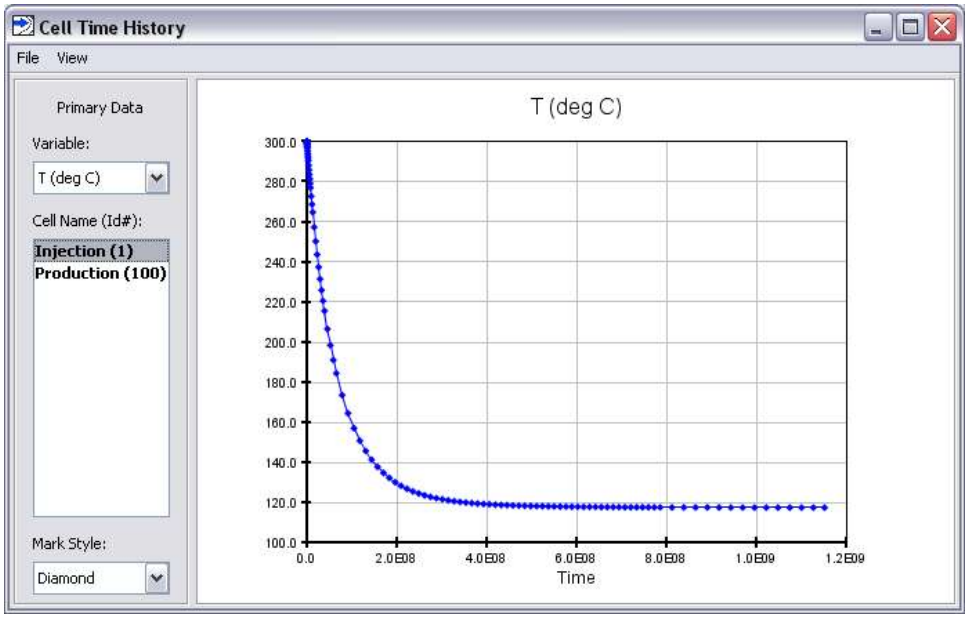



**Figure 3-8: Cell time history**

# 4. PetraSim Basics

## Work Flow in a Typical Analysis

Many problems will be run in two stages: (1) an analysis that establishes a steady state initial condition, and (2) an analysis that loads the steady state results as an initial condition and then proceeds with a transient disturbance, such as a spill or production from a reservoir. PetraSim makes it easy to load the results of a previous analysis as the starting condition of a new analysis.

The PetraSim interface helps guide the user through the steps of an analysis. These include:

- Selecting an EOS.
- Defining the problem boundaries, creating a conceptual model, and creating a mesh.
- Selecting the global options to be used in the analysis.
- Specifying the material properties.
- Defining the default initial conditions for the model, either directly or by loading the results of a previous analysis.
- Defining cell-specific data, such as material, sources, sinks, and initial conditions.
- Setting the solution and output options.
- Solving the problem.
- Post-processing of results using contour and time history plots.

The user must recognize that this process is seldom linear. It will likely be necessary to iterate as new understanding of the model and physics is obtained. New users are especially tempted to immediately proceed with a complex model. Don't do this! It is always recommended that the user perform 1D and 2D analyses before a 3D analysis.

A suite of examples taken from the TOUGH user guides is available at

https://www.rockware.com/petrasim-documentation/.

## Terminology

PetraSim divides the problem space into two sections. There is a **Conceptual Model** and a **Solution Mesh**. The **Conceptual Model** defines all the high-level features of the model, such as a model boundary, geologic layers, internal boundaries, and regions. The **Solution Mesh** defines cells and connections that divide the conceptual model into pieces for the TOUGH simulator. The conceptual model and solution mesh are further discussed in the topics, Conceptual Model and Solution Mesh.

- **Boundary** – this defines a 2D path around the problem space that limits the X,Y coordinates in the model.
- **Layers** – these define the stratification of the problem space.
- **Internal boundaries** – define surfaces that split the layers into sub-regions.
- **Regions** – sub-regions that result when a layer is split by an internal boundary. Each region can have its own set of properties parented by the layer's properties.

- **Cell** – a piece of the solution mesh that tries to conform to a portion of the conceptual model. Each cell has its own properties, such as initial conditions, sources/sinks, etc.

## PetraSim Interface

PetraSim uses multiple views to display the model and results:

- 3D View. Used to rapidly view the model, including internal boundaries and wells and define cell-specific parameters including sources and sinks and initial conditions.
- Tree View. Used to display and select regions in the model, materials, wells, and extra cells.
- 3D Plots. Used to display isosurfaces and contour plots of results.
- Time History Plots. Used to display detailed cell results as a function of time.

## 3D View

### Navigation

To navigate using the 3D model use the navigation toolbar:

- To **spin** the 3D model, select the **Orbit Tool** ( ) and left-click and hold on the model and move the mouse. The model will spin as though you have selected a point on a sphere.
- To **zoom**, hold the **Alt** key and drag the mouse vertically with the **Orbit Tool** or use the **Zoom Tool** ( ).
- To zoom to a window, use the **Zoom Box Tool** ( ).
- To **move** the model, hold the **Shift** key and drag to reposition the model in the window using the **Orbit Tool** or use the **Pan Tool** ( ).
- To **reset** the model, type "r" or click **Reset View** ( ).
- To change to a standard view, select for a **top** view, for **front** view, and for a **side** view.
- To go through the view history, use and .

### View Mode

PetraSim provides three modes for viewing the model that can be selected through the **View Mode Toolbar**:

- **Boundary Mode**: This mode shows the conceptual model with the layer sides visible as shown in Figure 4-1. Regions and layers can be selected and edited in this mode.
- **Layer Mode**: This mode shows only the conceptual model with the layer sides invisible as shown in Figure 4-2. Like the **Boundary Mode**, this mode allows regions and layers to be selected and edited.
- **Mesh Mode**: This mode shows only the solution mesh and internal boundaries and allows cells to be selected and edited, Figure 4-3.

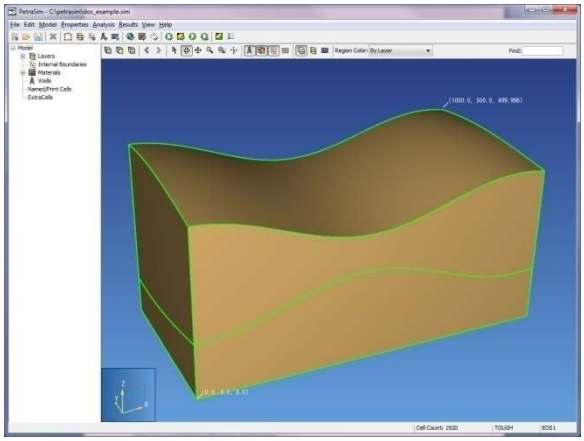


**Figure 4-1: Boundary Mode**

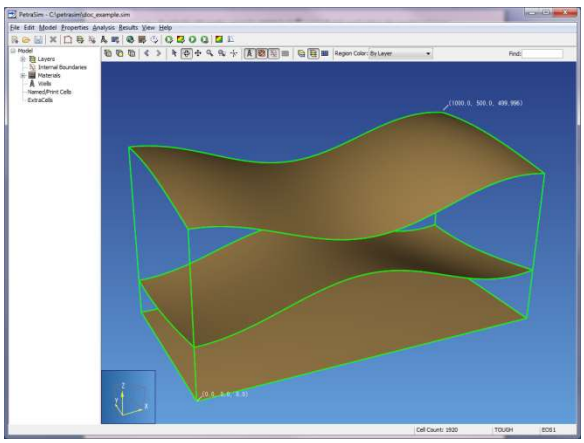


**Figure 4-2: Layer Mode**

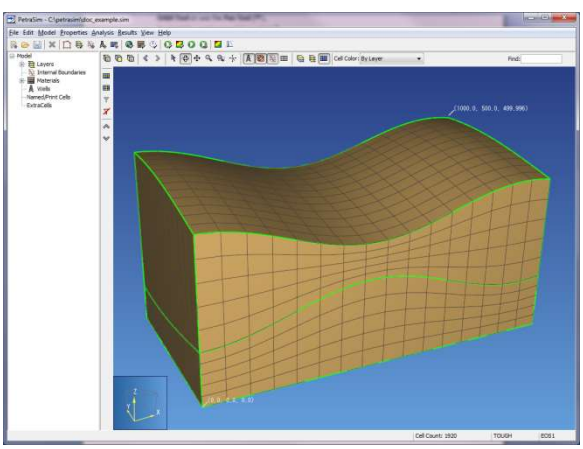


**Figure 4-3: Mesh Mode**

## Colors

Depending on the current **View Mode**, visible elements can be colored by various properties using the **Cell Color** option:

- **By Layer** – The visible cells or regions are colored by the layer to which they belong. The layer color is specified in the **Edit Layers** dialog as discussed in Defining layers with the layer manager.
- **Color Scheme** – All cells or regions are colored by the current color scheme, which can be changed under **View->Color Scheme**.
- **Material** – The cells or regions are colored by their currently set material. The material color is set in the **Edit Materials** dialog as discussed in Materials.
- **Print Flags** (only available in **Mesh Mode**) – If a cell has print flags set, the cell will be colored red, otherwise grey.
- **Fixed State** (only available in **Mesh Mode**) – If a cell is marked as Fixed State, the cell will be colored red.
- **Source/Sink** (only available in **Mesh Mode**) – If a cell is marked as a Source or Sink, the cell will be colored red.
- **All others** – All other properties come from the boundary conditions and material values for the element and are displayed with a color legend. If the property is inapplicable for a particular element, the element will be colored grey.

## Selection

Selection in PetraSim allows actions to be performed on specific objects in the model. Selection can be performed in either the **Tree View** or the **3D View**. Once an object is selected, actions can be performed on it through the **Edit** menu or right-click context menu.

In the **3D View**, selection can be performed with the **Orbit Tool** ( ) or **Selection Tool** ( ). Single-clicking an item in the **3D View** will select one item and Ctrl-clicking will select multiple items. With the **Selection Tool**, multiple items can be selected by left-clicking and dragging a box around the desired items. This selection box will select all items in the box and will penetrate through the model.

Additional items can be selected by holding the Alt and Shift modifier keys while clicking the desired objects. The additional items that are selected depend on the current **View Mode**.

### *Selecting Regions and Layers*

Selecting regions and layers in the **3D View** can only be performed when either the **Boundary Mode** or **Layer Mode** is active as discussed in View Mode. In either of these modes, the default selection action will select regions. If the owning layer should be selected instead, hold Alt while selecting the region.

### *Selecting Cells*

Selecting cells in the **3D View** must be performed in the **Mesh Mode** ( ) as discussed in the View Mode section. When using the **Orbit Tool** or **Selection Tool**, the default selection action will select individual cells. The following tools from the Mesh Toolbar Selection can be used to select specific groupings of cells:

- **Select Mesh X Slice** – Select a complete slice of cells on the X-plane. Alternatively, holding X while selecting a cell will select the entire slice.
- **Select Mesh Y Slice** – Select a complete slice of cells on the Y-plane. Alternatively, holding Y while selecting a cell will select the entire slice.
- **Select Mesh Layer** – Select a complete slice of cells on the Z-plane. Alternatively, holding Alt while selecting a cell will select the entire layer.
- **Select Mesh Column** – Select a column of cells. Alternatively, holding the Shift key while select a cell will select the complete.

For some concept-level objects, such as layers, regions, and wells, the cells that belong to that object may be selected all at once. To do so, select the layer, region, or well from the **3D View** or **Tree View**, right click it, and from the context menu select "Select Cells."

## Show/Hide/Filter Objects

PetraSim provides a variety of ways of limiting the currently visible objects. Some objects can be shown/hidden by classification, such as showing/hiding all wells or internal boundaries. Others can be shown/hidden several at a time, such as cells.

The following classes of objects can be shown or hidden with one of the buttons on the **Filter Toolbar**:

- Shows/Hides all wells
- Shows/Hides all background images and textures
- Shows/Hides all internal boundaries
- Shows/Hides all disabled cells

### *Show/Hide/Filter Cells*

When in the **Mesh Mode** ( ) cells can be hidden to reveal inner portions of the mesh. There are several ways to show and hide cells, some of which are chosen from the **Mesh Toolbar**:

- **Show only a subset of cells (filter)** – select the cells that should be visible and either select the **Filter** button ( ) from the **Mesh Toolbar** or right-click the selection and select "Show Only Selected Cells."
- **Show all cells** – select the **Show All Cells** button ( ) from the **Mesh Toolbar** or right-click in any view and from the context menu select "Show All Cells."

- **Show cells in only one mesh layer** – the ⌃ and ⌄ buttons in the **Mesh Toolbar** show only one layer of cells at a time. ⌃ will move the visibility to the next layer up from the current visible layer. ⌄ will move visibility to the next layer down. If any cells are selected when using these buttons, the buttons will maintain the selection in the cell column.
- **Hide individual cells** - select the desired cells, right-click the selection, and then from the context menu select "Hide Cells."
- **Hide all cells above a mesh layer** – select a cell on the layer that should be visible, right-click it, and from the context menu select "Hide Cells Above." This will leave the selected cell and all on its layer and below visible and hide the rest.

## Tree View

The Tree View (on the left of the 3D window) is used to display, select, and edit layers, regions, internal boundaries, materials, wells, and cells. Expand the list and then double-click on an object to edit its properties or right-click to show an additional context menu.

- Layers – Lists all layers in the model. Under each layer are all the sub-regions in that layer. Both layers and layer sub-regions can be edited by double-clicking the layer or region.
- Internal Boundaries – Lists all internal boundaries in the model.
- Materials – Lists all materials in the model.
- Wells – Lists all wells in the model.
- Named/Print Cells – Lists all cells that have either been given a name or been marked as a print cell.
- Extra Cells – Lists all extra cells that have been defined in the model.

## Units

All input uses metric (SI) units, such as meters, seconds, kilograms, degrees C, and the corresponding derived units, such as Newton, Joules, and Pascal for pressure. In some dialogs, the unit may be entered using a different scale. For instance, in the **Solution Controls** dialog, the time quantities may be entered in seconds, days, or years by following the number with the appropriate abbreviation.

Users can specify units according to their own preferences. To customize units:

1. On the **View** menu, click **Unit System…**
2. For each unit type, select the preferred units from corresponding drop-down list.
3. Click **OK** to apply the change.

Additionally, unit preferences can be cleared by clicking **Reset** in the Unit System menu. This sets each unit to its default SI value. The **Customize Units Dialog** is shown in Figure 4-4.

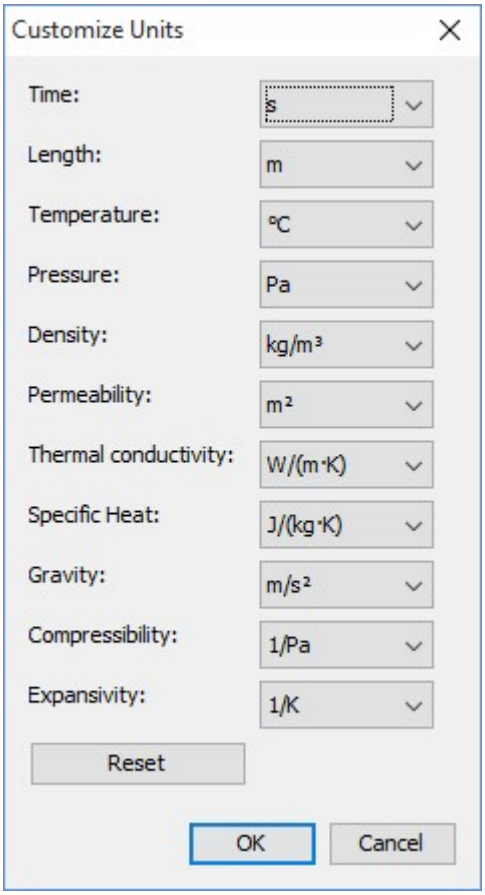



**Figure 4-4: Customize Units dialog**

## Displaying a Surface Image on the Model

It is possible to display a surface image on the model. This can be useful to help relate underground features with the surface image or to enhance the visual display. There are two ways to specify an image. One is as a floating background image that can exist at any Z location and the other is to drape an image over the terrain of the top layer.

### Floating Background Image

A floating background image is a flat image that can be specified at any Z location and with transparency. This type of image is useful for orienting underground features. To specify this type of image:

1. Save the image file (.bmp, .gif, .jpg, .jpeg, .png).
2. On the **View** menu, click **Background Image…**
3. In the **Background Image Dialog**, click the file selection icon, and select the image file.
4. The **Origin** defines the position of the lower left corner of the image in the model coordinates.
5. The **Extent** defines the length of the image in the model coordinates.
6. The **Z-Coord** defines the position of the image in the Z direction.

7. The **Transparency** slider defines the amount of transparency used to display the image. Move the slider to the left to minimize transparency.

An example surface image is shown in Figure 4-5.

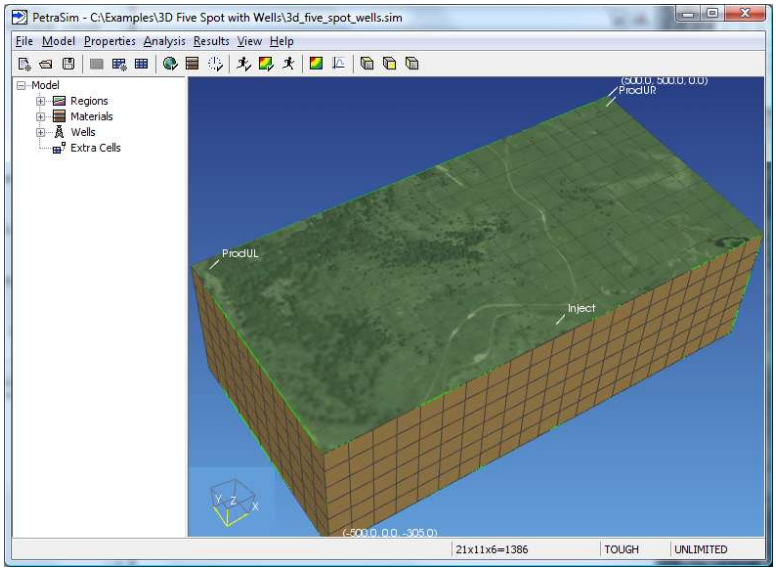



**Figure 4-5: Example background image**

## Draped Image

A draped image appears as a texture on the top of the terrain as shown in Figure 4-6. It conforms to the terrain on the top layer of the model and can be viewed in any **View Mode**. When viewed in **Mesh Mode** it is draped on the top layer of visible cells. To add a draped (top) image: on the **Model** menu, click **Set Top Image**.

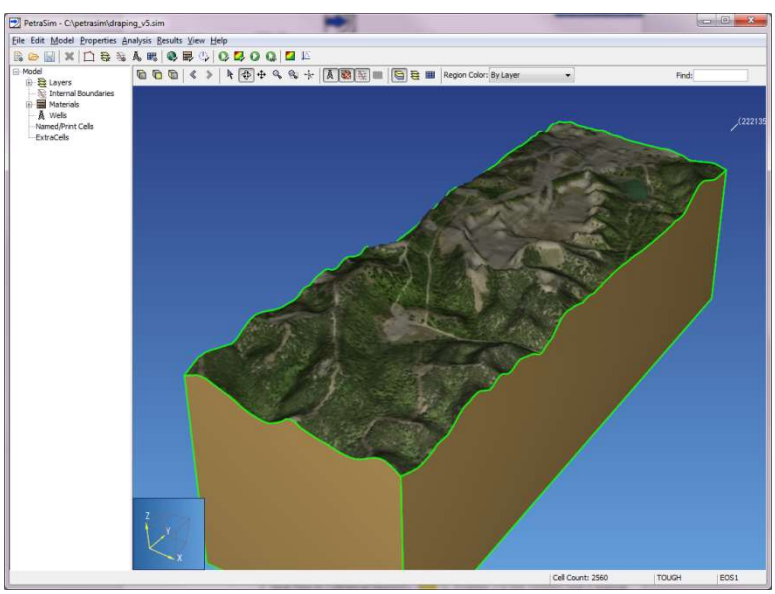



**Figure 4-6: Example draped image**

## User-Defined Labels

It is possible to add labels to the model in addition to those automatically created by the boundary and wells. To define labels:

1. On the **Model** menu, click **Labels...**
2. In the **Labels** dialog, add the **X, Y, and Z** coordinate data and **Name** text for each label.
3. Each label will now be displayed in the **3D View**. You can control the display of the labels in the **View** menu.

# 5. Working with Files

Several files are used when performing an analysis using PetraSim. These include the PetraSim model file, the TOUGH input file, and TOUGH output files. It is important to understand the differences between these files to take full advantage of PetraSim's features.

## PetraSim Model File (SIM)

The PetraSim model file (SIM) is a binary file that represents a PetraSim model. The SIM file contains all information needed to write a TOUGH input file.

**The SIM file can be used to save the model and share with other PetraSim users.**

## TOUGH Input File (DAT)

Execution of TOUGH is integrated into PetraSim. Before PetraSim executes TOUGH, a TOUGH input file (DAT) is automatically written. This file is then read by the TOUGH executable. The TOUGH input file contains all information needed for a TOUGH analysis. The DAT file is an ASCII text format file.

Most PetraSim users will never need to explicitly create or edit the TOUGH input file. In special cases, such as when a user has developed a special version of TOUGH, the user may need to edit the TOUGH input file before an analysis. In this case, PetraSim provides the option to export this file **File/Write TOUGH2 File…** for manual editing. For more information on the TOUGH files written during an analysis, see the Restart section in this document.

**PetraSim users should not use the DAT file to share models, since this file does not contain information needed to reconstruct a model in PetraSim.**

## Creating and Saving a New PetraSim Model

When PetraSim is started, it begins with an empty model. The user can immediately begin work on a new model. If another model has already been opened, select **File->New...** to clear the current model and start a new empty model. PetraSim always has one (and only one) active model.

To save the new model, select **File->Save...** and give the file name. Because the files written by TOUGH have a fixed name, it is recommended that the user create a new directory for each model. If this is not done, the TOUGH results from a first analysis will lost when a second model is run, even if the PetraSim model has a different name.

## Open a Saved PetraSim Model

To open a saved model, select **File->Open...** and select the file. To speed model selection, a list of recently opened files is available under **File->Recent PetraSim Files...**.

## Contour Files

Externally generated contour data can be used to define initial conditions, the geometry of layer divisions for the conceptual model, or internal boundaries.

The format of the contour file is given below. In the current implementation, the depth data is not used. The contour data defines contours (lines) in the X and Y plane on which a value is specified. If the contour is being used to define a layer or boundary, the contour value is interpreted as the Z value. If initial conditions are being defined, the Z value is interpreted as the value of the state variable being defined (pressure, temperature, etc.).

The data consists of the depth (not used) followed by a definition of contours. In the following example, the "!" and following comments are included only for description. These should not be included in an actual file.

```
Define top of reservoir    ! The first line is a description
<top origin>               ! Include this line (not used at this time)
<depth>                    ! Keyword to indicate beginning of a contour set
    0.                     ! The Z coordinate for this contour set
<contour>                  ! Keyword to define a contour at the given depth
    0.     1               ! Value of contour followed by number of points
-1000.  1000.              ! X and Y coordinates of the point(s)
<contour>                  ! Start of a new contour
  200.     3               ! Value (200.0) and number of points (3)
 -100. 1000.               ! X and Y coordinates of the point(s)
 -300.  800.               ! X and Y coordinates of the point(s)
-1000.  200.               ! X and Y coordinates of the point(s)
<contour>                  !
  100.     4               ! Complete the contours at this depth.
  200. 1000.
    0.  600.
 -400.  200.
 -800.    0.
<contour>
    0.     4
  400. 1000.
  200.  600.
 -200.  200.
 -600.    0.
<contour>
    0.     2
 1000.    0.
 1000. 1000.
                           ! Repeat <depth> and <contour> data
```

## XYZ (and TXT) Files

XYZ (or TXT) files may be used to define the geometry of layer divisions and internal boundaries as discussed in the topic, Conceptual Model. The can also be used to define initial conditions.

The XYZ file format consists of a list of XYZ points. PetraSim triangulates these points to form a surface. If initial conditions are being defined, the Z value is interpreted as the value of the state variable being defined (pressure, temperature, etc.). Following is a typical file.

```
-1000.  1000. -500.
 -100. 1000.  -300.
 -300.  800.  -300.
-1000.  200.  -300.
  200. 1000.  -400.
    0.  600.  -400.
 -400.  200.  -400.
 -800.    0.  -400.
  400. 1000.  -500.
  200.  600.  -500.
```

```
-200.  200.  -500.
-600.    0.  -500.
1000.    0.  -500.
1000. 1000.  -500.
```

## DXF Files

PetraSim contains limited support for DXFs to define layer divisions and internal boundaries as discussed in the topic, Conceptual Model. They can also be used to define initial conditions, although this would likely require the user to edit the file. If initial conditions are being defined, the Z value is interpreted as the value of the state variable being defined (pressure, temperature, etc.).

The DXF file is limited to 3DFACE entities and Polyface meshes. These must be the top objects in the hierarchy, not embedded in blocks.

## Petrel Files

PetraSim provides limited support for importing exported Petrel cell data into a PetraSim model. In order to be properly read by PetraSim, Petrel data must be written in an ASCII format, readable by the ECLIPSE reservoir simulator also maintained by Schlumberger. Presently the only data that can be directly read is the porosity data denoted by the ECLIPSE keyword PORO.

# 6. Conceptual Model

The conceptual model defines the high-level features of the model. These are detailed descriptions of entities as they exist in the world, including a problem boundary, geologic layers, regions, and internal boundaries. The conceptual model is independent of the solution mesh and is used to generate the solution mesh as discussed in the topic, Solution Mesh.

## Problem Boundary

The problem-space is limited in scope by defining a problem boundary. This is a 2D polygon that can be thought of as cutting a section out of the earth. The boundary polygon may be any shape, concave or convex, as long as it does not self-intersect. Some examples of boundaries are shown in Figure 6-1.

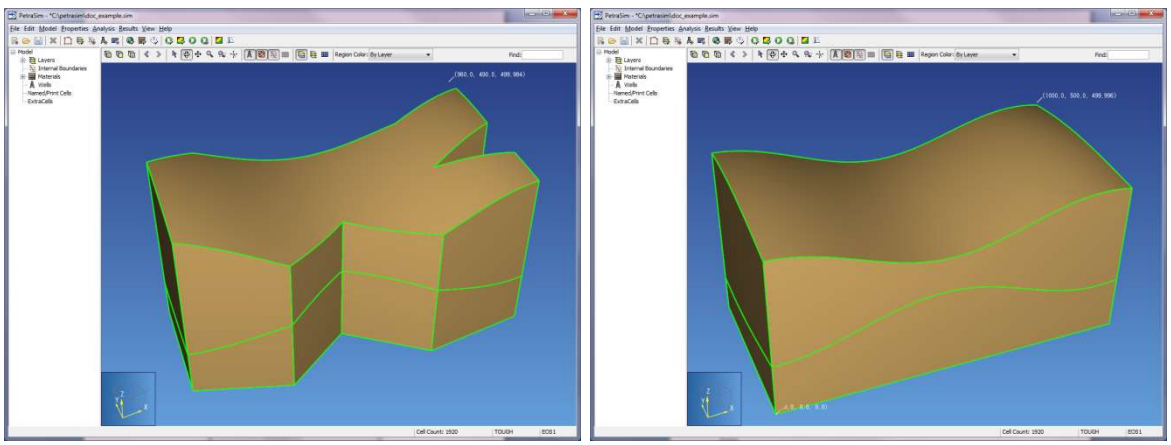


**Figure 6-1: Examples of different model boundaries**

The model boundary may be defined at any time, but it is preferable to define it either when starting to build the model or just after creating the layers. There are two ways to define the boundary. It can either be done when creating a new model or with the **Boundary Editor**.

### Defining boundary with a new model

To define the boundary as part of a new model, select **File->New** to create the new model. The **New Model** dialog is shown as in Figure 6-2. A rectangular boundary can be specified in this dialog by entering the **X Min, X Max, Y Min,** and **Y Max**.

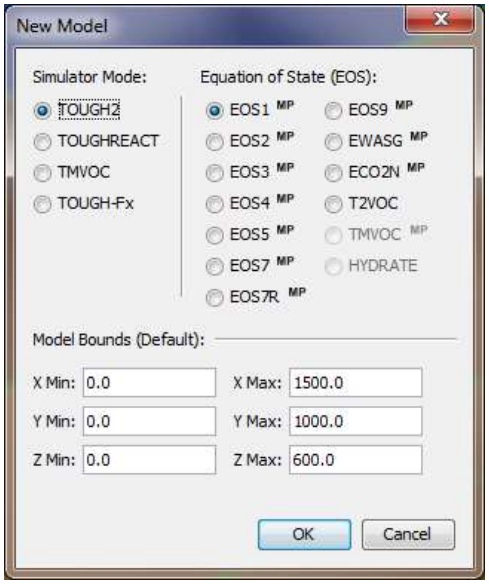



**Figure 6-2: Entering a boundary in the New Model dialog**

## Defining boundary with the boundary editor

To edit the boundary once a model has been created, open the **Boundary Editor** dialog by going to the **Model** menu and choosing **Edit Boundary…** ( ). The **Boundary Editor** dialog is shown in Figure 6-3.

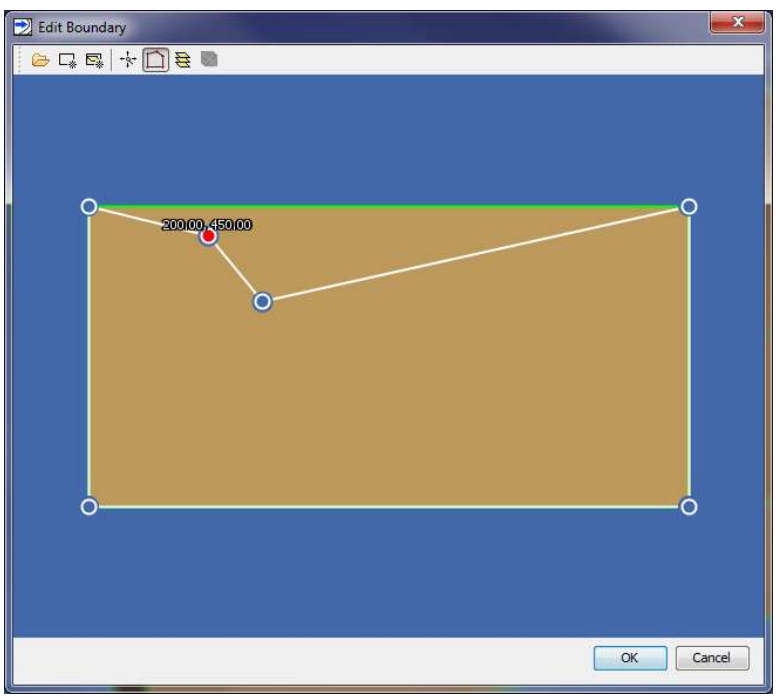



**Figure 6-3: Boundary editor**

This dialog shows an overhead view of the model along with the current boundary path. An existing point on the path can be edited either by clicking and dragging the point with the left mouse button or right-clicking a point and selecting "Edit…" from the context menu to set the point to a specific

coordinate. A point can be added to the boundary by clicking on one of the edges. The point will be added at the set point. Existing points can also be deleted by right-clicking the point and selecting "Delete" from the context menu.

There are also several ways to create the boundary from scratch using the toolbar:

**From a file** – Select this option to use an XY input file to create the boundary. This input file is similar to XYZ files discussed in the topic,

- XYZ (and TXT) Files. The main difference is that the XY file doesn't require a Z coordinate and must specify the coordinates in the proper order to form a polygon describing the boundary.
- **Quick Set Min/Max** – Select this to create a boundary that is an axis-aligned box using min/max x and y bounds as shown in Figure 6-4.
- **Auto Size to Layers** – Select this option to automatically create a boundary from the current layers if their divisions were generated from input files, such XYZ, Contour, or DXF files. Because the geometry in the input files may make different shapes or may not overlap in coordinates, another dialog will ask how to generate the resulting boundary as shown in Figure 6-5.
    - If the **Bounding Box** option is chosen for shape, the resulting boundary will be an axis-aligned box that fits the outer points of the input files.
    - **Convex Hull** will make the boundary a convex polygon that fits the points in the input files. This option is only relevant if the input points were not specified as a rectangular array of points in the input file.
    - The input for the shape is determined by combining the geometry from the different layer divisions in the model. The geometry can either be a **Union** of the shapes or an **Intersection**.
    - Different combinations of shape and layer-combining are shown in Figure 6-6.

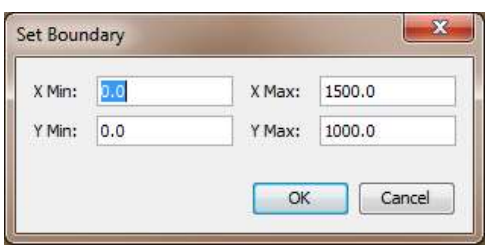



**Figure 6-4: Quick Set Boundary dialog**

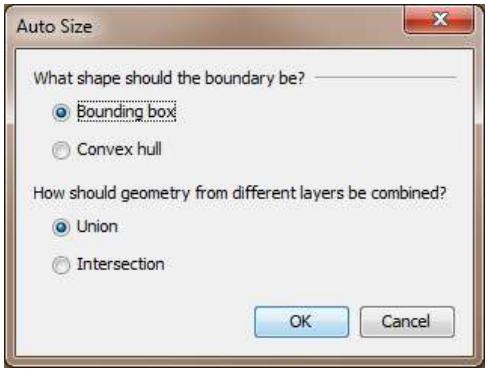



**Figure 6-5: Auto Size Boundary dialog**

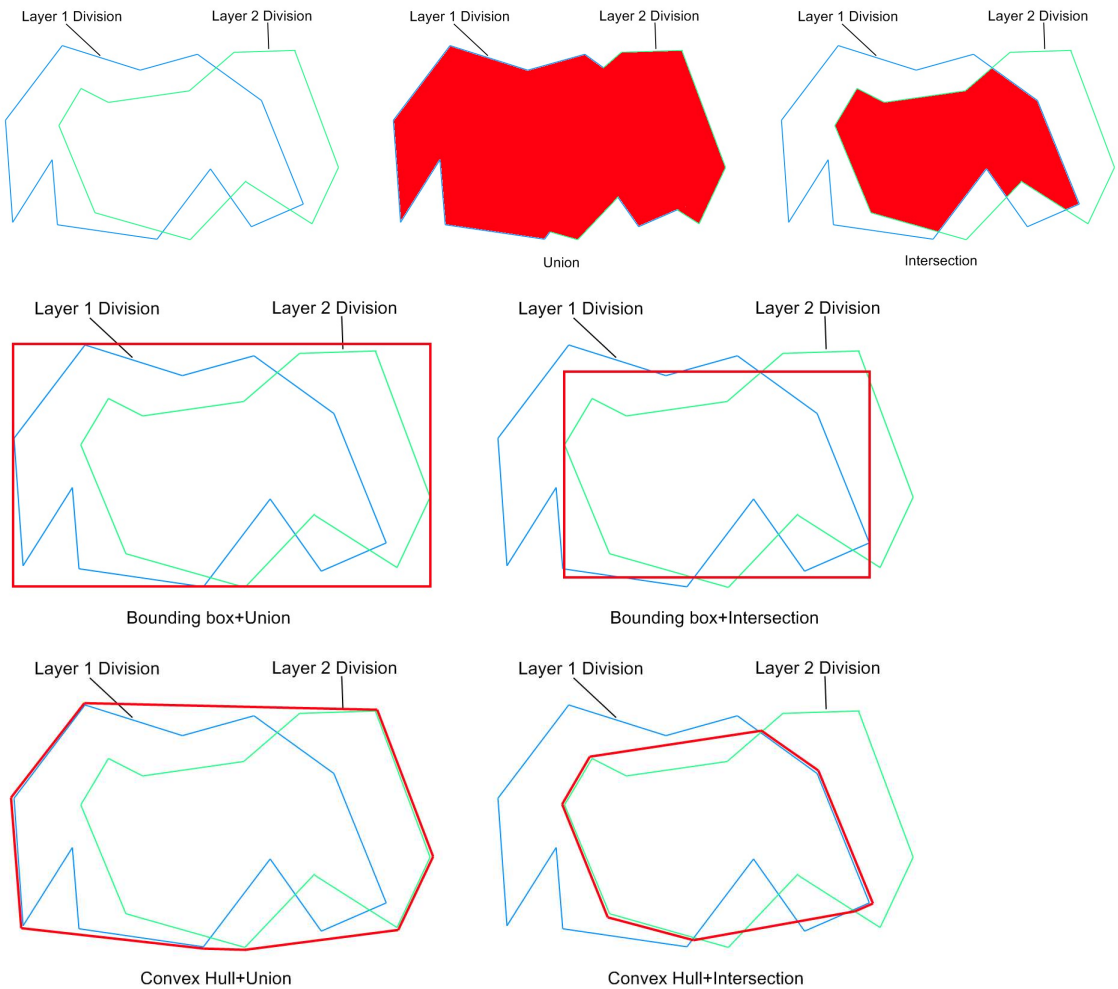



**Figure 6-6: Auto Size Boundary combinations**

## Layers

Layers can be used to describe the stratigraphy of the model. Layers are horizontal regions that are stacked on top of each other in the Z direction. A model can be composed of any number of layers, each having its own set of properties, including name, material, color, number of divisions in the solution

mesh, and initial conditions. Figure 6-7 shows several layers within one model. As can be seen in the figure, a layer does not have to extend to the boundary.

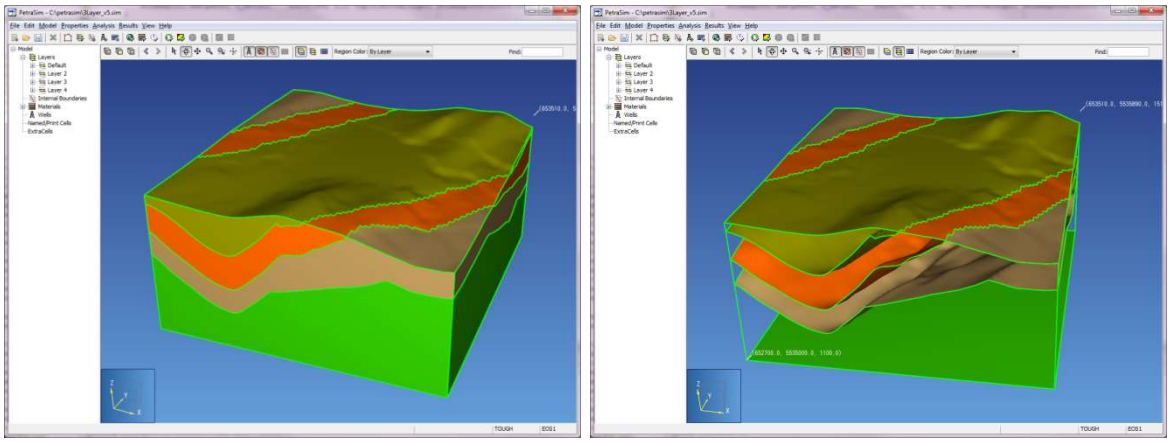


**Figure 6-7: Example of layers**

In PetraSim layers are defined by the geometric surfaces, or divisions, between each layer. Each division may be created by using a constant Z value, a planar function, or an input file for more complex surfaces. There will always be one more division than there are layers in the model. This extra division is used to define the top of the model. In Figure 6-7 it can be seen in the left image that there are four layers and in the right image there are five divisions defining the layers. PetraSim always associates the top two divisions with the top layer, and each subsequent layer is defined only by its lower division (each subsequent layer's upper division is implicitly defined by the next higher layer's lower division). The colors of the divisions in Figure 6-7 (right) demonstrate which division is associated with which layer.

The following guidelines are strongly suggested for layer divisions:

- Layer divisions should extend to the boundary of the model. If an input file does not do so, PetraSim will automatically extend the geometry to the boundary in the X,Y direction as shown in Figure 6-8. This may result in unintended geometric artifacts.
- Layer divisions are allowed to touch along areas, pinching the layer, but they should not cross within the model boundary. While PetraSim does not enforce this rule, it is best practice to make sure this rule is followed since it reduces ambiguities in determining the order of the layers along the Z direction. An example of invalid divisions is shown in Figure 6-9. PetraSim cannot reliably determine which layer should be the top, middle, and bottom. The model in this image could be fixed by changing the boundary to only include the portion of the model to the left or right of the divisions' intersection as shown in Figure 6-10.

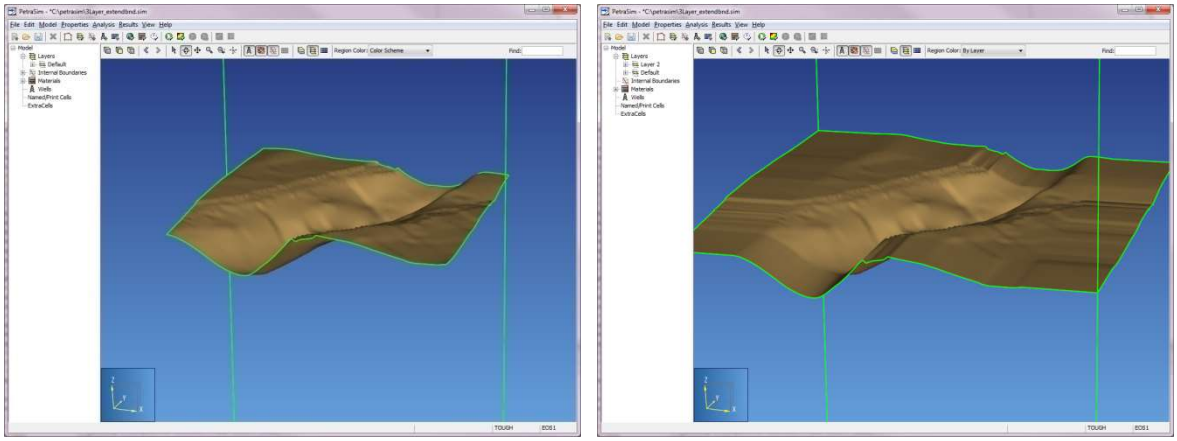


Figure 6-8: Example of extending an input file boundary

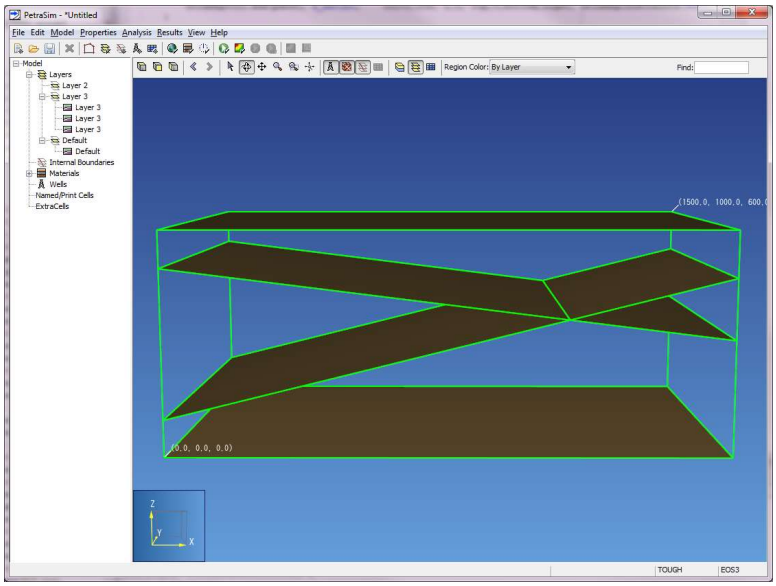



Figure 6-9: Example of invalid layer divisions

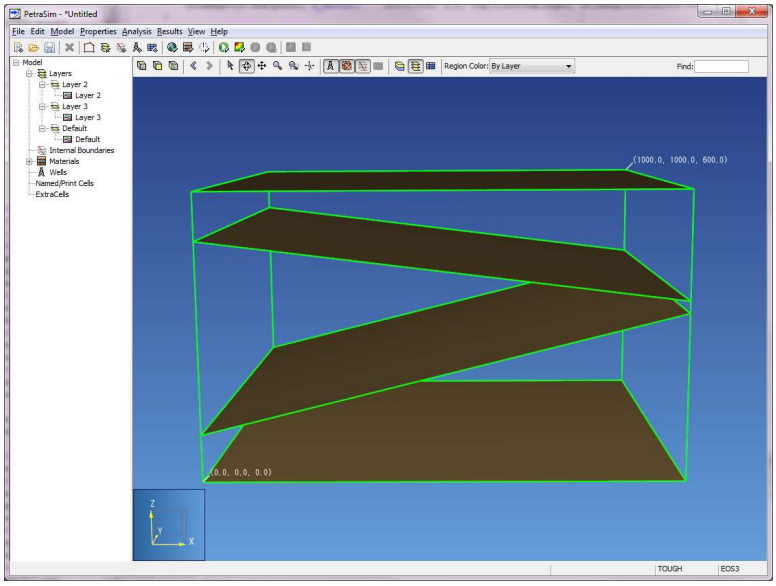



**Figure 6-10: Fixed layer divisions**

In PetraSim, there must always be at least one layer. For every new model there is, by default, one layer defined by two Z-planar divisions. These divisions can be specified when creating the new model. In addition, layers may be added, edited, and removed after the model is created.

## Defining the default layer with a new model

The divisions of the default layer may be specified when creating a new model. To do so, on the **File** menu, click **New**…. The **New Model** dialog appears as shown in Figure 6-2. Enter the desired **Z Min** and **Z Max**. The default layer divisions are always Z-planar.

## Defining layers with the layer manager

At any time while working on a model, layers may be added, edited, and removed through the **Layer Manager** dialog. On the **Model** menu, click **Edit Layers…** ( ). This will open the layer manager as shown in Figure 6-11. The current model layers appear in the left-hand list in the layer manager, and the properties of the selected layer are shown in the right-hand pane.

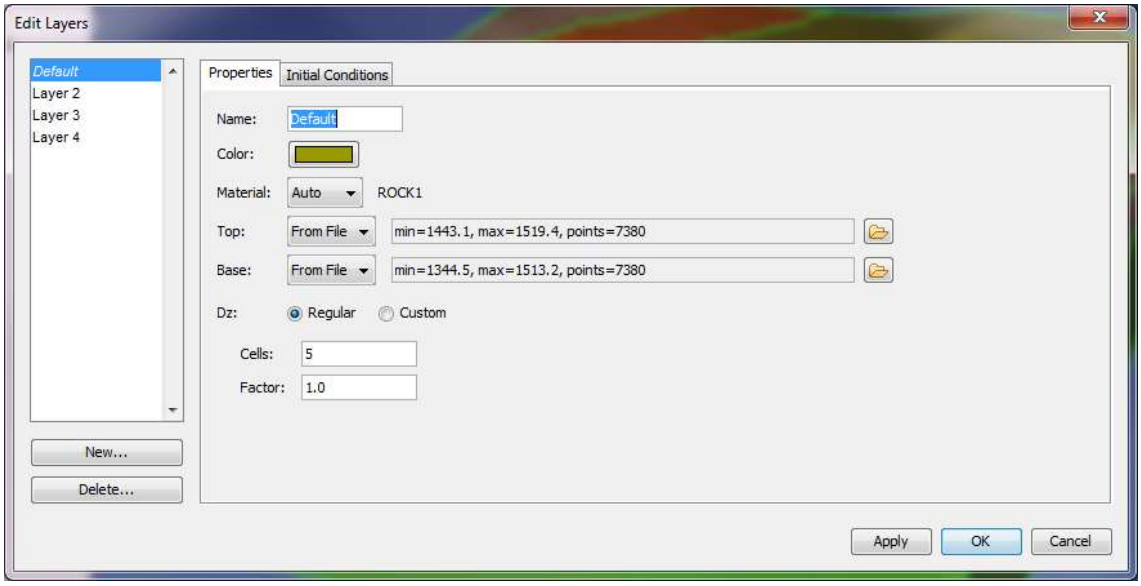



**Figure 6-11: Layer manager dialog**

### *Create a new layer*

By default, there is always one layer in the model. To create a new layer, click the **New…** button in the layer manager dialog. This will open the **New Layer** dialog shown in Figure 6-12. Specify the name of the new layer and the geometry defining its bottom (base) division. Then click **OK**. The geometry may be defined as follows:

- **Constant** – Specifies a Z location such that the division will be a plane located at Z=the entered value.
- **Function –** Specifies a planar division defined as $z = A + Bx + Cy$.
- **From File –** Allows the division's geometry to be defined by an input file. The geometry may be an XYZ file, Contour file, or DXF file as described in the Working with Files section.

The new layer will automatically be sorted and inserted into the list of layers based on its based division.

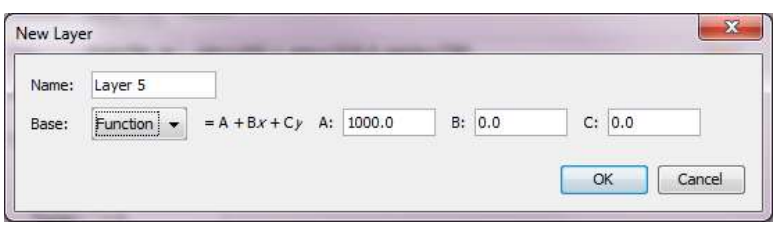



**Figure 6-12: New Layer dialog**

### *Delete a layer*

To delete an existing layer, first select it in the list and then click the **Delete…** button.

### *Edit a layer*

To edit an existing layer, first select it in the list. Its properties will be shown in the right-hand pane.

- **Name** – the layer name
- **Color** – the layer color. This will define how geometry is to be colored when the Region or Cell color is set to "By Layer" as discussed in the topic, Colors.
- **Material** – the layer material. All regions and cells in the layer will inherit this material unless the material is individually overridden by the layer or cell.
- **Top** – the top division. This field may only be edited on the top layer. See Create a new layer for a description of division input.
- **Base** – the bottom division. See the Create a new layer section for a description of division input.
- **Dz** – the divisions used to create the solution mesh. This is described in the Setting Z Divisions section.
- **Initial Conditions** – these are discussed in the Boundary and Initial Conditions section.

Once changes have been made to a layer, either press **Apply** to commit the changes and keep the dialog open or **OK** to commit the changes and close the layer manager dialog.

## Regions

Regions are portions of the model that have non-zero volume. They are the basis for creating high-level features in the model, such as faults. With no internal boundaries in the model, each layer consists of one region. Regions may be divided into smaller regions by adding internal boundaries as discussed in the next section. Regions are always parented by layers, and can be found in the **Tree View** as shown in Figure 6-13. This figure shows four layers that have been divided by an internal boundary, creating two regions in each layer.

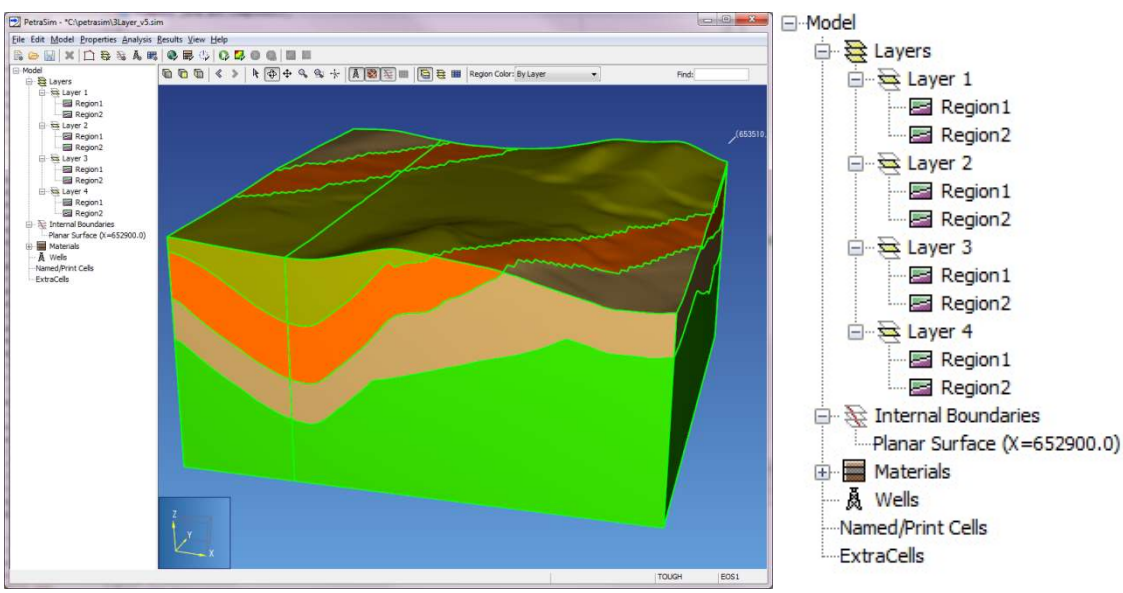



**Figure 6-13: Example of layers split into multiple regions**

Each region may have its own set of properties, which can be accessed by double-clicking a region in the **Tree View** or in the **3D View**. The region properties window is shown in Figure 6-14.

**Figure 6-14: Region properties dialog**

- **Name** – the name of the region.
- **Material** – the region's material. Cells in this region will inherit this material if they have not explicitly set a material in their properties. If this value is set to "Auto" the material will come from the owning layer.
- **Enable Region** – whether to include this region in the simulation. If this is unchecked, all cells in this region will be disabled and excluded from the simulation.
- **Initial Conditions** – see Layer and Regional Initial Conditions.

## Internal Boundaries

Internal boundaries are used to divide layers into multiple regions. Material properties and initial conditions can then be defined by region. Select **Model->Add Internal Boundary...** or to open the Add Internal Boundary dialog, Figure 6-15.

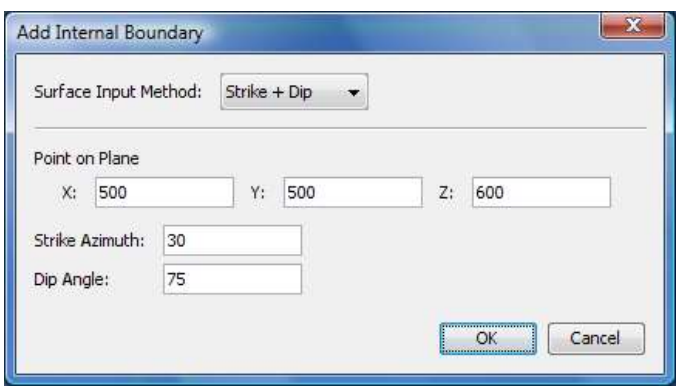



**Figure 6-15: Defining an internal boundary**

There are four options for specifying an internal boundary: **Strike + Dip**, **Three Points**, **Point + Normal**, and **Input File**. The first three options create planar divisions, each containing a different set of options to specify the plane. Figure 6-15 shows the input using the **Strike + Dip** option.

For the **Strike + Dip** option, the data include:

- Point on Plane – The coordinates of a point on the boundary plane.

- Strike Azimuth – The degrees from North (the positive Y axis) in a clockwise direction.
- Dip Angle – Degrees from horizontal of the plane. If the viewer is facing the azimuth direction, the dip is to the viewer's right.

For the **3 Points on a Plane** option, the data include:

- Points on Plane – The coordinates of three points on the boundary plane.

For the **Point + Normal** option, the data include:

- Point on Plane – The coordinates of a point on the boundary plane.
- Normal to Plane – The components of a vector normal to the plane. They do not need to be normalized.

For the **Input File** option, a 3D contour can be defined using the contour, XYZ, or DXF file formats (see Working with Files). An example is shown in Figure 6-16.

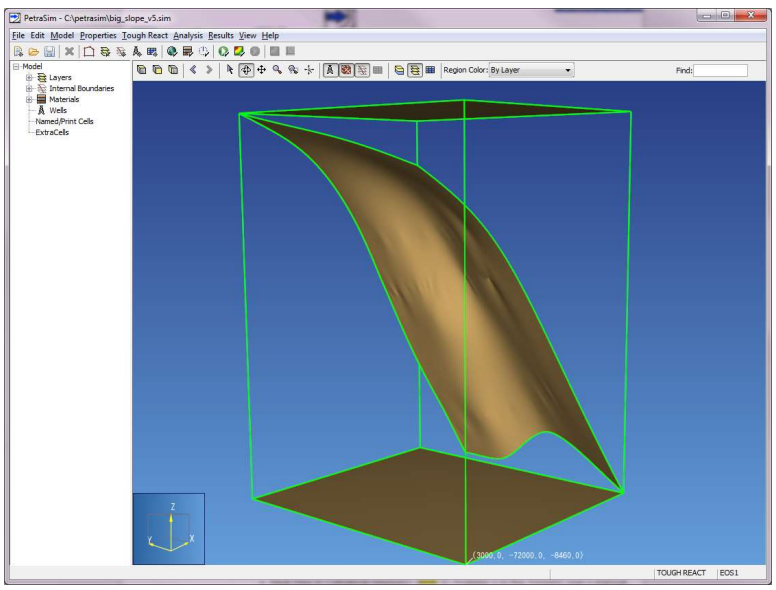



**Figure 6-16: The internal boundary shown in the model**

*NOTE:* Internal boundaries from input files are not automatically extended to the model boundary as layer divisions are. This means that the internal boundary will only split off new regions if it touches or intersects all surrounding geometry. If it does not, it will be added to the model as a geometric surface floating in the middle of the model as shown in Figure 6-17.

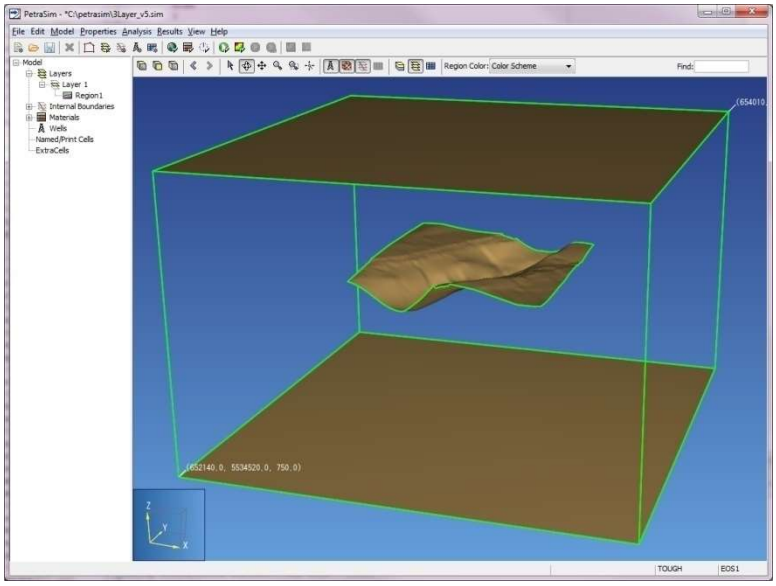
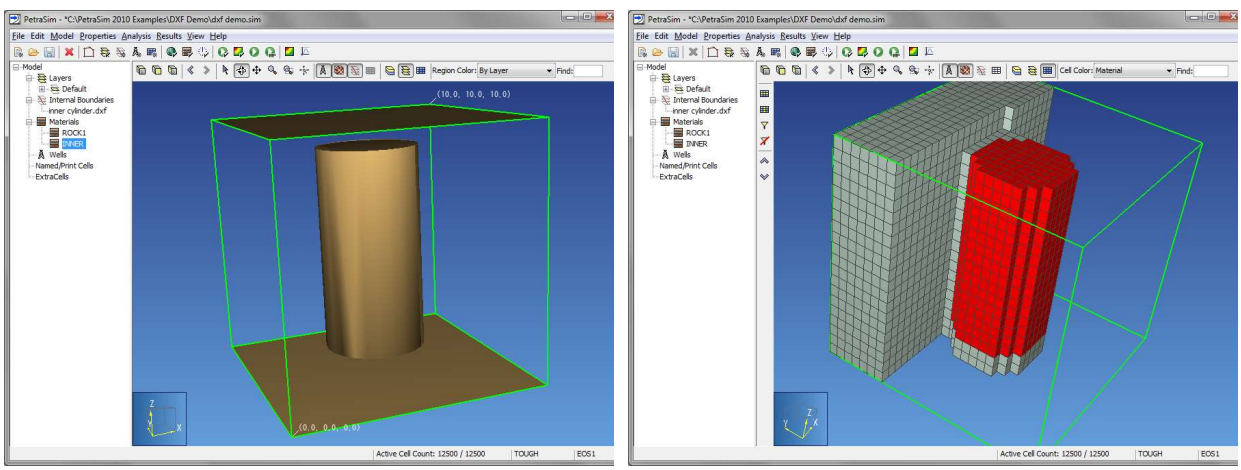



**Figure 6-17: Example of floating internal boundary**

Programs such as Sketchup or AutoCAD can also be used to create internal boundaries. In the images below, Sketchup was used to define a cylindrical region inside a rectangular mesh, so that different material properties can be associated with that region, Figure 6-18.




a. Closed internal region defined using DXF file

b. Mesh created using material properties assigned by region

**Figure 6-18: A cylindrical region defined using a DXF file**

## Faults

Faults are not explicitly modeled in PetraSim, but they can be created using internal boundaries and regions. To do so, add two internal boundaries to split off a new region. This new region between the boundaries corresponds to the fault. The fault properties can then be specified by editing the region as discussed in the previous section.

With more complex models with several layers, the fault may be split into many regions, spread across several layers as shown in Figure 6-19. This may make it difficult to find the fault regions using just the **Tree View** or **3D View**. To more easily find the regions, perform the following steps:

1. Select the two internal boundaries defining the fault from the **Tree View**.
2. Right click on one of the boundaries in the **Tree View**, and from the context menu, select "Select Regions Inbetween."

This will select and highlight the fault regions as shown in Figure 6-19.

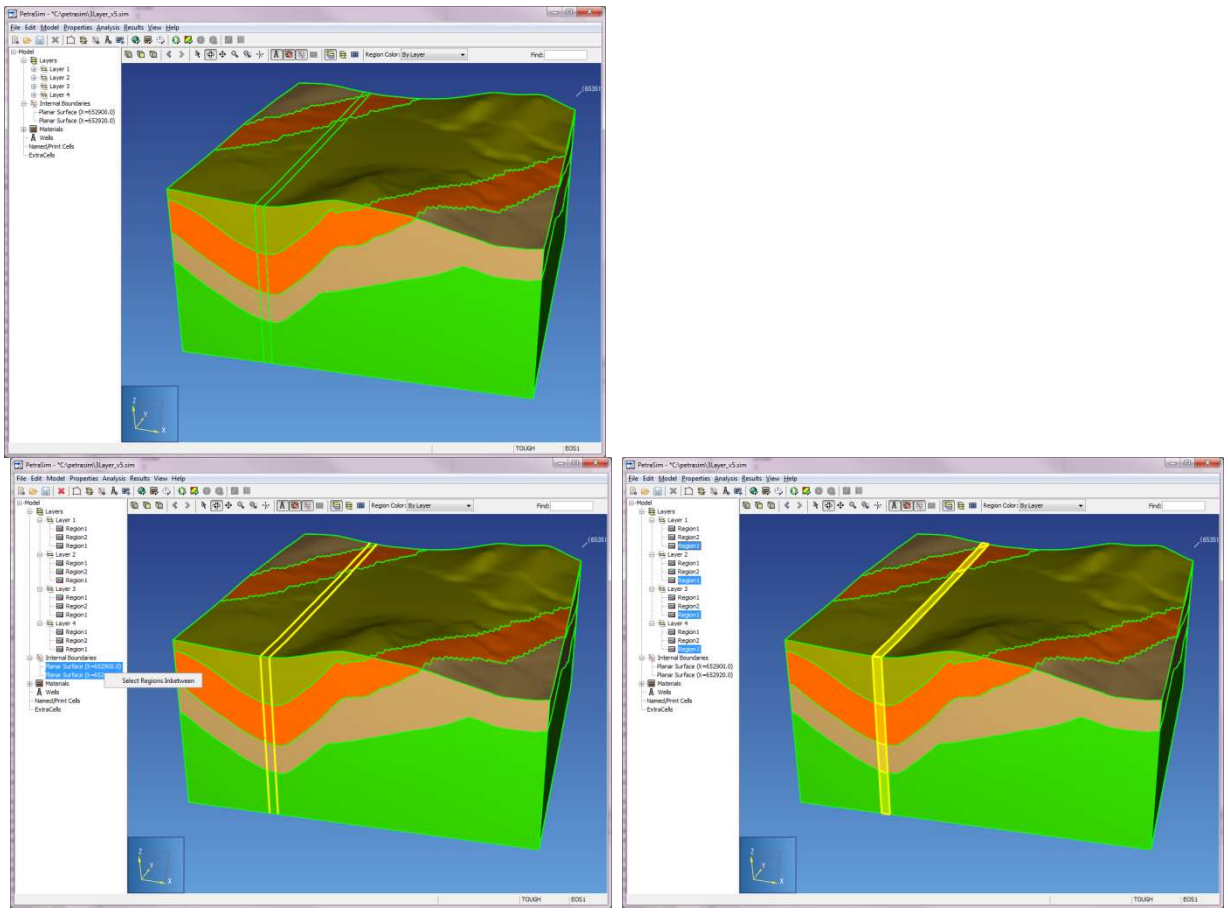


**Figure 6-19: Selecting fault regions**

## Cleaning Up the Model

Sometimes after making many changes to a model, such as adding and deleting internal boundaries or layers, the conceptual model may appear to have extraneous edges or other irregularities as shown in Figure 6-20. To fix these problems and clean up the model, from the **Model** menu select **Regenerate Conceptual Model**. This will rebuild the conceptual model. This should be a safe operation that will maintain all model properties and should make the model appear cleaner, but it is recommended to save the model before performing this operation.

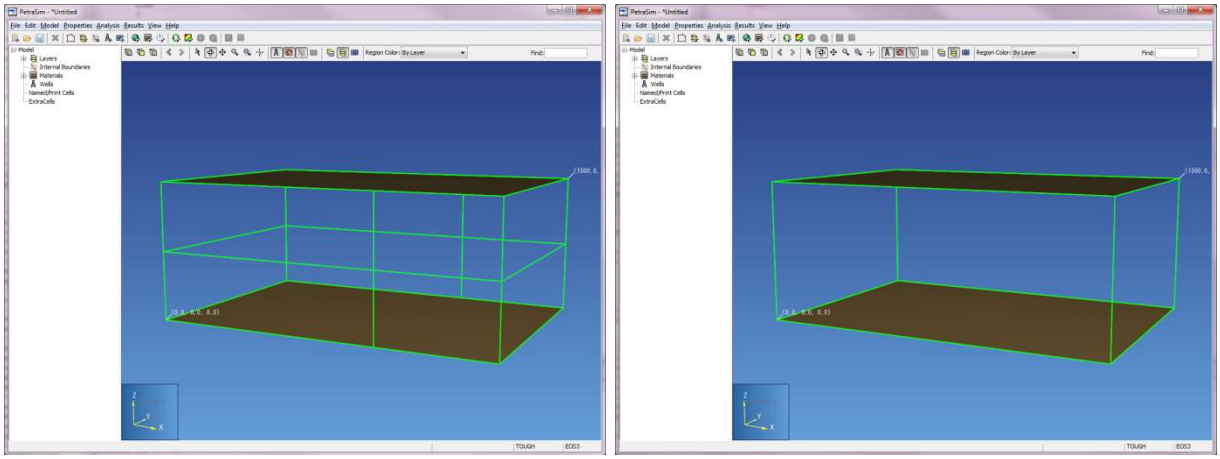


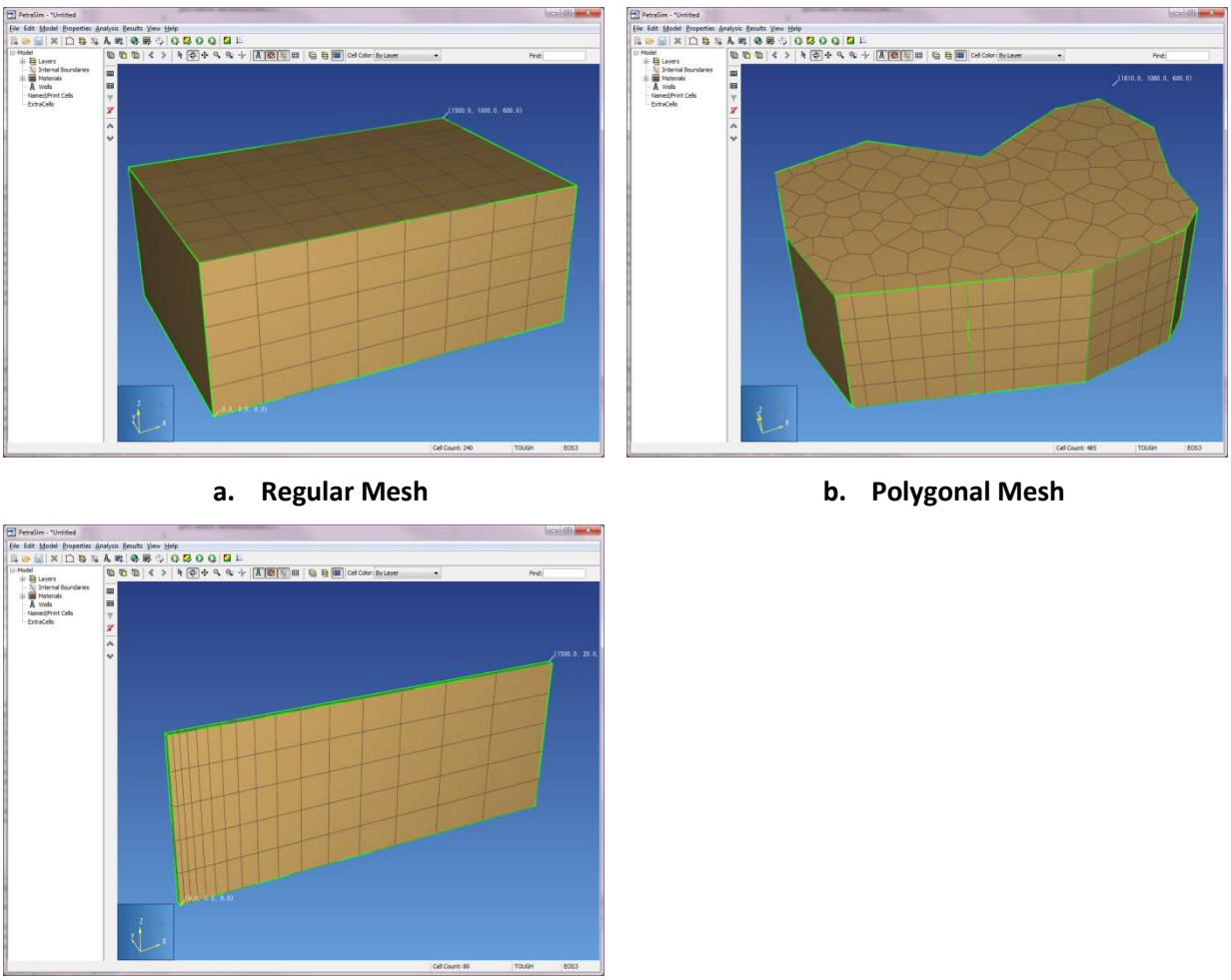
**Figure 6-20: Cleaning a conceptual model**

# 7. Solution Mesh

PetraSim provides three types of solution meshes:

- **Regular** – cells are rectangular hexahedrons.
- **Polygonal** – uses extruded Voronoi cells to conform to any boundary and support refinement around wells.
- **Radial** – represents a slice of an axisymmetric cylindrical mesh. This is based on the **Regular** mesh, but it only allows 1 Y-division.

Figure 7-1 shows the different types of meshes.



**a. Regular Mesh**

**b. Polygonal Mesh**

**c. Radial Mesh**

**Figure 7-1: Types of solution meshes**

All meshes in PetraSim conform to the layers of the model in the Z direction, so if a layer slopes upward, the mesh cells will also slope upward to conform. An example of this is shown in Figure 7-2.

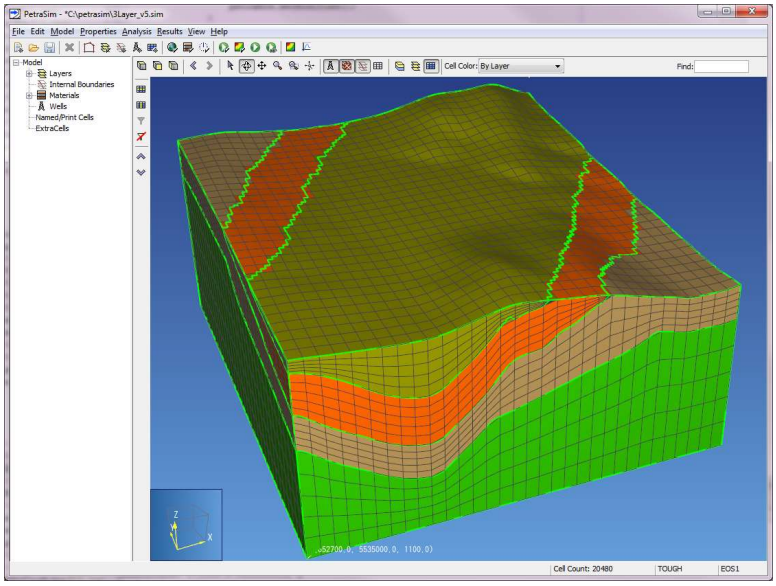



**Figure 7-2: Example of a mesh conforming to the model layers**

# Defining a Solution Mesh

Defining a solution mesh requires two steps. First the Z divisions must be specified per-layer in the **Layer Manager** dialog. Then a mesh of the desired type must be created with the **Create Mesh** dialog.

In the following sections, it is important to note the distinction between a **model layer** and a **cell layer**. A **model layer** is a layer defined in the conceptual model to define stratigraphy or other model properties. A **cell layer** is a portion of the model layer that corresponds to the solution mesh. Each model layer may be split into any number of cell layers.

## Setting Z Divisions

The Z divisions control how many cell layers are created per model layer. When a new mesh is created, each model layer is divided into a number of cell layers as seen in Figure 7-2 and then each cell layer is further refined in the XY dimensions based on the type of mesh created as discussed in the following section.

To edit the Z divisions for a layer, open the **Layer Manager** dialog as described in Defining layers with the layer manager. The Z divisions are entered in the Dz section. If Dz is set to **Regular**, the layer will be divided evenly into a constant number of cell layers when creating a new mesh. If this is set to **Custom**, a table will appear, allowing the cell layer divisions to be entered as custom sizes. Figure 7-3 shows an example of creating custom Dz. This Dz table allows the divisions to be entered such that a *Fraction* of the layer will be divided into the specified number of *Cells*. Each row in the table is ordered such that going down in the table corresponds to increasing Z values.[1]

[1] If a solution mesh already exists in the model and Dz is changed for a layer, the mesh will NOT automatically update with the new number of layer divisions. The mesh must be recreated to update the divisions.

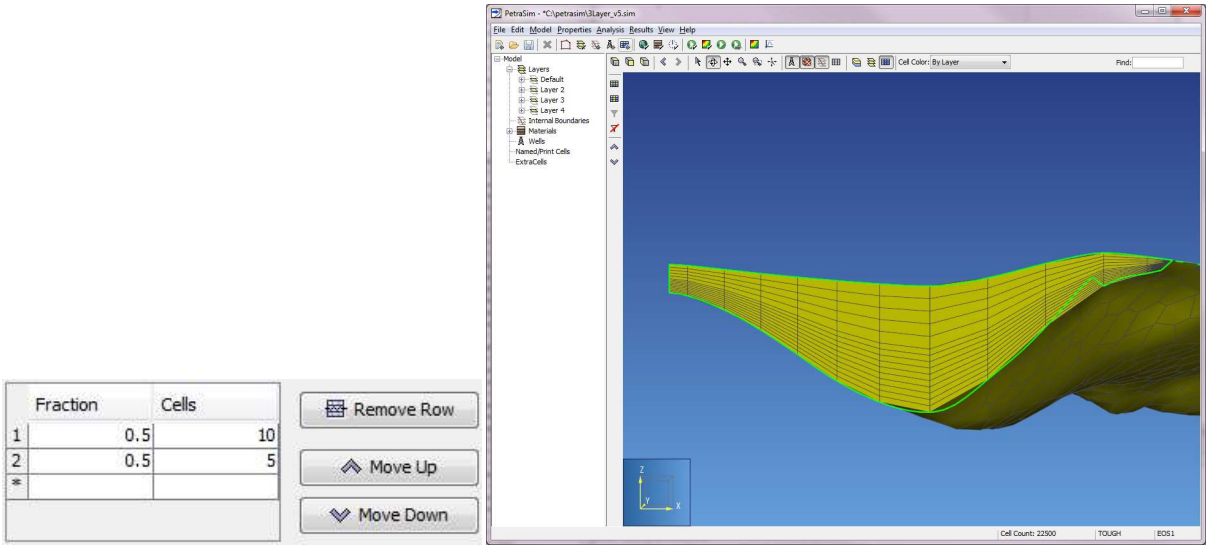



**Figure 7-3: Creating custom layer Dz**

## Creating the solution mesh

Once the Z-divisions have been set per layer, a mesh may be created in the **Create Mesh** dialog. The parameters entered in the **Create Mesh** dialog control how each cell layer is divided into horizontal pieces. To create the mesh, from the **Model** menu select **Create Mesh…** or click to open the **Create Mesh** dialog, Figure 7-4. Choose the desired **Mesh Type** from the drop-down box, and enter the required parameters as described in the following sections.

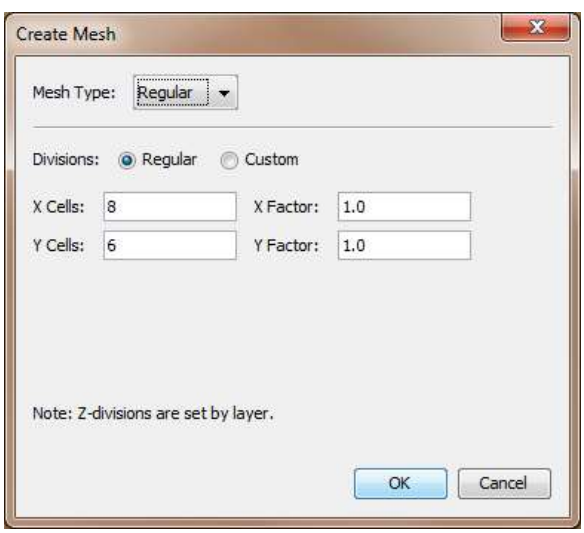



**Figure 7-4: The Create Mesh dialog showing regular parameters**

### *Regular Mesh*

A regular mesh is rectangular and is made of six-sided cells. It is created such that it fits the bounding box of the model. Because a model boundary does not necessarily have to be a rectangle, any cells outside the model boundary are disabled. The parameters for controlling cell sizes in the X and Y

directions are shown in Figure 7-4. Cell sizes can either be constant in the x and y directions using the **Regular** division type or vary in either direction using the **Custom** division type or size factors.

If **Regular** divisions are specified, **X Cells** and **Y Cells** correspond to the number of cells in the X and Y directions. A factor can be used to increase or decrease element size. If the factor is 1.0, then all cells in that direction have the same size. If not, the relations in Figure 7-5 can be used to calculate the cell size that will result for a given initial size and factor.

$$l = l_0 + l_1 + l_2 + \ldots + l_{n-1}$$
$$l = l_0 f^0 + l_0 f^1 + l_0 f^2 + \ldots + l_0 f^{n-1}$$
$$l = l_0 \sum_{i=0}^{n-1} f^i$$

**Figure 7-5: Calculating cell size when the factor is not 1.0**

Cell sizes can also be more finely controlled using the Custom division option. The sizes are entered into a table as shown in Figure 7-6. The cells are defined in the direction of increasing coordinate (X, Y, or Z) and the user gives the direction, number of cells, and size of those cells. This must be defined for each direction and the sum of all cell sizes must match the boundary length in each direction.

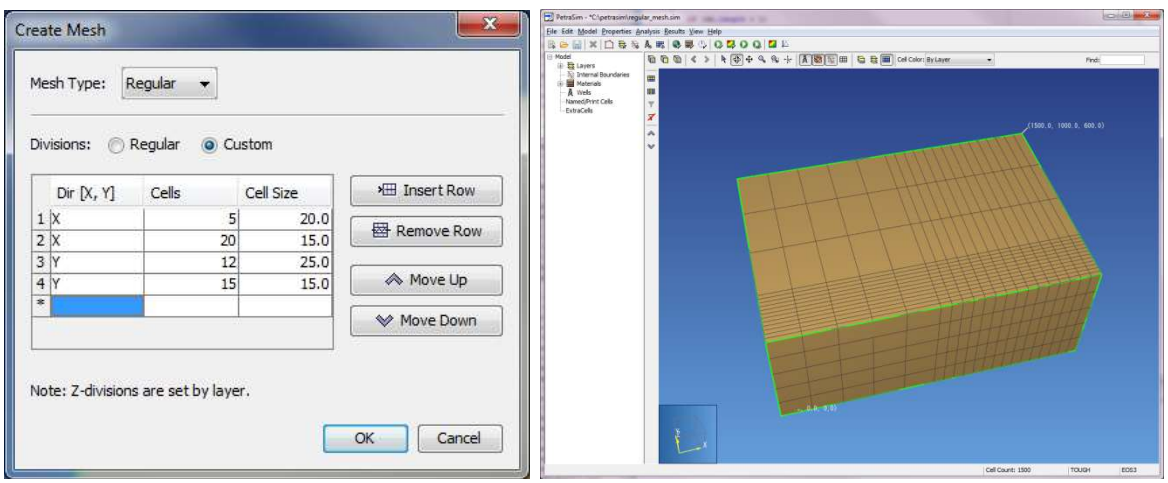



**Figure 7-6: Example of custom divisions for a regular mesh**

### *Polygonal Mesh*

A polygonal mesh can be used to match an arbitrary boundary or provide additional refinement around wells. The parameters for creating a polygonal mesh are shown in Figure 7-7.

- **Maximum Cell Area** –defines an approximate value for the maximum area of each cell in the XY plane.
- **Min Refinement Angle** – controls how quickly the area near wells disperses. The smaller this value is, the more quickly the cells will return to the maximum cell area extending radially out from the well.
- **Refine Wells** –specifies whether or not the area around wells should be automatically refined

- **Max Area near Wells** –defines an approximate XY cell area near wells.
- **Additional Refinement** –defines **X** and **Y** coordinates at which to apply refinement to the mesh. The **Area** defines an approximate XY cell area near the specified point of refinement.

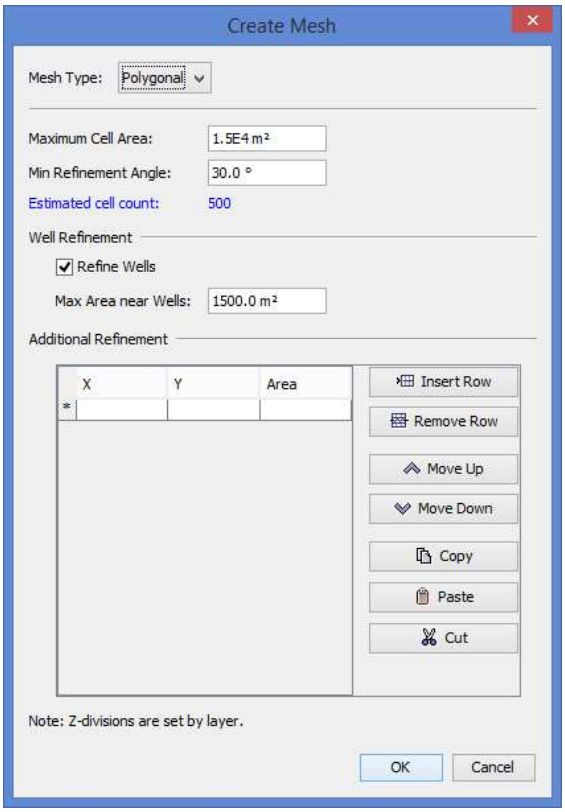



**Figure 7-7: Parameters for a polygonal mesh**

### *Radial Mesh*

The user can also create a radial RZ (axisymmetric) mesh. An RZ mesh is modeled as a 2D slice through a cylinder centered at (0,0,0) as shown in Figure 7-8. In this slice, the red line is the portion of the cylinder that is modeled by the RZ mesh. It appears in the model as a 2D regular mesh with the X divisions representing the radial divisions and the number of Y divisions being 1.[1]

[1] While the radial mesh will be displayed as a rectangular mesh with only one Y division, all cell data is displayed and written to the TOUGH input file with the correct cell volumes and connection areas to represent the cell revolved around the center of the cylinder.

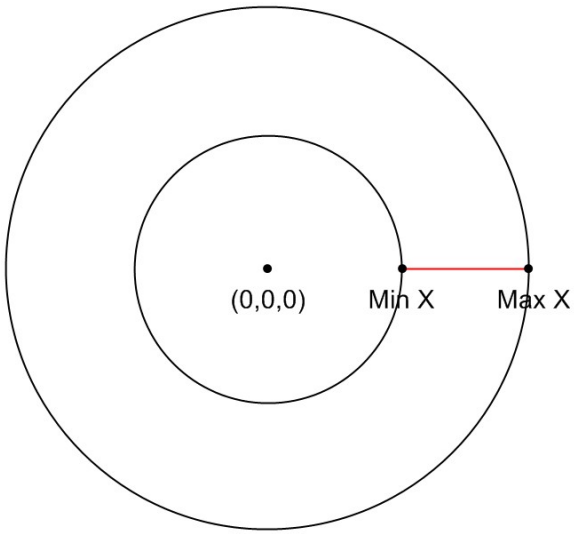



**Figure 7-8: Radial mesh representation in PetraSim**

To create a radial mesh, select the radial mesh option in the **Create Mesh** dialog as in Figure 7-9. The only parameter needed to create the mesh is the radial divisions, which correspond to the X divisions in the resulting mesh. These are specified similarly to the divisions in a **Regular Mesh**.

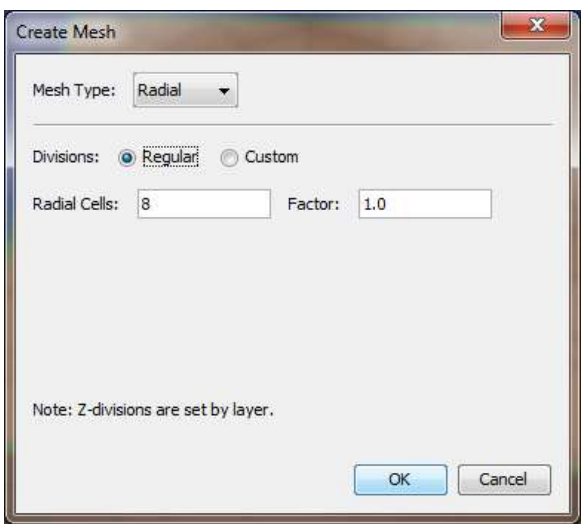



**Figure 7-9: Parameters for a radial mesh**

## Editing Cells

Once a mesh has been created, every cell will be assigned to a region in the conceptual model based on the center of the cell. This allows each cell to inherit the properties of the owning region, such as materials and initial conditions. Each cell may be edited to provide more fine-grained control over its properties. The user can edit the properties of a cell from the **3D View** or **Tree View** by double-clicking the desired cell or selecting the desired cells, right-clicking on one, and selecting **Edit Cells…** from the context menu as shown in Figure 7-10. The **Edit Cells** dialog is shown in Figure 7-11.

- **Cell Name** - A descriptive name that can be used to access cell results for plotting. If this name is not empty, the cell will be displayed in the **Tree View** under "Named/Print Cells".
- **Cell ID** - This is calculated by PetraSim, not editable.
- **X, Y, and Z Center** - The center of the cell, not editable.
- **Volume** - The volume of the cell calculated based on dimensions, not editable.
- **Volume Factor** - A multiplier on the volume that is used to obtain the final volume sent to the TOUGH input file.
- **Permeability Modifier** – A multiplier for the permeability of the cell sent to the TOUGH input file.
- **Porosity** – Sets the porosity of the cell. Because TOUGH interprets a value of 0.0 for this field as the same value as is set in the **Material** porosity, this field must be greater than 0.0.[1]
- **Material** - The material for the cell.[2]
- **Type** – The cell type. See Enabled, Disabled, and Fixed State Cells for further details.

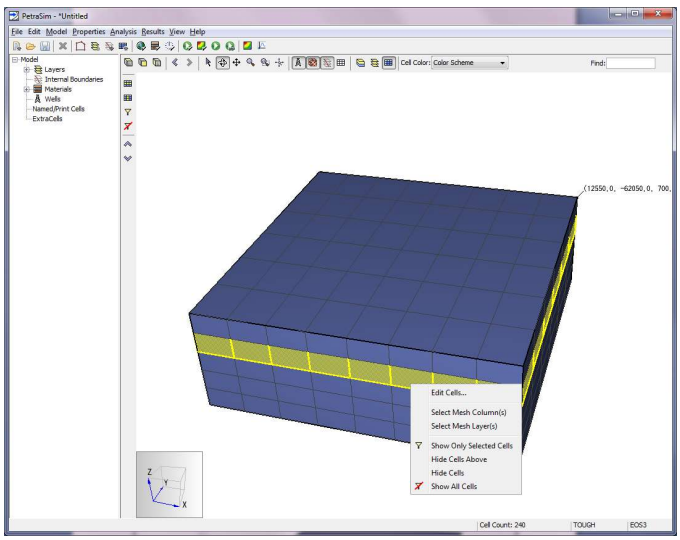



**Figure 7-10: Editing a cell in the 3D View**

[1] If "Auto" is selected in the drop-down, the property will be taken from the cell's selected material.
[2] If "Auto" is selected in the drop-down, the property will be taken from the cell's owning region.

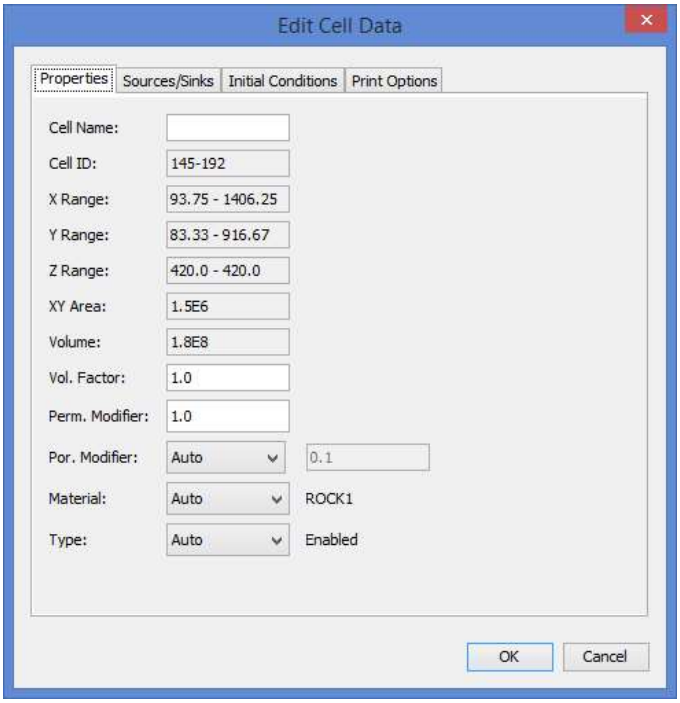



**Figure 7-11: Editing cell properties**

The Sources/Sinks and Initial Conditions tabs will be described in Boundary and Initial Conditions.

The Print Options tab is used to output cell data every time step for the selected cells (this is the FOFT file as used by TOUGH). In addition, connection data can be written (this is the COFT file as used by TOUGH).

### Enabled, Disabled, and Fixed State Cells

In the cell editor, a cell can be set to Type **Enabled**, **Disabled**, or **Fixed State**, with the following meanings:

- An **Enabled** cell is a standard cell in the analysis.
- A **Disabled** cell will not be included in the analysis. No information about this cell will be written to the TOUGH input file. It will not be included in the results.
- A **Fixed State** cell is used to set boundary conditions. The cell is included in the analysis, but the state of the cell (Pressure, Temperature, etc.) will not change. In the TOUGH2 User's Guide, such cells are named "Inactive". It was necessary for us to use a different name to distinguish between Fixed and Disabled cells.

## Extra Cells

There are times when the capability to add non-geometric "extra" cells is useful. These extra cells can be used to define special boundary conditions or in other ways to "trick" the model into representing some special feature.

Support for "extra" cells is provided in PetraSim through dialogs. Since these cells are not geometric, the user must define the volume and connections of these cells to the regular grid cells. To create an extra cell, on the **Model** menu**,** click **Add Extra Cell...**. Figure 7-12 illustrates the definition of the basic cell properties. These basic properties are similar to that of a normal cell as discussed in Editing Cells.

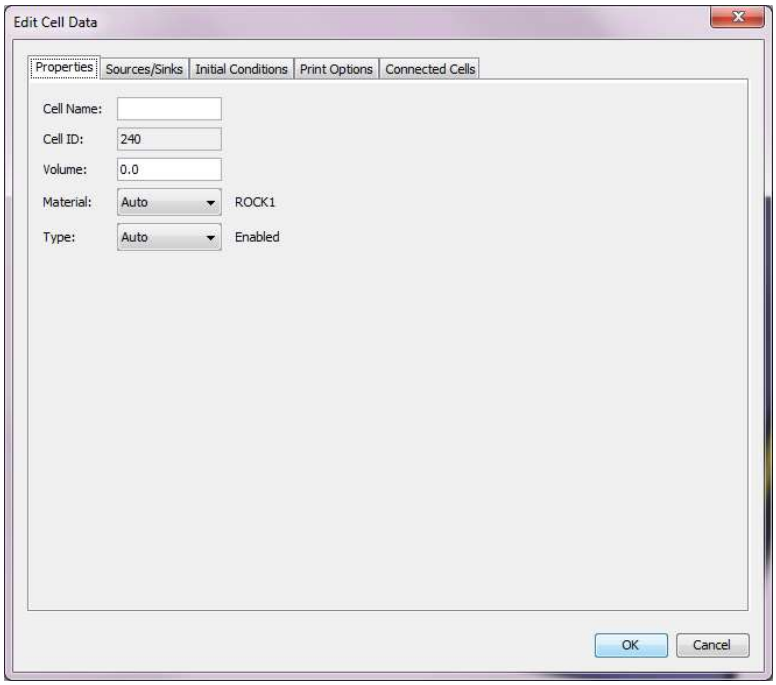



**Figure 7-12: Defining the basic extra cell properties**

The Sources/Sinks, Initial Conditions, and Print Options for an extra cell are the same as a standard cell.

The connections of the extra cell to the grid are specified by selecting the Connected Cells tab, Figure 7-13. The user must manually specify the connection data required by TOUGH. This includes:

- **To Cell** - This is the cell to which the extra cell is connected. This will be the cell ID of a cell in the mesh. You can find the cell ID of any cell using the Grid Editor and then viewing the cell properties.
- **Orientation** - This is must be 1, 2, or 3 and corresponds to the PermX, PermY, or PermZ definitions in the material data.
- **Dist. This** - The distance of the connection in the extra cell. See TOUGH concepts "Spatial Discretization."
- **Dist. To** - The distance of the connection in the connecting cell.
- **Area** - The cross-sectional area of the connection.
- **Gravitational Acceleration** - The cosine of the angle between the gravitational acceleration victor and the line between the two elements. If positive, the extra element is above the connecting "To" element.
- **Radiative Heat Transfer** - "Radian emmittance" factor for radiative heat transfer. Usually left as 0.0.

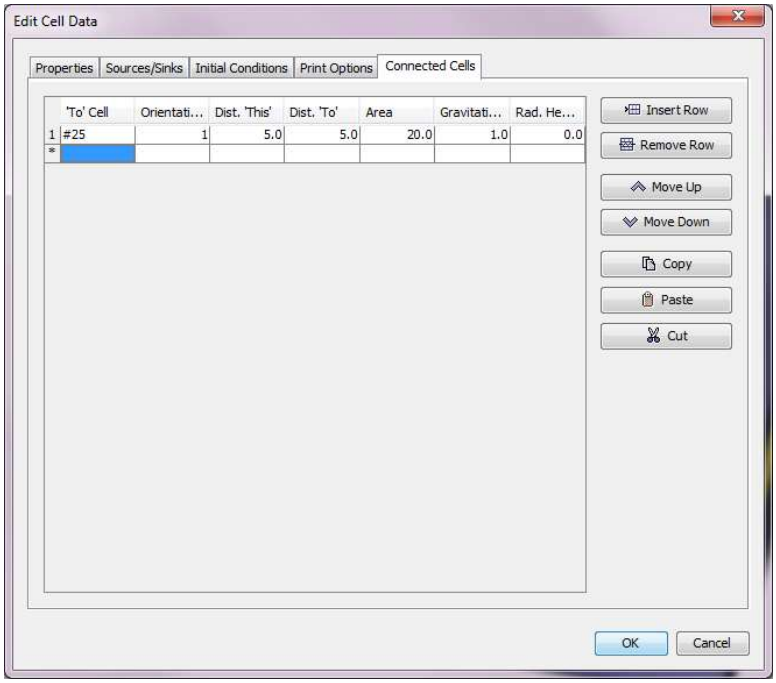



**Figure 7-13: Defining the extra cell connections to the model**

To edit an extra cell, double click on the extra cell in the Tree View.

# 8. Materials

Materials are used to define the permeability and other properties in an analysis. Each cell is associated with a material. Materials can be assigned by layer (select a layer and edit the layer properties), by region (select a region and edit the region properties), or to individual cells (select the cell and edit the cell properties). PetraSim uses inheritance to determine any particular cell property: it first looks in the cell; if the property is not found there, it looks in the region; then it looks in the layer; finally it looks in the default model.

When a new model is started, there is one default material. Material data is edited by selecting . In this dialog, the user can edit, create, and delete materials, Figure 8-1. The basic material data includes (many are self-explanatory):

- **Name** - The material name that will be written to the TOUGH input file, limited to five characters.
- **Description** - A longer description for user clarity.
- **Color** – The color that will be used in the **3D** and **Results** Views to color cells and regions when the cell or region color option is set to "Material."
- **Rock Density** - Density.
- **Porosity** - Porosity
- **X, Y, and Z Permeability** - The permeability is defined along each axis.[1]
- **Wet Heat Conductivity** - Wet conductivity
- **Specific Heat** - Specific heat.

[1] When using a **Polygonal** mesh, only an XY and Z permeabilities may be specified. The XY permeability is used between cells in one cell layer.

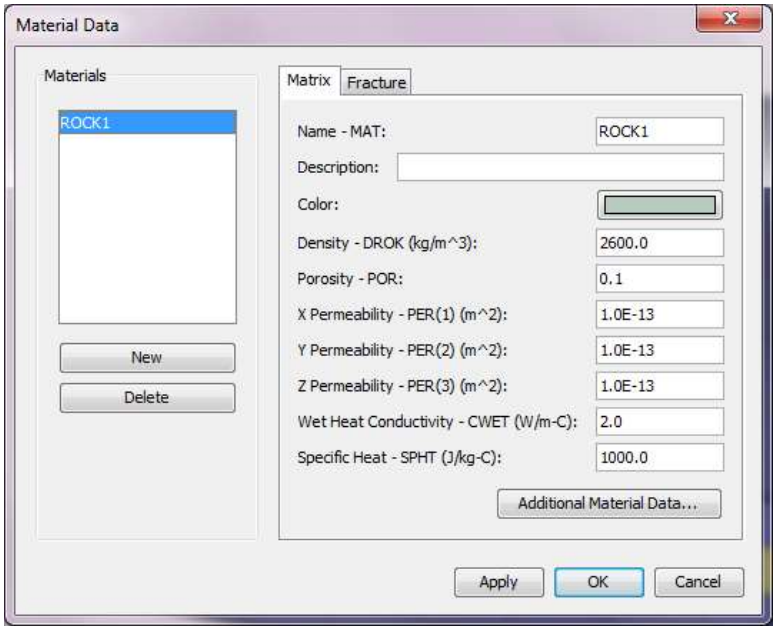



**Figure 8-1: Material properties**

## Relative Permeability

Selecting the **Relative Perm...** button displays the **Additional Material Data** dialog. The first tab is used to define Relative Permeability, Figure 8-2. The user selects the desired relative permeability function and then defines the parameters used by that function. A graph will display the permeability (magenta is gas; blue is liquid) as a function of liquid saturation.

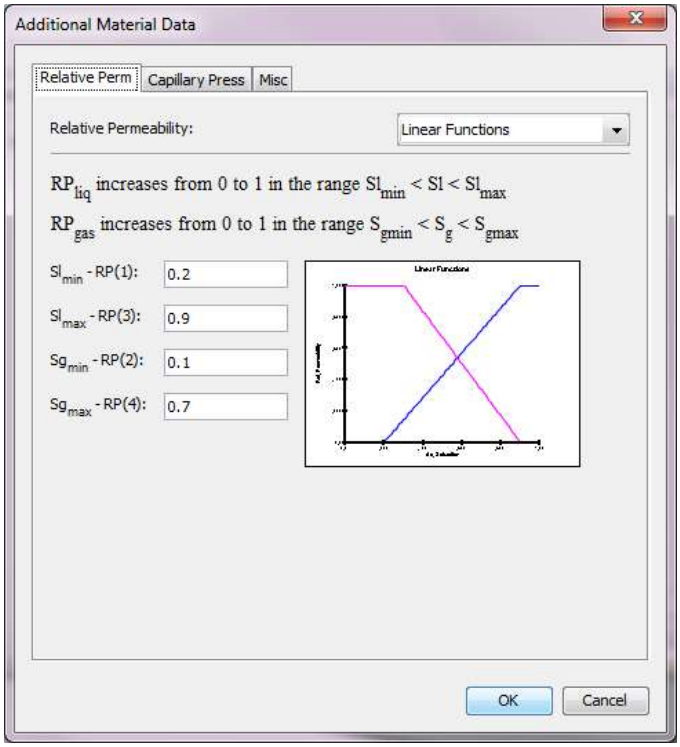



**Figure 8-2: Relative permeability functions**

## Capillary Pressure

Select the Capillary Pressure tab to define the capillary pressure function, Figure 8-3. The user selects the desired capillary pressure function and then defines the parameters used by that function. The value of ICP corresponds to the TOUGH function ID. The PetraSim Tools website provides a spreadsheet to plot the capillary pressure functions: https://www.rockware.com/petrasim-tools/.

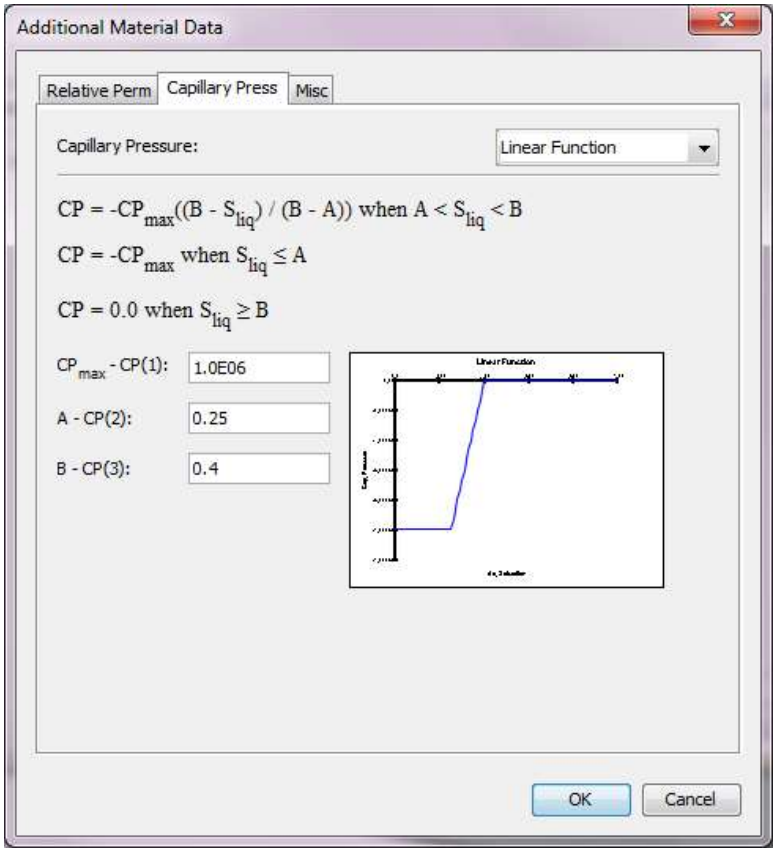



**Figure 8-3: Capillary pressure functions**

## Miscellaneous Material Data

Select the **Misc** tab to define additional material properties, Figure 8-4. These include:

- **Pore Compressibility** - This defines how the pore volume changes as a function of pressure. This is used when storativity is to be included in the model, such as when performing a well test analysis. In most cases, this is not used and remains 0.0.
- **Pore Expansivity** - This defines how the pore volume changes with temperature. In most cases, this is not used and remains 0.0.
- **Dry Heat Conductivity** - Used with the wet heat conductivity to change the thermal conductivity of the rock.
- **Tortuosity Factor** - The user is referred to Appendix D of the TOUGH2 User's Guide for a detailed discussion of this factor. In most cases, this is not used and remains 0.0.
- **Klinkenberg Parameter** - The user is referred to Appendix A of the TOUGH2 User's Guide for a detailed discussion of this factor. In most cases, this is not used and remains 0.0.

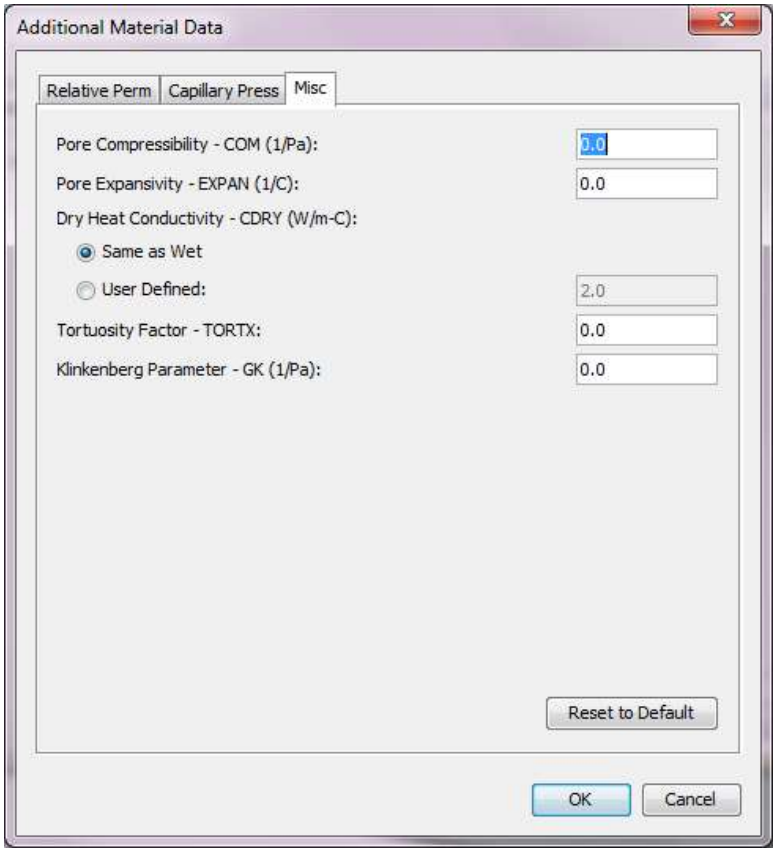



**Figure 8-4: Miscellaneous material data**

## Assigning Different Materials by Cell

To support the use of geostatistical data, PetraSim allows the user to import a table of material assignments for all cells. This is useful if the user has an independent representation of the model that can be queried to obtain a spatial definition of materials. PetraSim provides two tools:

- The capability to write a file with cell IDs and X, Y, Z coordinates.
- The ability to paste a table of material types for all cells.

To write a file with cell IDs and X, Y, Z coordinates, on the **File** menu, click **Write Grid Data...**. The resulting file defines the cell coordinates in their PetraSim order that allows you to query a separate material database.

On the **Model** menu**,** click **Assign Cell Materials...** to open the **Assign Cell Materials** dialog, Figure 8-5. You can either type or paste a list of materials to be assigned to each cell. All materials must have already been defined. Values in the **Material Name** column must match the name of a material stored in the current model.

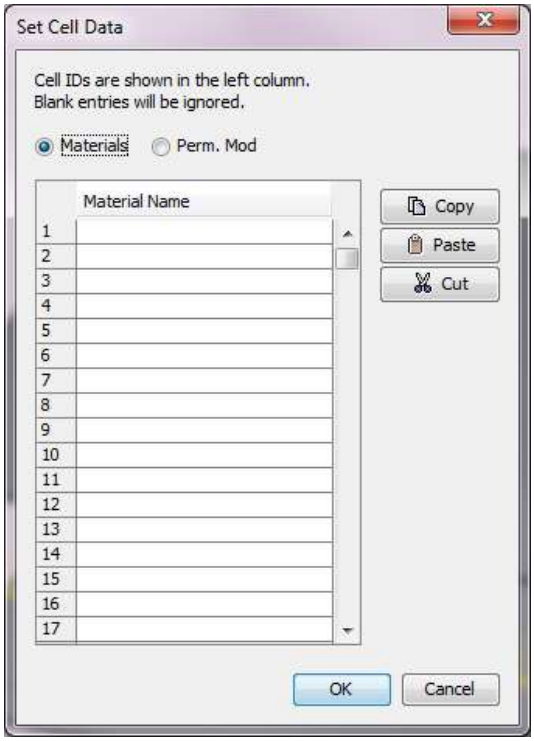



**Figure 8-5: Assign Cell Materials dialog**

# 9. Boundary and Initial Conditions

## Initial Conditions

Initial conditions are used to define the initial state of each cell. When generating the simulator input file, a hierarchy is used to determine values for each cell: if a value is defined at the cell, that value is used; if defined at the region, the region's value is used; if defined at the layer, the layer's value is used; finally, the default model initial conditions will be used.

The specific initial conditions are different for each EOS. For any specific EOS, there are at least single- and two-phase initial conditions, as well as options for different components. The user is referred to Chapter 3, Tough Concepts for a discussion of components and an example of setting single- and two-phase initial conditions.

Only for the simplest models will the initial conditions be uniform over the model. In most realistic analyses, a steady state simulation will be used to reach an equilibrium solution. For example, this will be used to reach gravity-capillary equilibrium in a vadose zone analysis or heat and fluid flow equilibrium in a geothermal reservoir analysis. The steady state results will then be used as initial conditions for the transient analysis. When this approach is used, two separate folders should be used to store the steady state analysis and the transient analysis.

Because of the complex physics represented in TOUGH, setting of the initial conditions can be challenging. The user is directed to the many examples available at the PetraSim web site for guidance on how others specify initial conditions.

### Default Initial Conditions

Default initial conditions are always defined for the model. To set these conditions, on the **Properties** menu**, click Initial Conditions...** ( ). This will open the Default Initial Conditions dialog, Figure 9-1.

You will then be provided all the available initial condition options that are valid for the EOS and selected components. Based on your knowledge of the problem, define these appropriately.

**Figure 9-1: Setting default initial conditions**

## Layer and Regional Initial Conditions

Initial conditions can also be set per layer or region. To do so, select the layer or region and then select **Edit->Properties...**. On the dialog, select the **Initial Conditions** tab. After selecting, **Specify by Layer/Region**, you will be able to define initial conditions, Figure 9-2. If you do not want region initial conditions to be used, deselect **Specify by Layer/Region** and the initial conditions will inherit from the parenting layer or default initial conditions for regions and layers, respectively.

**Figure 9-2: Setting region initial conditions**

## Cell Initial Conditions

To define initial conditions by cell, open the **Edit Cells** dialog as discussed in Editing Cells. On the Initial Conditions tab of the Edit Cell Data dialog, select **Specify Initial Conditions by Cell**, Figure 9-3. You will then be able to define initial conditions for a cell. If you do not want cell initial conditions to be used, select **Use Region (or Global) Initial Conditions**.

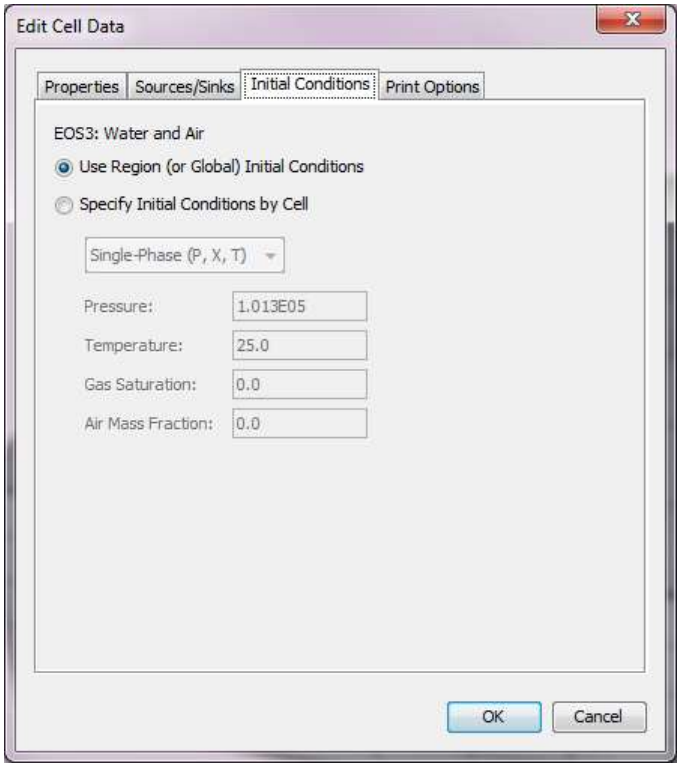



**Figure 9-3: Setting cell initial conditions**

### Loading Previous Results as Initial Conditions (Restart)

To read initial conditions from a previous analysis, select **File->Load Initial Conditions...** and read a previous SAVE file. The model used to write the SAVE file must have the same geometry as the model for which you are reading data. See the Restart section in this document for more details. Because the new analysis will over-write the existing SAVE file, save the PetraSim model to a new directory before starting the restart analysis. You can change the start time of the restart analysis to match the end time of the first analysis.

## Boundary Conditions

### Fixed Boundary Conditions

Boundary conditions where the pressure, temperature, and other variables do not change with time (called "essential" or Dirichlet boundary conditions) are typically set using "Fixed State" option in a cell. This is done by editing the cell (see Editing Cells for details).

A cell with fixed conditions will act as a source/sink for fluid and heat flow.

"Tricks" can be used to selectively fix the pressure or temperature independently. For example, to fix the pressure, the material of the cell can be changed so that the thermal conductivity is zero. Then, only fluid will flow to the cell and the cell will act as a fixed pressure. Similarly, the permeability could be set to zero for the cell to act as a fixed temperature condition.

## Sources and Sinks

Sources and sinks are used to define flow into or out of the cell. These are typically used to define production from or injection into a cell. This is used for situations such as a well in a reservoir or rainfall on the surface.

The rates can be defined as constant or using a table to give time/rate pairs. By default, PetraSim assumes a step change when a time history of input is specified. This can be changed in the Solution Parameters options.

To define a source or sink, open the **Edit Cell** dialog as discussed in Editing Cells. Select the **Sources/Sinks** tab as shown in Figure 9-4. The user has several options:

- **Heat** - The rate of Heat In can be defined as a constant or through a table as a function of time. Use a negative number to remove heat. If a flux is selected, the flow rate is equal to the flux multiplied by the area of the cell projected on the XY plane (the flux is in the Z direction).
- **Mass Out** - This defines the mass (or mass flux) rate produced from the cell.
- **Well on Deliverability** - This defines a boundary condition where the cell produces to a fixed pressure. The user defines the Productivity Index and the pressure. See page 64 of the TOUGH2 User's Guide for instructions on calculation of the Productivity Index.
- **Well from File** - This is a coupled wellbore flow model. See page 66 of the TOUGH2 User's Guide for instructions on its use.
- **Injection** - Injection parameters will vary depending on the EOS being used. In general, the user will specify injection rate (or flux) and enthalpy[1].

[1] In the case of simultaneously injecting multiple components into the same cell, specifying each of their individual enthalpies is not recommended because it would cause the simulator to disregard mixing effects. Instead, a separate simulation run should be performed with a single mixed element at desired initial conditions to calculate the correct mixed enthalpy. Then that enthalpy should be used for each component being injected into the same cell.

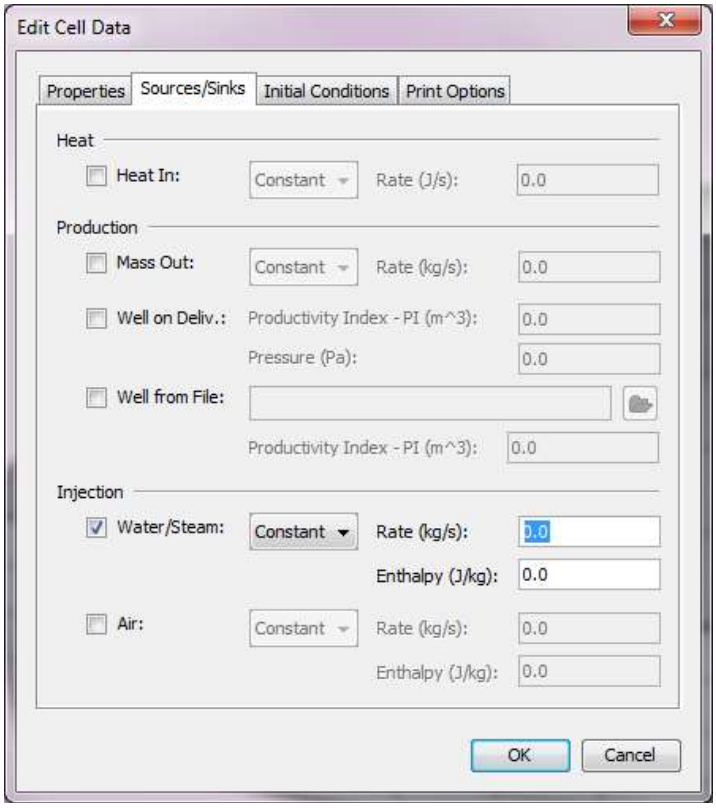



**Figure 9-4: Defining a cell as a source/sink**

## Load Cell Flow Rates

Basic source and sink data can be loaded from a data file. The first line of the file will list a series of cell names, separated by spaces. Each of these cell names must be defined in the PetraSim model. The second line gives the generation type (MASS, HEAT, COM1, etc.) for either injection or production at the given cell. The following lines each contain a time followed by pairs of flow rate and enthalpy for each cell. Enthalpy is required, but not used, for production wells. The content of an example input 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
```

This input file expects that there exist cells named P1, P2, and I1, defined before import. In this file, P1 and P2 are mass production wells, and I1 is an injection well (the injection type is EOS dependent). In the example, production occurs from only P1 for one year, then production from P2 and injection from I1 begin after one year. This table input is provided to allow spreadsheet editing for all well data.

## Using Wells in PetraSim

PetraSim provides a basic option to define wells as geometric objects (lines in 3D space). Injection or production options are assigned to the well and PetraSim handles the details of identifying the cells that are intersected by the well and applying the appropriate boundary conditions to each cell. This is not a true coupled well model; it is a means of identifying the cells that intersect a well and creating the individual sources/sinks for each cell. It also provides a way to label and display wells. The cells intersecting a well can be easily viewed and selected by right-clicking the well in the **Tree View** and selecting "Select Cells." Additional mesh refinement may be achieved around wells by using Polygonal meshes as discussed in the topic, Polygonal Mesh.

Adding a well and defining the boundary conditions is a two step process. Define the well coordinates by selecting **Add Well...** on the **Model** menu or from the main toolbar. This will open the **Add Well** dialog as shown in Figure 9-5. Name the well and give the coordinates in order, either starting at the top or bottom of the well. The new well will be displayed in the tree view.

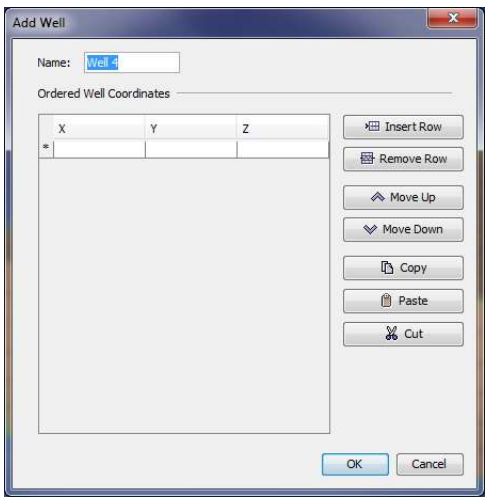



**Figure 9-5: Add Well dialog**

To edit the well, double-click it in the **Tree View**. This will show the **Edit Well** dialog as shown in Figure 9-6.

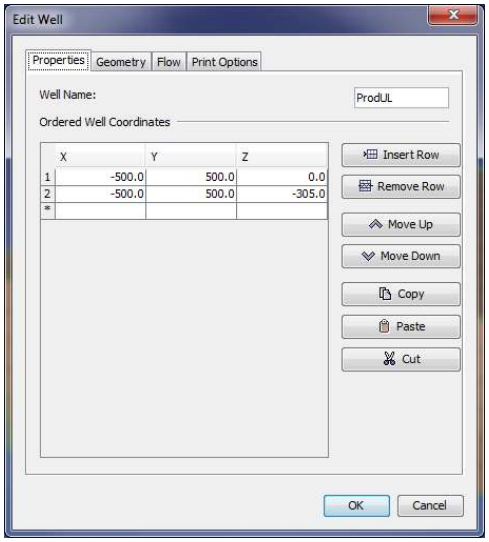



**Figure 9-6: Edit Well dialog**

The minimum and maximum Z coordinates of the completion interval (the range over which the well can flow to the porous media) can be edited under the **Geometry** tab. In the **3D View**, the completion interval is the red portion of the well as shown in Figure 9-7. For models that will use the **Well on Deliverability** option, it is best if these completion bounds correspond to gridlines in the model. This is because the entire cell depth is used when calculating the **Well on Deliverability** flow. If the well will use **k*h** or **Uniform** options to distribute the flow, then the completion interval does not need to correspond to the gridlines.

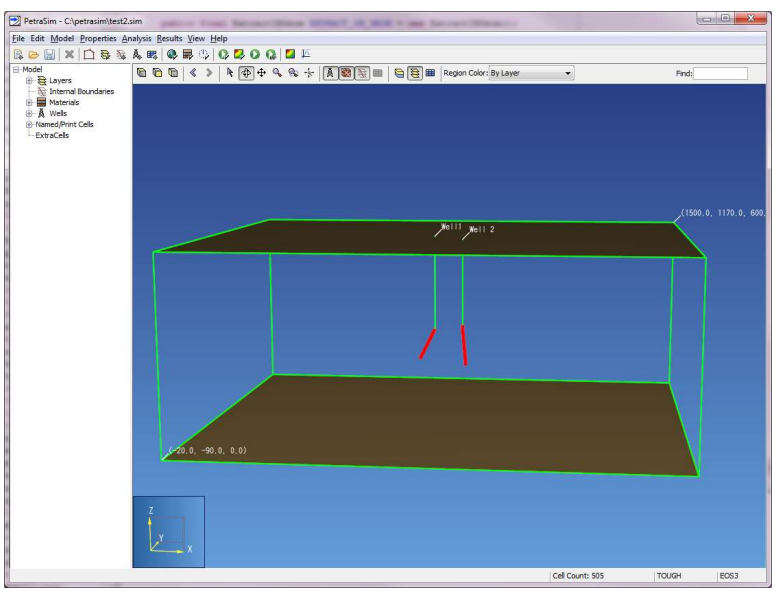



**Figure 9-7: Well completion interval in 3D View**

Select the appropriate production or injection options under the **Flow** tab. When flow rates are specified, the number is for the entire well. Flow into each cell the well intersects is apportioned either by k*h (permeability*height) or uniformly. If k*h is used, the total k*h is calculated for the entire well

and then the flow into each cell is determined by the permeability and height (intersection length) for that cell. Using this approach, more flow is injected (produced) into cells with higher permeability. The uniform distribution proportions flow by the intersection length of each cell. In either of these cases, PetraSim creates individual sources/sinks for each cell intersected by the well. These sources/sinks are independent of each other.

For the **Well on Deliverability** option, some additional methods are available to control how the well input is generated. When the **By Well** specification method is selected, the user can select the **Well Model** or **User Defined** gradient. The **Well Model** option activates the TOUGH2 well on deliverability model, where the pressure gradient is calculated using a depth dependent flowing density in the wellbore (see the TOUGH2 user manual). In this case, the specified pressure corresponds to the pressure at the center of the top cell in the well. If the **User Defined** gradient is selected, the pressure is that at the top of the completion interval and the user specifies the gradient directly. For both cases, follow the TOUGH2 guidelines for calculating the Productivity Index.

An alternative to the **By Well** specification method is to manual enter values for productivity index and pressure for each cell intersected by the well using a table. To enter manual well data, select **By Intersected Cells** and click Edit.

Output for the well can be controlled under the **Print Options** tab.

### *Reading and Writing Well Data*

PetraSim supports the import and export of well data. This feature can be used to edit wells in bulk, or to import known well data from an external source. To import wells, select **File->Load Well Data…**. Likewise, to export your well data for edit, select **File->Write Well Data…**.

For more information about the well data file format, see Appendix A.

## Time-Dependent Essential (Direchlet) Boundary Conditions

Although TOUGH2 provides an easy way to set constant essential (Dirichlet) boundary conditions using the "Inactive" cell option, there is no similar provision for time-dependent boundary conditions. There are two reasons for this decision:

- This places a significant burden on the user to ensure that all specified states would be physically meaningful.
- "The user could get into terrible problems when phase compositions change in the boundary cell, because then primary variables get switched. The user could end up interpolating between one number that means temperature, and another that means saturation." (15)

The alternate approach is to rely on TOUGH2 to handle any phase change by injecting or withdrawing mass and/or heat from boundary condition cells, thus using natural (Neumann) boundary conditions to obtain the desired essential boundary conditions in the cell. However, since this is an indirect way to accomplish the desired goal, the user needs some guidance on how to accomplish this.

The boundary condition cells should be thought of as cells that are not part of the solution. Therefore, we can set material properties and other parameters in ways that are not tied to the actual problem to be solved. The following sections describe some useful "tricks."

### *Use a Very Large Volume*

The first concept is to make the volume of the cell with the boundary condition "very large" relative to the other cells in the grid. There is no absolute definition of "very large" but the concept is that the volume should be so large that flow in and out of the boundary condition cell to model cells will have negligible effect on temperature or pressure in the boundary condition cell. A typical value could be a volume of 1.0E50 $m^3$. In PetraSim, this can be accomplished by setting the volume multiplication factor to a large number (see Editing Cells).

### *Setting a Temperature Condition*

For a simple temperature boundary condition, we do not want flow into or out of the cell. This can be accomplished by making a special material that has zero permeability and small porosity and applying it to this cell. It is also necessary that the connections between the temperature boundary condition cells and the other cells in the model have a non-zero length in the boundary condition cell. The use of zero permeability and small porosity has two effects:

- Because of the small porosity, calculating the necessary heat input/output to change the cell temperature is easy, since there is negligible fluid in the cell and the rock specific heat can be assumed for the entire cell.
- Because of zero permeability, no fluid will flow from this cell into any connected cells (the non-zero length connections are also necessary). Note: Although zero permeability is the correct approach, the user should be aware that for upstream weighting of absolute permeability (MOP(11) = 0 or 1), it is still possible to force flow into a cell with zero permeability and non-zero nodal distance (15).

The user then sets the desired initial temperature and then specifies the heat flow into (or out) of the cell to obtain the desired change in boundary condition cell temperature.

This method is directly applicable in PetraSim.

### *Setting a Pressure Boundary Condition*

Setting a pressure boundary condition can be accomplished in a similar manner as that used to set a temperature. In this case, a new material is created with zero thermal conductivity and assigned to the cell. As before, it is also necessary that the connections between the temperature boundary condition cells and the other cells in the model have a non-zero length in the boundary condition cell. The pressures in the cell can now be controlled by flow into and out of the cell (see the following example).

This method is directly applicable in PetraSim.

*Caution: If the specified pressure results in flow from the boundary condition cell to model cells, the heat transported by that flow will affect the temperature in the model cells.*

### *Combined Pressure and Temperature Boundary Conditions for Single Phase Liquid*

Experienced TOUGH2 users often apply simultaneous temperature and pressure boundary conditions by creating two boundary condition cells, as described above, and then connecting both boundary condition cells to the same cell in the model. TOUGH2 accommodates this, since it is not required that connections represent physically meaningful geometries. PetraSim supports this option through the use of "extra cells."

In the following we describe a way to accomplish the same objective, but using only physically meaningful geometry. This method also handles the combined pressure and temperature conditions in a way that usually corresponds to the desired physical behavior with respect to heat transport by flow out of the boundary condition cell.

Setting combined pressure and temperature boundary conditions will use the following concepts:

- A "very large" volume in the boundary condition cell. Consequently, heat or mass flow to connected model cells will have negligible effect on the temperature or pressure in the boundary condition cell.
- A "somewhat larger" permeability in the boundary condition cell (maybe 1000 times the normal value). This allows fluid flow into or out of the boundary condition cell and ensures that the pressure drop in the boundary condition cell will be approximately zero. Note: Pruess does not recommend changing the permeability due to possible numerical problems, but instead suggests changing the nodal distance to be small (1.0E-10).
- A "small" value for the porosity of the boundary condition cell. As a result, the rock heat capacity can be used to calculate the required heat flow to change temperatures.
- A "large" value of pore compressibility. This means that water compressibility can be neglected in the calculation of pressure changes due to flow into or out of the boundary condition cell and that changes in volume due to temperature changes will have negligible effect on pressure.
- Specification of heat flow to the boundary condition cell to obtain the desired time-dependent boundary temperature.
- Specification of fluid flow to the boundary condition cell to obtain the desired time-dependent boundary pressure.

### *Multi-Phase Pressure and Temperature Boundary Conditions*

For multi-phase conditions, the pore compressibility can be left as zero, since the gas phase will serve the same purpose. The flow to control pressure would use the gas phase and would need to account for the mixture compressibility.

### *Solution Controls*

The solution cannot resolve transients to a level finer than the time step. Therefore, it is necessary to limit the maximum time step. For example, if the period of a transient is one day, it will be necessary to divide the day into several time steps (5 to 10) to capture the transient response.

By default, TOUGH2 averages the flow data at the beginning and end of the time step. This is fine if the transient is smooth and several time steps are used during to resolve the transient. If larger time steps are used, it is important to activate the rigorous step rate option (In PetraSim, Solution Controls/Options).

### *Example*

The following example is based on a desire to specify time-dependent temperatures and pressures that represent the conditions for a stream in a groundwater calculation. The desired values are given in Figure 9-8 and Figure 9-9.

| Days | Time (sec) | Temperature (C) | Pressure (Pa) |
|---|---|---|---|
| 0 | 0 | 19.160000 | 105409.8525 |
| 1 | 86400 | 18.640000 | 110401.2634 |
| 2 | 172800 | 19.550000 | 116677.8879 |
| 3 | 259200 | 19.520565 | 116229.5576 |
| 4 | 345600 | 18.891391 | 111297.9241 |
| 5 | 432000 | 17.938530 | 109414.9367 |
| 6 | 518400 | 17.251983 | 113001.5793 |
| 7 | 604800 | 17.701749 | 115841.0046 |
| 8 | 691200 | 17.527829 | 112015.2526 |
| 9 | 777600 | 17.680223 | 108936.7177 |
| 10 | 864000 | 17.528930 | 107621.6154 |
| 11 | 950400 | 17.303951 | 106904.2869 |
| 12 | 1036800 | 16.662827 | 106426.0679 |
| 13 | 1123200 | 15.904299 | 106067.4037 |
| 14 | 1209600 | 15.329595 | 106515.734 |
| 15 | 1296000 | 14.898715 | 120653.0834 |
| 16 | 1382400 | 14.901659 | 115512.2291 |
| 17 | 1468800 | 14.768427 | 114346.5702 |
| 18 | 1555200 | 14.879019 | 112702.6924 |
| 19 | 1641600 | 15.213435 | 110102.3765 |
| 20 | 1728000 | 15.042283 | 108906.829 |

**Figure 9-8: Desired boundary conditions**

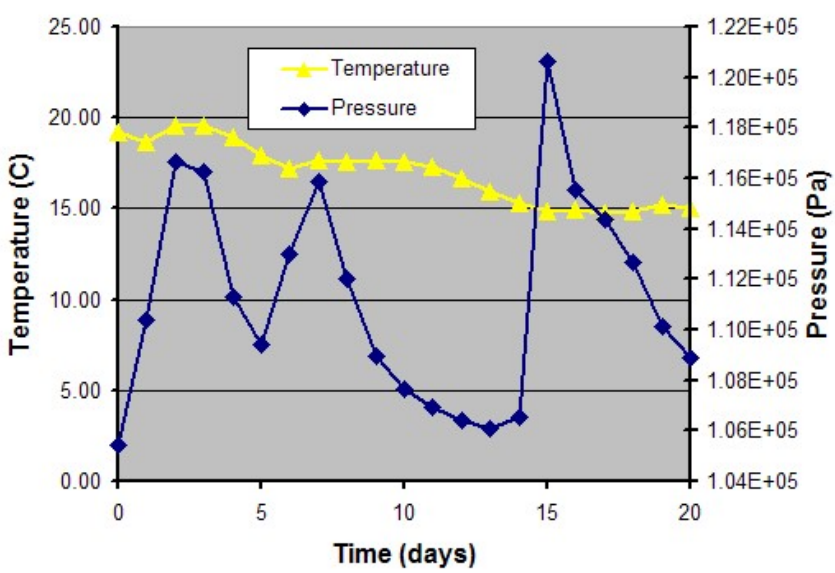



**Figure 9-9: Graph of desired boundary conditions**

For the example, create a cell with dimensions of 1 m on each side, but set the volume factor to be 1.0E50. We set the material properties as Figure 9-10.

| Property | Value |
|---|---|
| Rock Density (kg/m3) | 2600 |
| Rock Porosity | 0.001 |
| Permeability (m2) | 1E-13 |
| Specific Heat (J/kg-C) | 1000 |
| Pore Compressibility (1/Pa) | 1.-E-6 |

**Figure 9-10: Desired boundary conditions**

We calculate the heat flux as follows:

$$\dot{Q} = V\rho c_p \frac{\Delta T}{\Delta t}$$

where $\dot{Q}$ is the heat flux, $V$ is the cell volume, $\rho$ is the rock density, $c_p$ is the rock heat capacity, $\Delta T$ is the change in temperature, and $\Delta t$ is the change in time. Note that since the porosity is very small, we only use the rock properties and apply this to the entire cell volume. The calculated values are shown in Figure 9-11.

| Time (sec) | Temperature (C) | Heat Flux J/s |
|---|---|---|
| 0 | 19.160000 | -1.564815E+51 |
| 86400 | 18.640000 | 2.738426E+51 |
| 172800 | 19.550000 | -8.857694E+49 |
| 259200 | 19.520565 | -1.893349E+51 |
| 345600 | 18.891391 | -2.867405E+51 |
| 432000 | 17.938530 | -2.065999E+51 |
| 518400 | 17.251983 | 1.353464E+51 |
| 604800 | 17.701749 | -5.233704E+50 |
| 691200 | 17.527829 | 4.585919E+50 |
| 777600 | 17.680223 | -4.552793E+50 |
| 864000 | 17.528930 | -6.770207E+50 |
| 950400 | 17.303951 | -1.929308E+51 |
| 1036800 | 16.662827 | -2.282607E+51 |
| 1123200 | 15.904299 | -1.729433E+51 |
| 1209600 | 15.329595 | -1.296630E+51 |
| 1296000 | 14.898715 | 8.859259E+48 |
| 1382400 | 14.901659 | -4.009296E+50 |
| 1468800 | 14.768427 | 3.328000E+50 |
| 1555200 | 14.879019 | 1.006344E+51 |
| 1641600 | 15.213435 | -5.150394E+50 |
| 1728000 | 15.042283 | 6.362092E+48 |
| | 15.000000 | |

**Figure 9-11: Calculated heat flux**

Similarly, we calculate the required fluid flow rates using:

$$\dot{m} = \rho_{water} \emptyset V C \frac{\Delta P}{\Delta t}$$

where $\rho_{water}$ is the density of water, $\emptyset$ is the porosity, $C$ is the pore compressibility, and $\Delta P$ is the change in pressure. The calculated values are shown in Figure 9-12.

| Time (sec) | Pressure (Pa) | Flow kg/s |
|---|---|---|
| 0 | 105409.8525 | 5.77132E+42 |
| 86400 | 110401.2634 | 7.25735E+42 |
| 172800 | 116677.8879 | -5.18382E+41 |
| 259200 | 116229.5576 | -5.7022E+42 |
| 345600 | 111297.9241 | -2.1772E+42 |
| 432000 | 109414.9367 | 4.14706E+42 |
| 518400 | 113001.5793 | 3.28309E+42 |
| 604800 | 115841.0046 | -4.42353E+42 |
| 691200 | 112015.2526 | -3.55956E+42 |
| 777600 | 108936.7177 | -1.52059E+42 |
| 864000 | 107621.6154 | -8.29411E+41 |
| 950400 | 106904.2869 | -5.52941E+41 |
| 1036800 | 106426.0679 | -4.14706E+41 |
| 1123200 | 106067.4037 | 5.18382E+41 |
| 1209600 | 106515.734 | 1.63463E+43 |
| 1296000 | 120653.0834 | -5.94411E+42 |
| 1382400 | 115512.2291 | -1.34779E+42 |
| 1468800 | 114346.5702 | -1.90073E+42 |
| 1555200 | 112702.6924 | -3.00662E+42 |
| 1641600 | 110102.3765 | -1.38235E+42 |
| 1728000 | 108906.829 | 0 |
| | 108906.829 | |

**Figure 9-12: Calculated flow rates**

These are input to TOUGH2. Note that this is a bit tricky, since injection and production must both be set on the same cell. This means that two separate conditions must be set. The injection for flow in and the production for flow out. Set these terms zero when the other is acting, that is, during injection, the production is zero and during production the injection is zero.

The resulting plots show excellent agreement between temperatures, and not quite as good agreement for pressures.

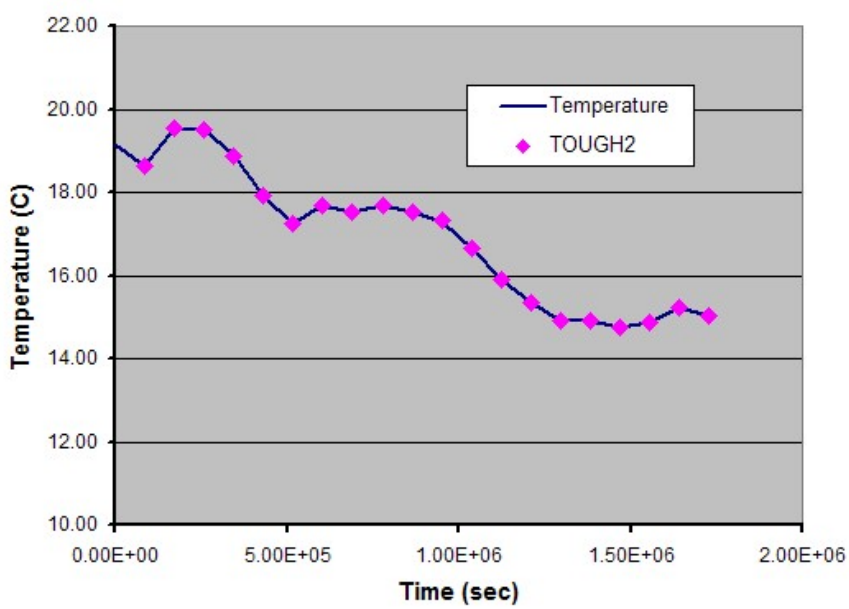



**Figure 9-13: Comparison of desired and calculated boundary condition temperatures**

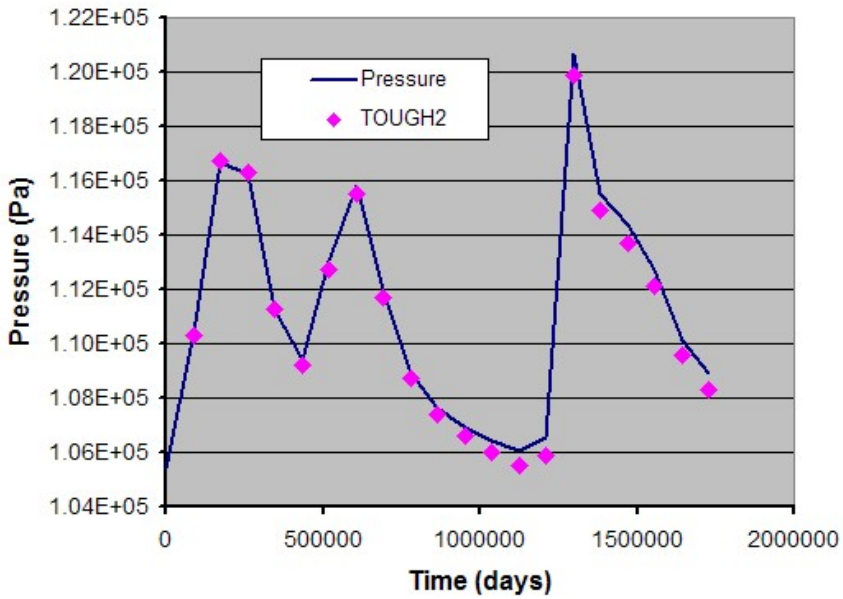



**Figure 9-14: Comparison of desired and calculated boundary condition pressures in TOUGH2**

These concepts are described in an example problem available on the PetraSim web site.

# 10. Solution and Output Controls

## Solution Controls

The Solution Controls dialog allows the user to specify all aspects that will be used by TOUGH in solving the problem. To set these controls, select **Analysis->Solution Controls…** or to open the Solution Controls dialog.

### Times Tab

Select the **Times** tab, Figure 10-1. This tab is used to input all data related to solution times and time step control.

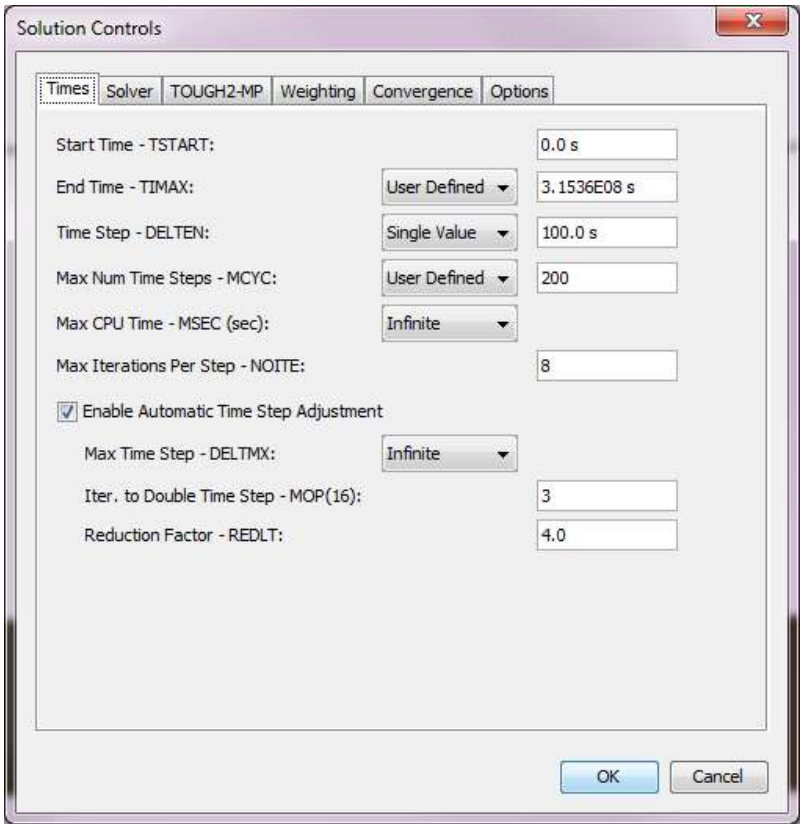



**Figure 10-1: The Times tab controls**

- **Start Time** - The start of the analysis. In most cases this will be 0.0.
- **End Time** - The end time of the analysis. Usually specified, but can be set to infinite and then solution will run for the Max Num Time Steps
- **Time Step** - User control of the time steps. If Automatic Time Step Adjustment is enabled (recommended), this is the initial time step used in the analysis. The user can also specify a table of time steps for the solution. If a list of time steps is given, the last time step will be used until the End Time is reached. If the user has selected to define the time steps in a table and enabled Automatic Time Step Adjustment, the specified table of time steps is used first, with

automatic adjustment after if the number of solution time steps exceeds the number of time steps in the list.

- **Max Num Time Steps** - The maximum number of time steps for the solution. If this number is exceeded, the analysis ends.
- **Max CPU Time** - A control to limit the maximum CPU time used in the analysis. If this number is exceeded, the analysis ends
- **Max Iterations per Step** - The maximum number of iterations for a time step. If exceeded and Automatic Time Step Adjustment is enabled, then time step will be reduced.
- **Automatic Time Step Adjustment** - If selected, the time step size will be automatically adjusted (recommended).
- **Max Time Step** - Maximum time step that will be used when adjusting the time step.
- **Iter. to Double Time Step** - If convergence is reached in this number of iterations, then time step size will be increased.
- **Reduction Factor** - If convergence fails in Max Iterations per Step, then time step will be reduced by this factor.

### Solver Tab

Select the **Solver** tab, Figure 10-2. TOUGH provides conjugate gradient and direct solvers, with several options. The user can select the solution method and options for that method. Either the Preconditioned Bi-Conjugate Gradient (default) or Stabilized Bi-Conjugate Gradient methods are recommended.

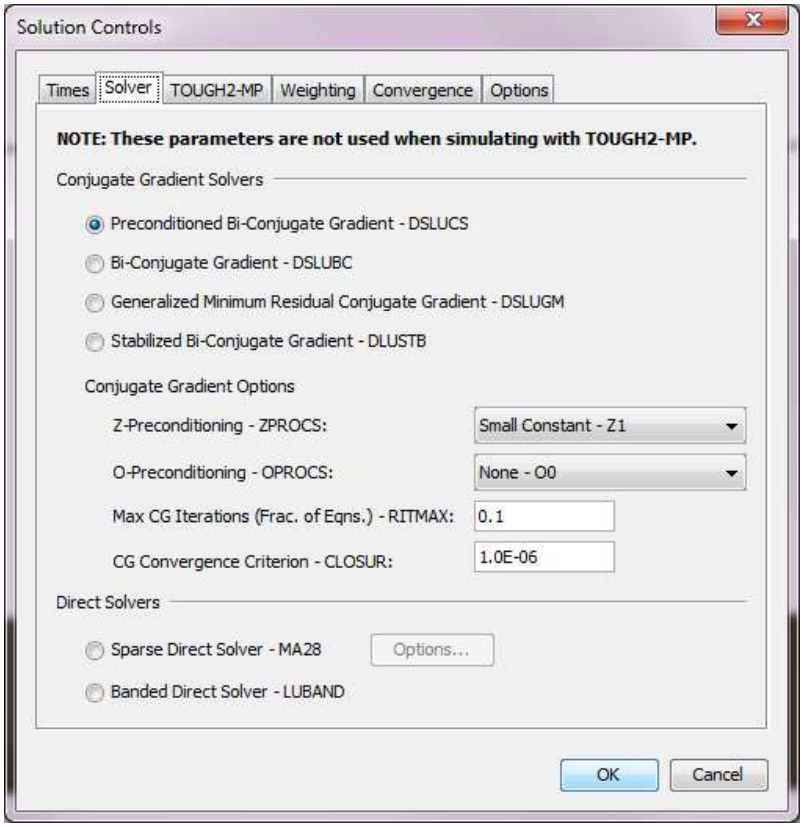



**Figure 10-2: The Solver tab controls**

## TOUGH2-MP Tab (TOUGH2-MP license only)

Select the **TOUGH2-MP** tab, Figure 10-3. These are options for the TOUGH2-MP simulator. The Additional N/R iterations after convergence option controls the value of MOP(21) in record PARAM.1. The simulator can be set to perform one additional Newton-Raphson iteration after convergence if needed.

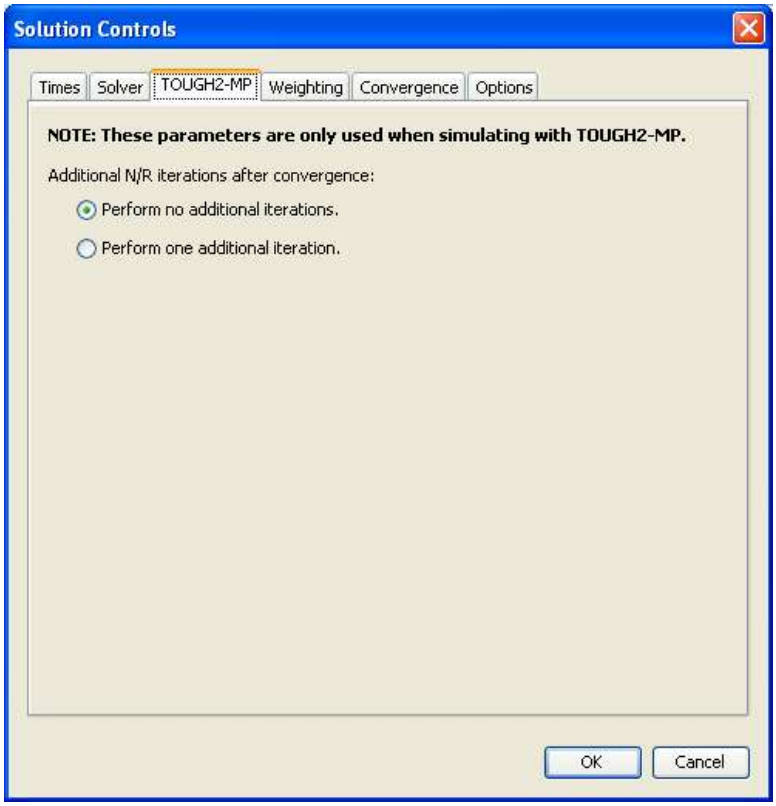



**Figure 10-3: The TOUGH2-MP tab controls**

## Weighting Tab

Select the **Weighting** tab, Figure 10-4. This tab provides several options about the weighting in calculations at interfaces.

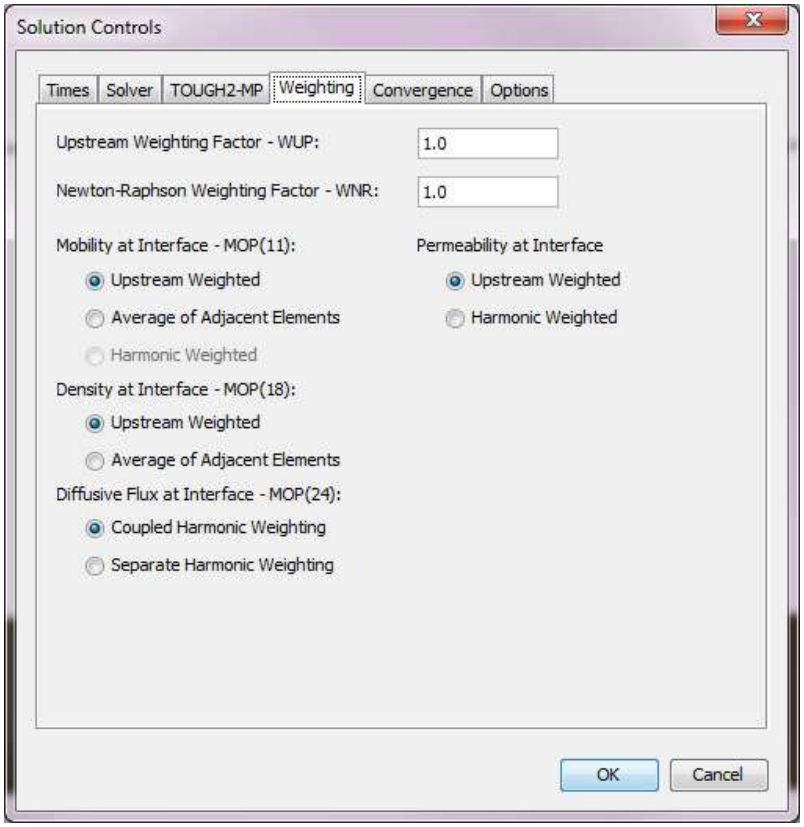



**Figure 10-4: The Weighting tab controls**

The Upstream Weighting Factor is used to calculate mobilities and enthalpies at interfaces, and must be a value from 0 to 1. The Newton-Raphson Weighting Factor is used to calculate increments in Newton-Raphson iteration, and must be a value from 0 to 1.

## Convergence Tab

Select the **Convergence** tab, Figure 10-5 to edit the Relative Error Criterion and Absolute Error Criterion. For more information on these values, see the TOUGH2 User's Guide.

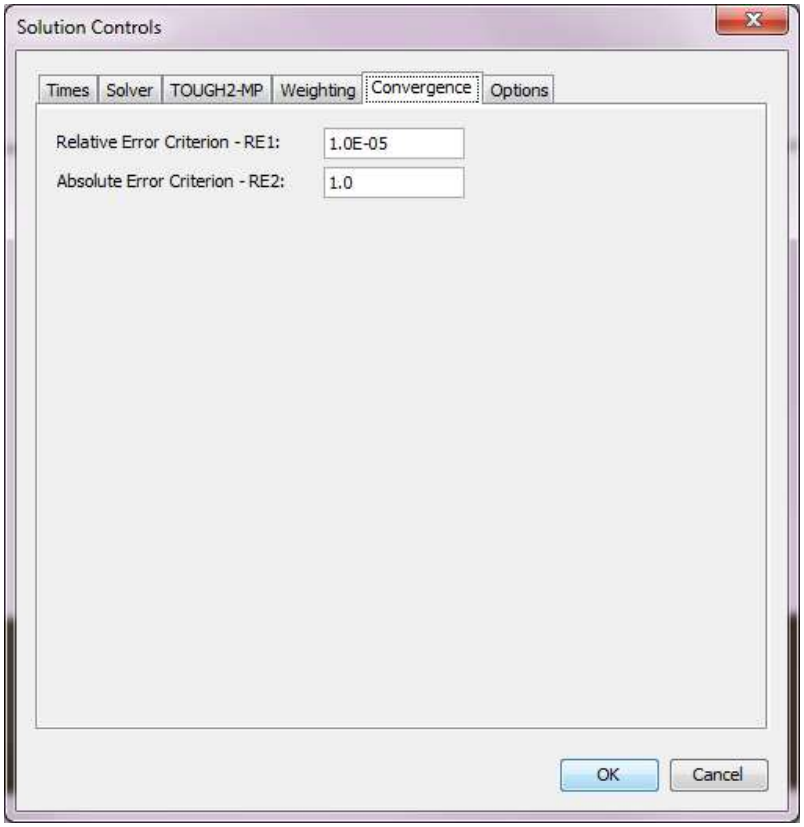



**Figure 10-5: The Convergence tab**

## Options Tab

Select the **Options** tab, Figure 10-6. This tab allows the selection of various other options provided by TOUGH2.

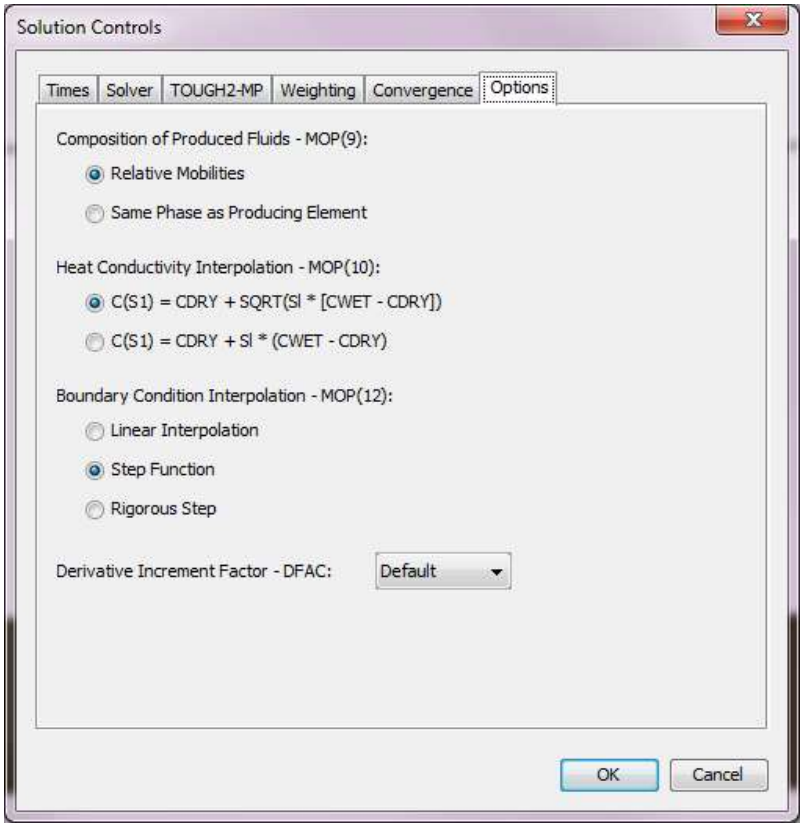



**Figure 10-6: The Options tab controls**

- **Composition of Produced Fluids** - The relative amounts of phases in the produced fluid are determined either according to the relative mobilities in the source element or the same as the producing element.
- **Heat Conductivity Interpolation** - The interpolation formula for heat conductivity as a function of liquid saturation ($S_l$).
- **Boundary Condition Interpolation** -The interpolation procedure for time dependent sink/source data (flow rates and enthalpies).
- **Derivative Increment Factor** – The increment factor for numerically computing derivatives.

## Output Controls

The Output Controls dialog allows the user to specify output options. To set these controls, on the **Analysis** menu**,** click **Output Controls…** ( ), see Figure 10-7.

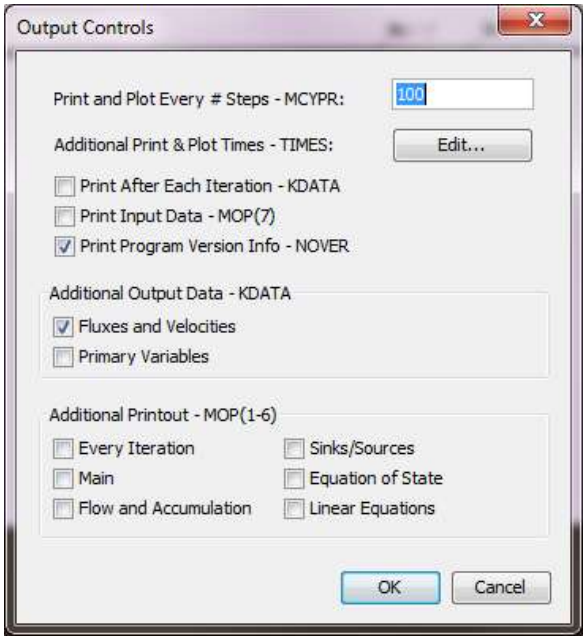



**Figure 10-7: Output controls dialog**

Output Controls options include:

- **Print and Plot Every # Steps** - Output will be written at the specified time step increment.
- **Additional Print and Plot Times** - This opens a table in which you can give specific times at which output is desired.
- **Additional Output Data** - Select fluxes and velocities to have the output data necessary to include flux arrows in the 3D plots. Selecting Primary Variables is usually only used for debugging purposes.
- **Additional Printout** - These options are usually only used for debugging purposes.

# 11. Running Simulation

## Running a Simulation

To run a simulation: on the **Analysis** menu, click **Run TOUGH2** ( ). This will first save the PetraSim model file and then the **Running TOUGH2** dialog will be displayed, Figure 11-1.

The **Running TOUGH2** dialog displays simulation time steps on the X-axis and the log of the time step on the Y-axis. As a rule of thumb, a growing time step is a good sign of simulation progress. If your time steps start to become smaller, it may indicate that the simulator is having a difficult time converging.

When the simulation finishes, a message will be displayed and the **Cancel** button will turn into a **Close** button. Click the **Close** button.

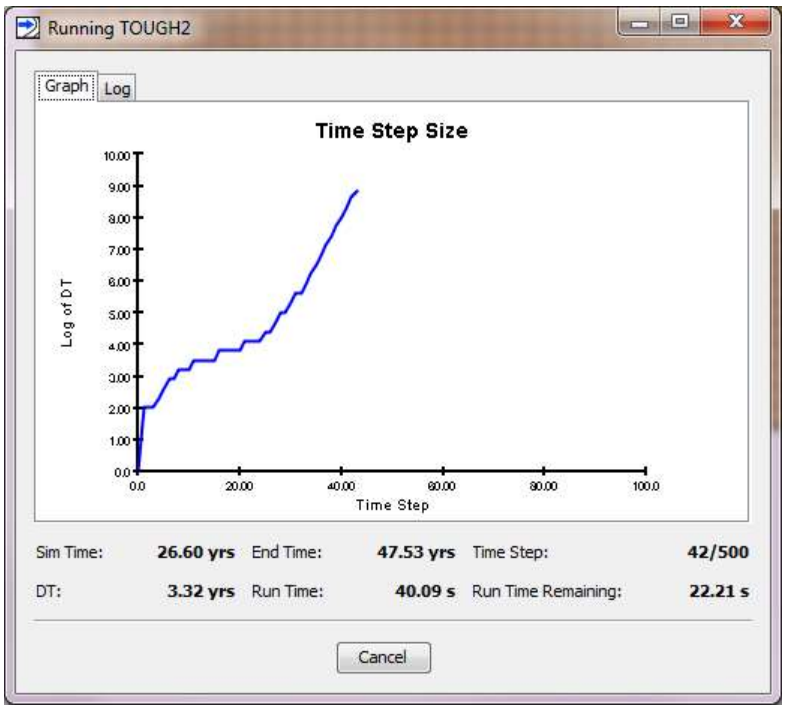



**Figure 11-1: Running the TOUGH analysis**

## Setting TOUGH2 Analysis Priority

A TOUGH2 analysis makes heavy demands of the computer processor; if you are running a single core computer, you may want to reduce the priority of the TOUGH analysis. Start the Task Manager (Ctrl+Alt+Delete or right-click on the lower toolbar). On the Processes tab, click on CPU to sort by the process using the most CPU (you many need to click twice to bring highest CPU users to the top of the list). You will see a process such as "EOS7.exe". Right-click on the process, select Set Priority and select Low. Close the dialog.

Setting the priority low will keep your computer response snappy to other tasks and allow the CPU to support the TOUGH analysis when not needed for other tasks.

## Monitoring Progress of TOUGH Analysis

During the TOUGH analysis, there are several ways to monitor progress. One way is to go to the problem directory and, using a text editor, open the *.out file as it is written by TOUGH. In this file will be text similar to the following:

```
*******************************************************
     260(  21,  3) ST = 0.209715E+09 DT = 0.104858E+09
     365(  22,  3) ST = 0.419430E+09 DT = 0.209715E+09
      51(  23,  4) ST = 0.838861E+09 DT = 0.419430E+09
     216(  24,  4) ST = 0.125829E+10 DT = 0.419430E+09
     258(  25,  4) ST = 0.167772E+10 DT = 0.419430E+09
```

The first number is the ID of the cell with the smallest time step. The first number in the parentheses is the time step counter and the second number is the number of iterations required for that step to converge. ST is the total solution time. DT is the solution time increment.

## Writing the Input File

Most users will not need to explicitly save a input file, since this is automatically written when the analysis is performed. However, if you are using a special executable, you can save the input file without attempting to run a simulation. To save the input file(s): on the **File** menu, click **Write TOUGH2 File...** to write the input file. If you are using another simulator (e.g. TOUGHREACT) the name of this action will be slightly different.

This file can then be edited (if necessary) and used to run your custom simulator from the command line. The results of custom compiles are not generally compatible with PetraSim's results visualization system. If you would like suggestions on how to modify custom binaries to generate PetraSim-compatible output, please contact technical support.

## Running TOUGH2-MP

TOUGH2-MP is a parallel version of TOUGH2 providing several improvements to the TOUGH2 code, including support for multiple processors and multiple machines, which can significantly reduce the time needed to run simulations. It also removes the cell count and cell connection limitations in TOUGH2, allowing multi-million cell problems.

Support for TOUGH2-MP is seamlessly integrated into PetraSim and can be purchased for nearly all EOS'. PetraSim supports TOUGH2-MP by running several processes on a single-computer with multiple cores. The number of processes to be used for TOUGH2-MP simulations may be specified in the **Preferences** dialog by going to the **File** menu and selecting **Preferences…**. By default, PetraSim will start TOUGH2-MP with as many processes as there are cores on the current PC. For instance, if the PC contains two, four-core processors (eight total), PetraSim will use eight processes to run the simulation.

TOUGH2-MP is run similarly to TOUGH2: after setting up the problem, under the **Analysis** menu, select **Run TOUGH2-MP** ( ). The same progress dialog is used to monitor the simulation as shown Figure 11-1. Viewing results is the same as in TOUGH2.

# 12. Plotting Results

PetraSim reads the TOUGH output files to make plots of results. The user can make 3D or time history plots of the data. When a plot is displayed, selecting **File/Export Data...** will allow the user to export the current plot data in either Tecplot or spreadsheet format.

## 3D Plots of Results

To make a 3D plot of results: on the **Results** menu, click **3D Results...** ( ). This will open a new window with a display of the model and pressure isosurfaces at the first output time, Figure 12-1.

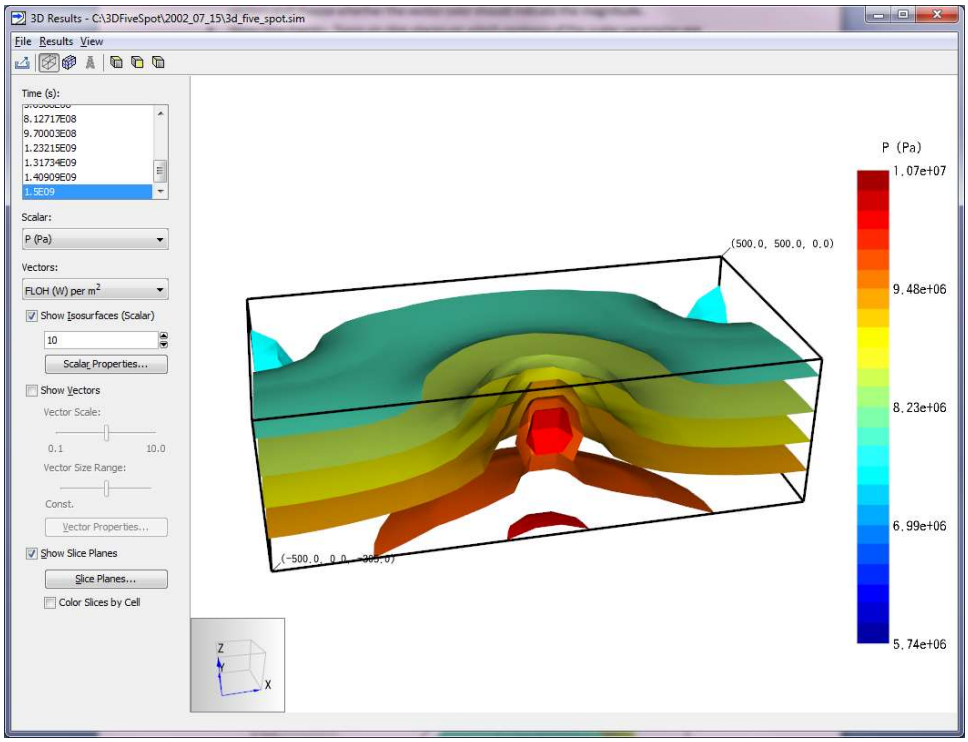



**Figure 12-1: The 3D results window**

Plot controls include:

- **Time (s)** - A window that displays all the available output times. Select one of these times for plotting.
- **Scalar** - Select the output parameter for plotting. The scalar parameter is the one that will be used for isosurfaces and contours on slice planes. The list of parameters is dynamically created from the TOUGH output file and will be different for each EOS.
- **Vectors** - If vector data was written to the output (this must be selected as one of the Output Controls options), this will display a list of available vector data. The list of parameters is dynamically created from the TOUGH output file and will be different for each EOS.
- **Show Isosurfaces** - This checkbox turns on the display of isosurfaces for the selected scalar. The number indicates how many isosurfaces will divide the plot range. Selecting the **Scalar**

**Properties...** button displays a dialog, Figure 12-2, on which you can specify a specific plot range, choose to use a logarithmic scale, and specify the number of colors used on contour plots.

- **Show Colorblock Plots** – Selecting this option will allow the visualization of grid cells in the 3D Results using the Cell Coloring options from the editor. This allows you to see the visualization of the results uninterrupted by interpolation between cells. When this option is selected, so too are the mesh selection tools, making it possible to isolate specific sections of the model for visualization.
- **Show Vectors** - If vector information is available, selecting the checkbox will turn on the display of vector data, Figure 12-3. The Vector Scale controls the scaling factor applied to the vectors and the Vector Size Range controls the relative size of the longest to shortest vectors. By default, both the relative size and color of the vectors correspond to the magnitude of the vector. Moving the Vector Size Range to the left will result in all vectors having the same length. Selecting the **Vector Properties...** button displays a dialog, Figure 12-4, in which the user can set the range for vectors and choose whether the vector color should indicate the magnitude.
- **Show Slice Planes** - Turns on slice planes on which contours of the scalar parameter are displayed. Select the **Slice Planes...** button to define the axes normal to the planes and the coordinates of the planes, Figure 12-5. Typical plots are shown in Figure 12-6. You can also view the slices as discrete values per cell as shown in Figure 12-7 by selecting **Color Slices by Cell**.

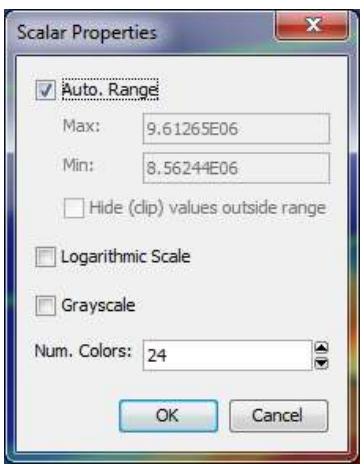



**Figure 12-2: Scalar Properties dialog**

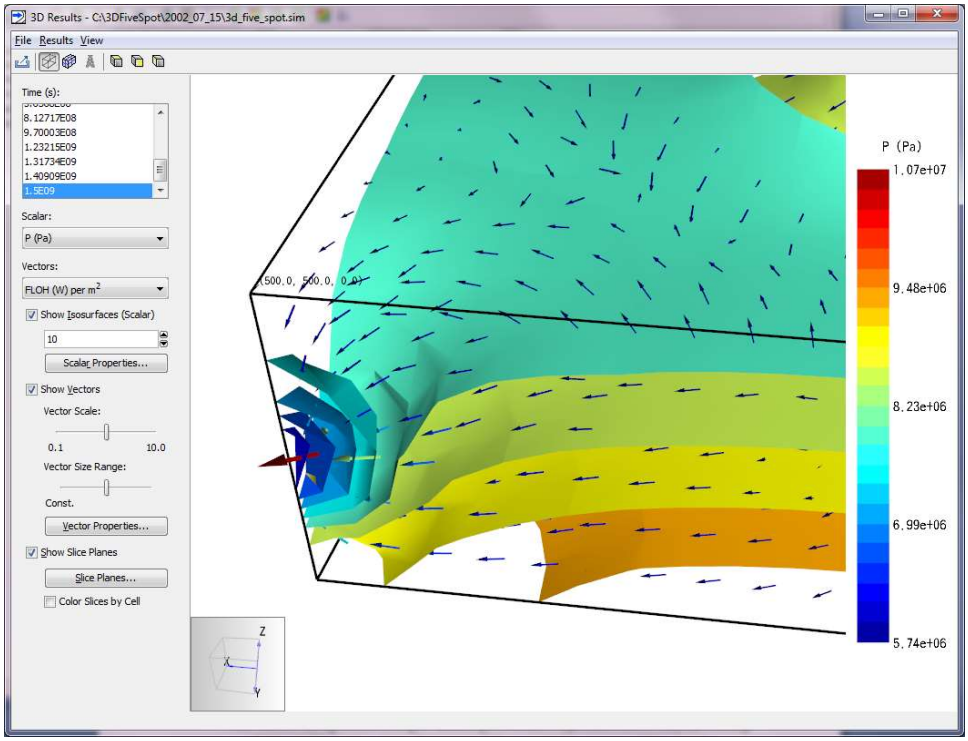



**Figure 12-3: 3D Vector results**

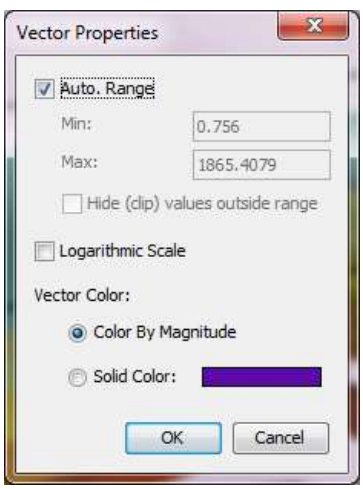



**Figure 12-4: Vector Properties dialog**

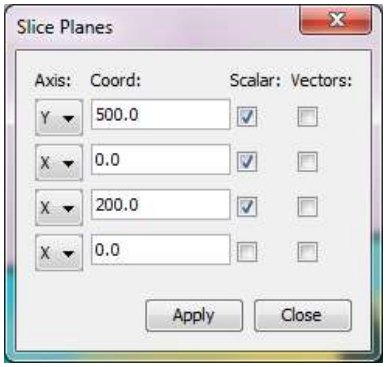



**Figure 12-5: Slice Planes dialog**

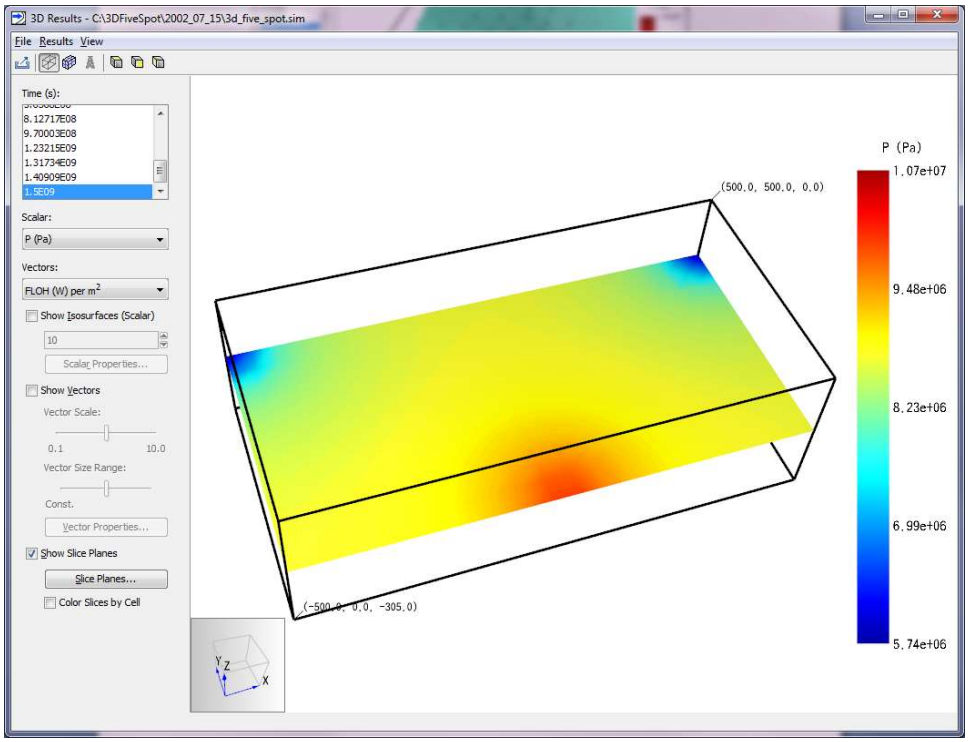



**Figure 12-6: Example of contours on slice planes**

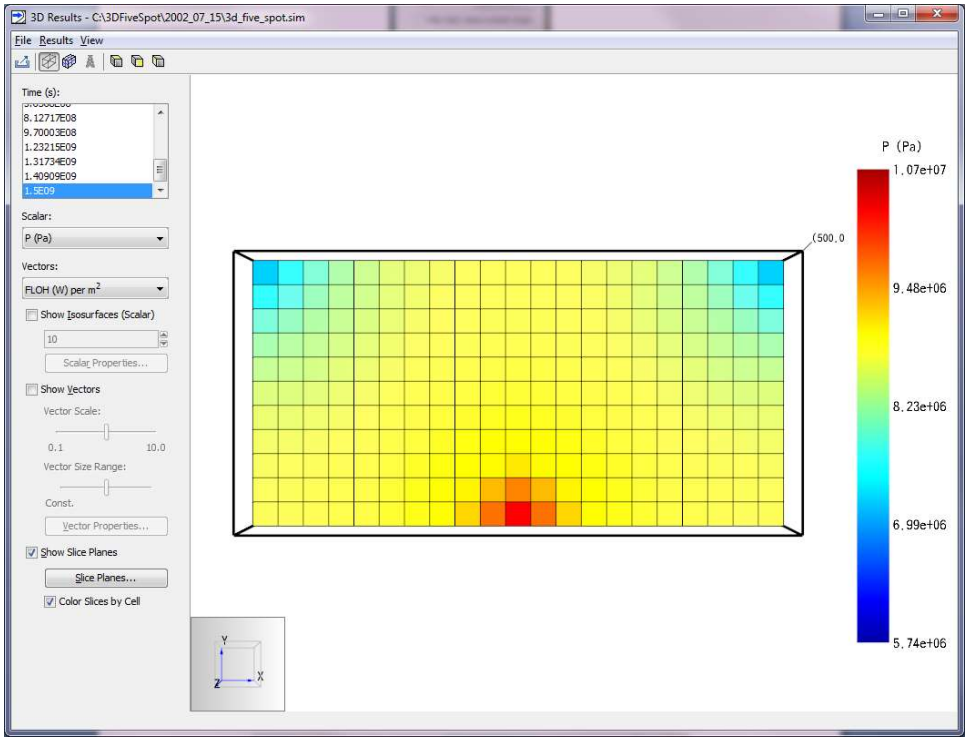



**Figure 12-7: Slice contours colored by cell**

To write a file that can be read into Tecplot: on the **File** menu, click **Export Data...** The format of the data will be a value and then the X, Y, and Z coordinates. The data can be written either at the center or corners of each cell.

## Line Plots of Results

A line plot, an XY plot of a variable along a line, can also be made from the **3D Results** window. Such a plot would be used to plot temperature along a well. To make a line plot, first open a **3D Results** window as discussed in 3D Plots of Results.

To make a line plot

1. On the **File** menu of the **3D Results** window, click **Line Plot...**.
2. In the **Point 1** coordinate boxes **(X, Y, and Z**) type the coordinates of the starting point of the line.
3. In the **Point 2** coordinate boxes (**X, Y, and Z**) type the coordinates of the ending point of the line.
4. Click **OK** to close the **Line Plot** dialog.
5. This will open a **Line Plot** window.
6. In the **Variable** list, select the variable for plotting.
7. In the **Time** list, select the time for which you want to plot the data.

The coordinates can be saved to or loaded from a Comma-Separated Value (CSV) file. To save the coordinates of the points:

1. Specify **Line** as the **Source** in the **Line Plot** dialog.

2. Click **Save** to write the coordinates into a CSV file.

To load the coordinates of the points:

1. Specify **Line** as the **Source** in the **Line Plot** dialog.
2. Click **Load** to retrieve coordinates from a CSV file.

To save time, a line plot can conveniently be generated along the coordinates of a well. To make a plot along the well depth:

1. On the **File** menu of the **3D Results** window, click **Line Plot…**.
2. Specify **Well** as the **Source**.
3. Click **OK** to close the **Line Plot** dialog.
4. This will open a **Line Plot** window.
5. In the **Variable** list, select the variable for plotting.
6. In the **Time** list, select the time for which you want to plot the data.

An example is shown in Figure 12-8. You can export this data to a comma separated value file for import into a spreadsheet.

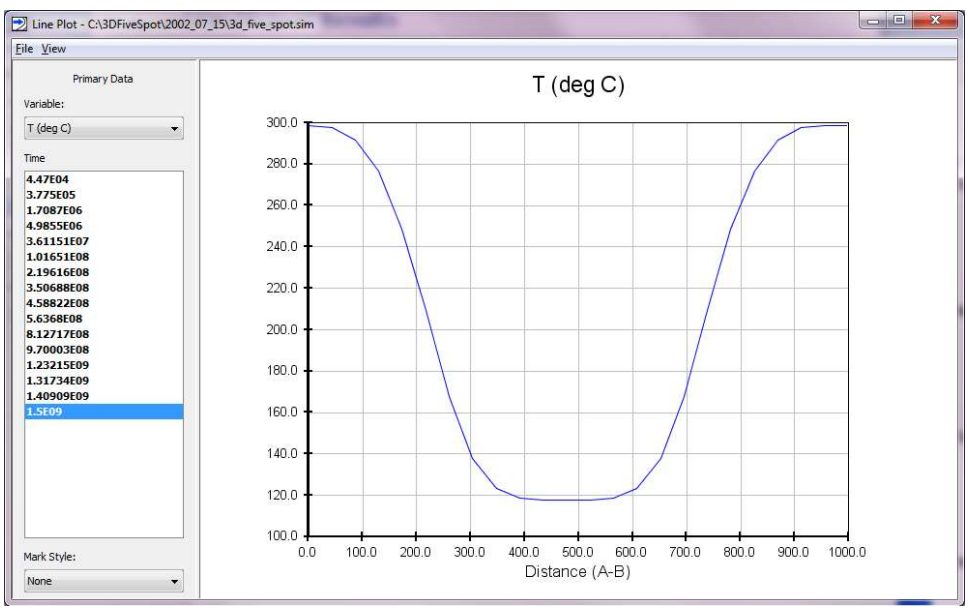



**Figure 12-8: Example line plot**

## Time History Plots of Results

To make a time history plot: on the **Results** menu, click **Cell History Plots…** ( ). This will open the window shown in Figure 12-9.

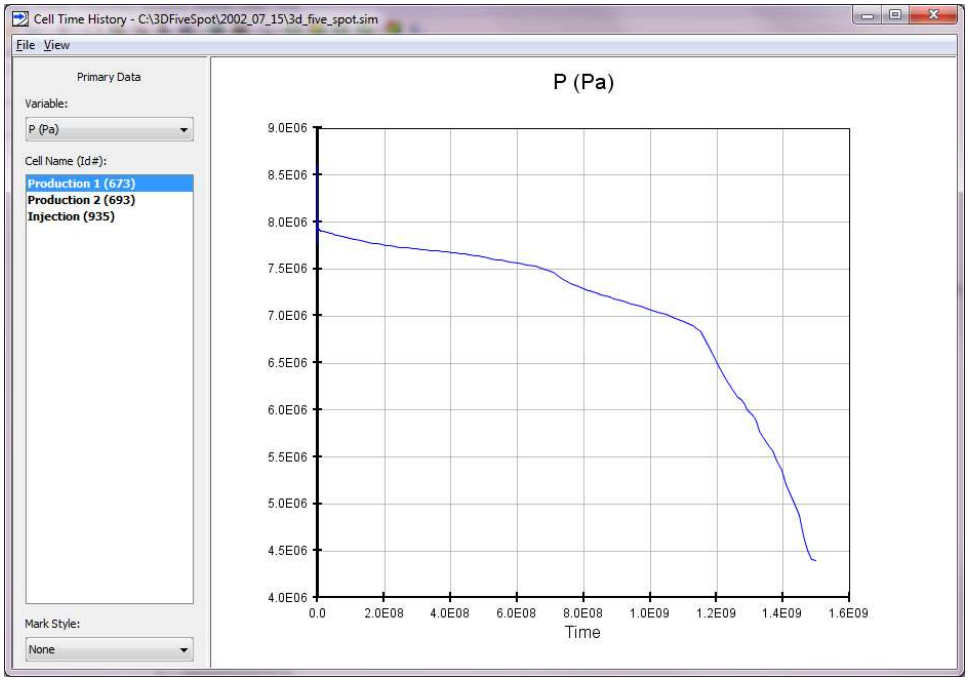



**Figure 12-9: Example time history plot**

You can select the variable and cell to plot. The **Cell Name** is the name given to the cell in the **Edit Cells** dialog. Time history plotting for a cell is also activated in **Edit Cells** dialog.

By default, only the cells for which time history data have been requested or which have been given a name are listed. To expand the list to show all cells: on the **View** menu, click **All Cells**. When all cells are selected, data will only be available at the times in the standard output file. For cells for which time history output was specified, the results are available at each time step.

## Source/Sink and Cell History Plots

This section explains the flow plots created by PetraSim and how to obtain time histories of cells that have sources or sinks.

The model used as an example represents production from a highly permeable layer at about 500m depth (average P = 5 MPa, constant T = 25 ÂºC, single-phase conditions). The model uses EOS1 and extends for 500x500x20m with a grid of 10x10x4 cells. An initial hydrostatic solution was run. In the production run, two of the boundaries are set to a fixed state and cell 169 uses a Well on Deliverability condition with a Productivity Index of 6.0E-9 and a Pressure of 5.0E6 Pa.

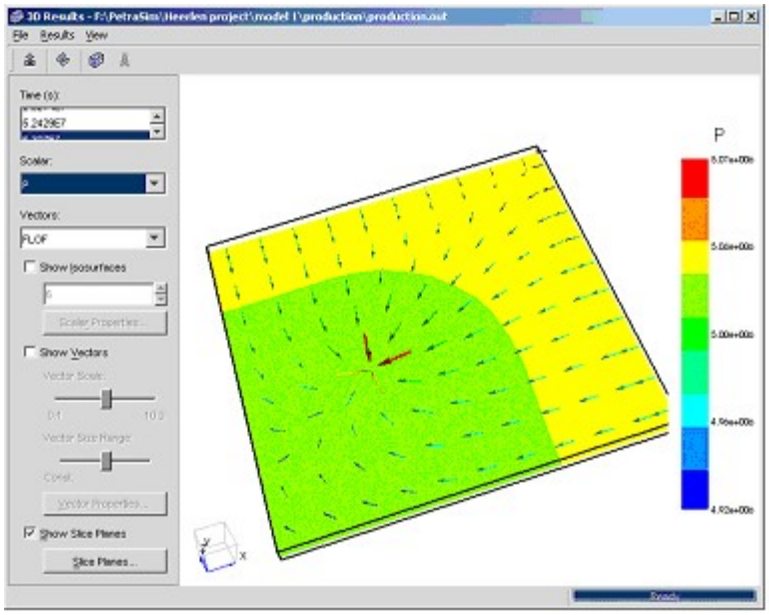



**Figure 12-10: Plot of production flow**

The most important piece of information for a source or sink is the flow rate into/out of the cell. On the **Results** menu, click **Source/Sink Plots...**, Figure 12-11. To make this plot, the Y Scale Range was adjusted to Min Y = -135.2, Max Y = 0.0 (use **View->Range...**). This plot indicates that the production rate is 135.0 kg/sec.

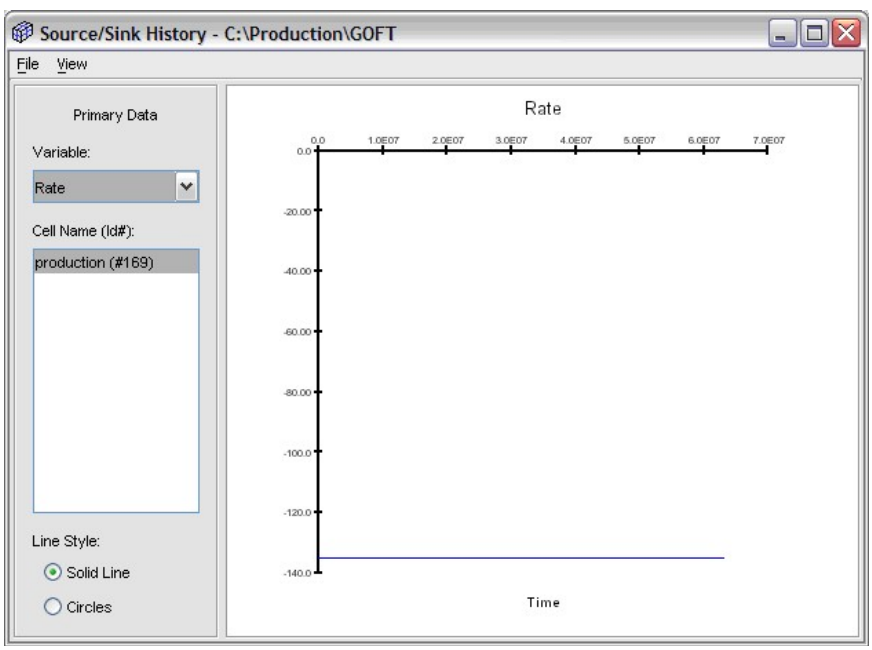



**Figure 12-11: Plot of production from cell 169**

This information can be verified by looking at the TOUGH2 output file. At the end of every printed time step, the source/sink (generation) data is given, as shown below. This data shows that the generation rate is -135.0 kg/s, which matches the PetraSim plot.

```
TOUGH2 Analysis

KCYC =   20  -  ITER =    1  -  TIME = 0.63070E+08

ELEM SRC INDEX    GENERATION RATE   ENTHALPY   X1        X2
                    (KG/S) OR (W)    (J/KG)

169  1   1        -0.13500E+03    0.10940E+06  0.10E+01  0.00E+00
```

To understand the cell history flow plots it is necessary to know the cell names and connections. Figure 12-12 shows the cells names and how they are physically connected for the cells adjacent to cell 169. The production cell is 169 and it is connected to adjacent cells in layer 2 and to cell 48 in layer 1 and cell 290 in layer 3.

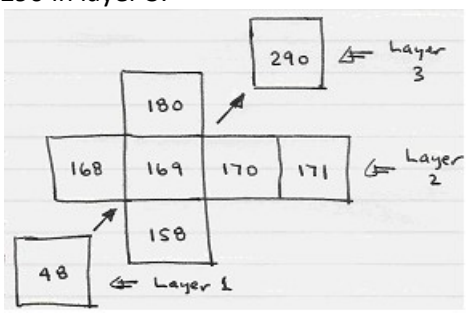



**Figure 12-12: Connections for cell 169**

We will first focus on the flow plot for cell 170, since that is the simplest. To see the plot shown in Figure 12-13:

1. On the **Results** menu, click **Cell History Plots...**
2. On the **View** menu, click **All Cells...**, then select FLOF(X) for cell #170

Select **File->Export Data...** to view the numerical value of -0.029 kg/s-m2.

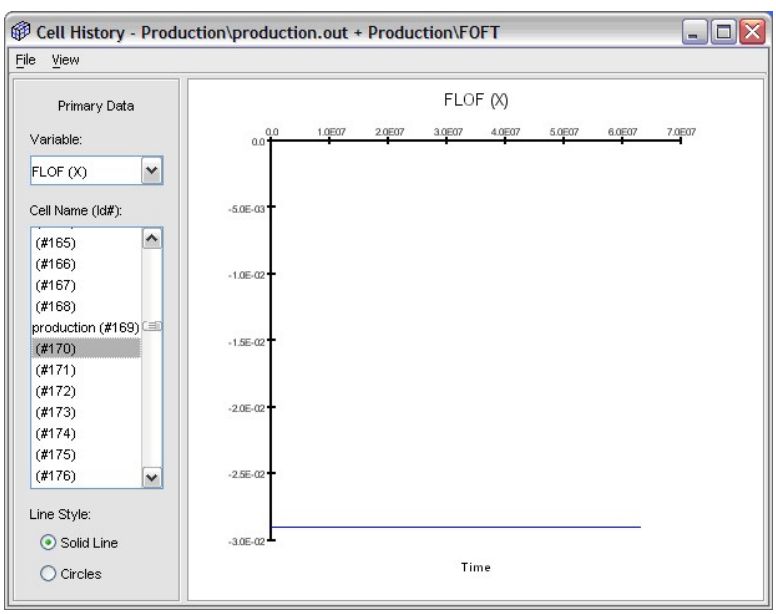



**Figure 12-13: Plot of FLOF(X) for cell 170**

The flow data plotted in the Cell History plot is the flux averaged at that cell. If we go to the output file, we can obtain the actual values of flow for each connection. A part of the file is shown below.

```
EL1  EL2  INDEX    FLOH       FLOH/FLOF       FLOF    FLO(GAS)     FLO(AQ.)  FLO(WTR2)
                    (W)         (J/KG)        (KG/S)    (KG/S)       (KG/S)    (KG/S)

169  170  385 0.107373E+07 0.109403E+06 0.981440E+01 0.000E+00 0.981440E+01 0.000E+00
170  171  386 0.513309E+06 0.109404E+06 0.469187E+01 0.000E+00 0.469187E+01 0.000E+00
171  172  387 0.340934E+06 0.109404E+06 0.311627E+01 0.000E+00 0.311627E+01 0.000E+00
172  173  388 0.268545E+06 0.109405E+06 0.245460E+01 0.000E+00 0.245460E+01 0.000E+00
173  174  389 0.233448E+06 0.109405E+06 0.213379E+01 0.000E+00 0.213379E+01 0.000E+00
```

For the connection between cells 169 and 170, the flow is 9.81 kg/sec. For the connection between cell 170 and 171, the flow is 4.69 kg/sec. To calculate the average X flux at cell 170, we average the two flows and divide by the area between the cells (250 $m^2$ since the cell face width is 50m and the cell height is 5m). The resulting value is 0.029 kg/s-$m^2$, which matches Figure 12-11.

In the plot the negative sign indicates that the X flux is in the negative X direction. This is consistent with the positive connection sign convention used by TOUGH2. For a connection between cell 1 and cell 2, a negative FLOF indicates a flow from cell 1 to cell 2. A positive FLOF indicates flow from cell 2 to cell 1.

We now look at the more complex case of flow into cell 169, which is a production cell. To see the plot shown in Figure 12-14:

1. On the **Results** menu, click **Cell History Plots...**
2. In the Variable box, click FLOF(X)

This is a graph of fluid flux in the X direction at cell 169. The value is -0.00368 kg/s-$m^2$. To view specific values: on the **File** menu, click **Export Data...**.

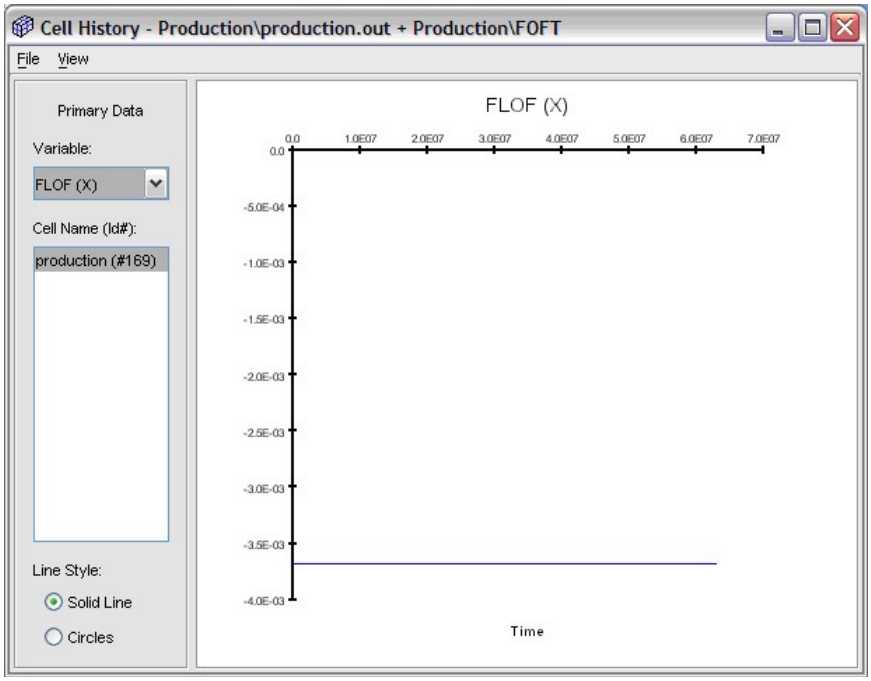



**Figure 12-14: FLOF(X) plot for cell 169**

If we look in the output file, we will find the following data for the connections, Table 12-1.

**Table 12-1: Data for connections to cell 169**

| Connection | FLOF |
|---|---|
| 168->169 | -7.97 |
| 169->170 | 9.81 |
| 158->169 | -7.95 |
| 169->180 | 9.95 |
| 48->169 | -34.32 |
| 169->290 | 64.98 |

Using these values and the sign convention for flows, the flows into cell 169 are represented in Figure 12-15.

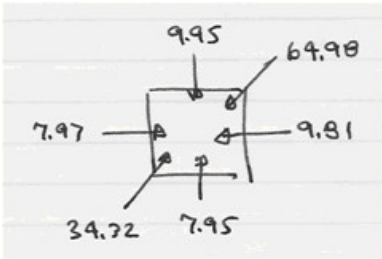



**Figure 12-15: Flows into cell 169**

If we sum these flows, the total is 135.0 kg/sec, consistent with previously discussed source/sink data.

Since this cell is a production cell, there is flow in from the left and in from the right. The average X flux is then ((7.97-9.81)/2)/250 = -0.00368 kg/s-m$^2$, which matches Figure 12-14.

Thanks to Hildenbrand Alexandra for providing this model.

## Well Plots

Well plots are used to show the accumulation of cell quantities for entire wells. Well plots can be enabled by opening the **Edit Well** dialog as discussed in Load Cell Flow Rates

Basic source and sink data can be loaded from a data file. The first line of the file will list a series of cell names, separated by spaces. Each of these cell names must be defined in the PetraSim model. The second line gives the generation type (MASS, HEAT, COM1, etc.) for either injection or production at the given cell. The following lines each contain a time followed by pairs of flow rate and enthalpy for each cell. Enthalpy is required, but not used, for production wells. The content of an example input 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

This input file expects that there exist cells named P1, P2, and I1, defined before import. In this file, P1 and P2 are mass production wells, and I1 is an injection well (the injection type is EOS dependent). In the example, production occurs from only P1 for one year, then production from P2 and injection from I1 begin after one year. This table input is provided to allow spreadsheet editing for all well data.

Using Wells in PetraSim, and under the **Print Options** tab, select “Print Time Dependent Flow and Generation (BC) Data.”

Well plots can be viewed after a simulation by opening the **Results** menu and selecting **Well Plots**. PetraSim calculates various quantities for wells based on the individual cell results for the well, including the following:

- **Flow Rate** –the total flow rate into/out of the well, calculated as $\sum_{k=1}^{n} \mathrm{F_k}$.
- **Flow Rate – Liquid** – the total flow rate of liquid into/out of the well, calculated as $\sum_{k=1}^{n} \mathrm{F_k}(1 - \mathrm{f_{kgas}})$.
- **Flow Rate – Gas** – the total flow rate of gas into/out of the well, calculated as $\sum_{k=1}^{n} \mathrm{F_k f_{kgas}}$.
- **Energy** – the total thermal energy moving into/out of the well, calculated as $\sum_{k=1}^{n} \mathrm{F_k H_k}$.

where n is the number of cells in the well, $\mathrm{F_k}$ is the flow rate in the $\mathrm{k^{th}}$ cell, $\mathrm{f_{kgas}}$ is the flow fraction of gas, and $\mathrm{H_k}$ is the enthalpy.

## General Use of the Comma-Separated Value (CSV) Files

In Version 4.0 of PetraSim a significant change was made in how output data is accessed for plotting. The TOUGH2 source code was modified to output all data in comma separated value (CSV) format. This approach made plotting significantly more robust. It also provides the user with direct access to results data. The output mirrors the data output in the standard TOUGH2 output file.

The following files are available in CSV format:

- **mesh.csv** – This file includes output for each cell for each output variable for all solution output times.
- **conn.csv** – This file includes output for each connection between cells for each output variable for all solution output times.
- **foft.csv** – If individual cells are selected for additional output, data is written to this file for those specific cells for every time step.
- **coft.csv** – If individual connections are selected for additional output, data is written to this file for those specific connections for every time step.
- **goft.csv** – This file includes output for each source/sink in the model.

If the user imports a CSV file into a spreadsheet, the filter options in the spreadsheet can be used to focus on specific details in the data. The CSV format also makes it easy for the user to write their own programs to read and manipulate the data.

The TOUGH3 simulator now also outputs data in this format when the OUTPU block is included in the input file. For TOUGH3 simulations the files are called OUTPUT_ELEME.csv (instead of mesh.csv) and OUTPUT_CONNE.csv (instead of conn.csv). These TOUGH3 files are loaded directly into the 3D results window. The foft, coft and govt CSV files output by TOUGH3 are not currently displayed in the PetraSim interface.

# 13. Flow in Fractured Media

## The MINC Approach

TOUGH uses the "Multiple INteracting Continua" (MINC) method to approximate modeling fluid and heat flow in fracture-porous media. As described in (16), "The method is applicable to flow processes in which an important aspect is the exchange of fluid, heat, or chemical species between fractures and unfractured rock. ... MINC can only be applied to media in which the fractures are sufficiently well connected so that a continuum treatment of flow in the fracture network can be made." If the fractures are not sufficiently connected, a discrete representation of the fracture should be used with a different porous material for flow in the fracture. A detailed explanation of MINC is provided in (17).

As described in (16), "The method is an extension of the double-porosity concept, originally developed by (18) and (19). It is based on the notion that fractures have large permeability and small porosity (when averaged over a reservoir subdomain), while the intact rock (the rock "matrix") has the opposite characteristics. Therefore, any disturbance in reservoir conditions will travel rapidly through the network of interconnected fractures, while invading the matrix blocks only slowly."

MINC is implemented in TOUGH as a mesh processor of the mesh. Additional cells and connections are created so that matrix blocks are "discretized into a sequence of nested volume elements which are defined on the basis of distance from the fractures. Continuum #1 represents the fractures, continuum #2 represents matrix rock in close proximity to the fractures, continuum #3 represents matrix rock at larger distance, etc. In response to an imposed disturbance in the fracture system, fluid and/or heat can migrate in the matrix blocks outward towards the fractures, or inward away from the fractures.

For a complete description, the user is referred to (16) and (17), copies of which are available on the PetraSim Tools webpage: https://www.rockware.com/petrasim-tools/. At the same location, you can find the document “Understanding and Using MINC” and MINC example problems.

In PetraSim, the initial condition data is applied to both the fracture and matrix. This means that reading restart data from the SAVE file will apply the fracture data to both the fracture and matrix for each cell. This can be used used as a “trick” to speed convergence to an initial state. If the user wants to preserve the matrix data, a manual restart should be performed. For more details, see the ***Command Line Execution of TOUGH2*** section in this document.

## Using MINC in PetraSim

To activate the MINC option in PetraSim: on the **Properties** menu, click **Global Properties...** ( ). Click the MINC tab, Figure 13-1. Select **Enable Multiple Interacting Continua (MINC)**. Then, the input data corresponds to that given in the TOUGH2 User's Guide.

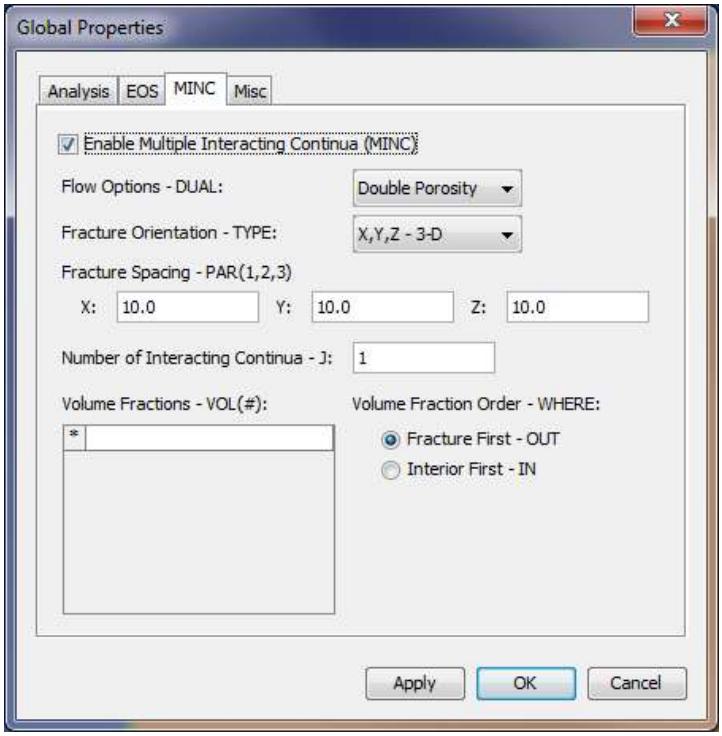



**Figure 13-1: Activating MINC in PetraSim**

Once the MINC option is activated, the user will need to specify the fracture material data on the Fracture tab of the Material Data dialog. This will be the data used for the fractures. The Matrix data will be used for the rock matrix.

# 14. TOUGH3 and TOUGH V2.1 Simulations

PetraSim is installed with TOUGH2 executables that are optimized to work with PetraSim, licensed through a contract with the US DOE. TOUGH3, which was officially released in January of 2018, is not included with PetraSim. However, PetraSim creates input files compatible with TOUGH3 and can also visualize CSV output from TOUGH3 simulations.

## TOUGH v2.1 Support

TOUGH v2.1 is no longer available or supported by LBL. If a customer purchased TOUGH v2.1 through RockWare or LBL in the past, RockWare can provide TOUGH v2.1 executables that are designed to work with PetraSim. Other than the addition of the ECO2M fluid property module, there is very little difference between TOUGH v2.1 and TOUGH2.

## Acquiring TOUGH3

TOUGH3 can be acquired through Lawrence Berkely National Lab. Pricing and licensing information can be found at: https://tough.lbl.gov/.

## Setting up a TOUGH3 Simulation

Simulations for TOUGH3 should be set up through the TOUGH Simulator Mode. The one exception to this is for the ECO2M simulator, which should be created through the TOUGH V2.1 Simulator Mode.

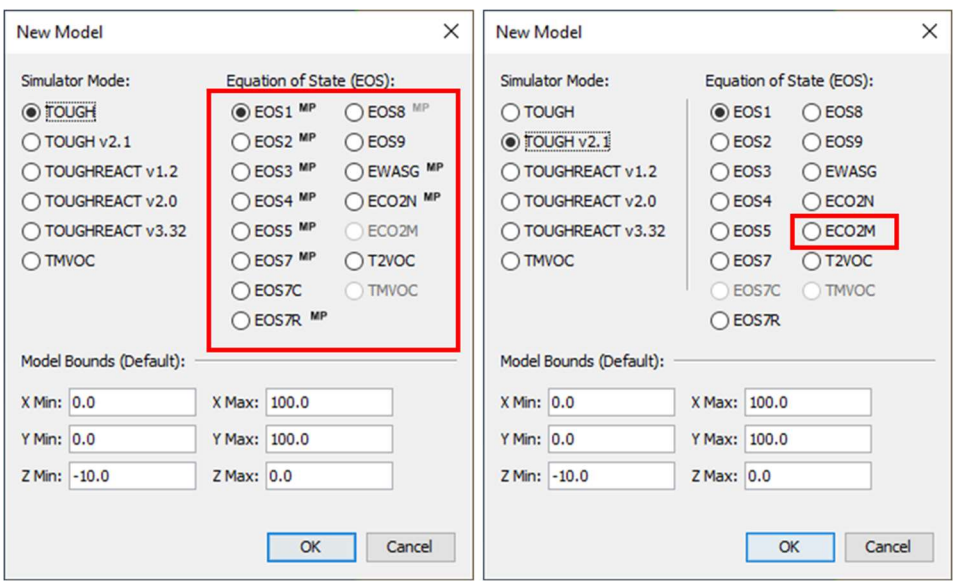



**Figure 14-1: Create TOUGH3 simulations with the TOUGH or TOUGH v2.1 (ECO2M only) interfaces**

## TOUGH3 OUTPU Block

PetraSim includes the option to write the TOUGH3 OUTPU block to the input file. This can direct the simulator to output data as CSV files that are compatible with PetraSim and can be plotted in both 2D and 3D. Access the OUTPU block settings through the **Analysis | Output Controls** menu item. The default text entered for the OUTPU block can be modified to output a custom suite of output

parameters. The user should refer to the TOUGH3 manual for additional information about the OUTPU block format (5).

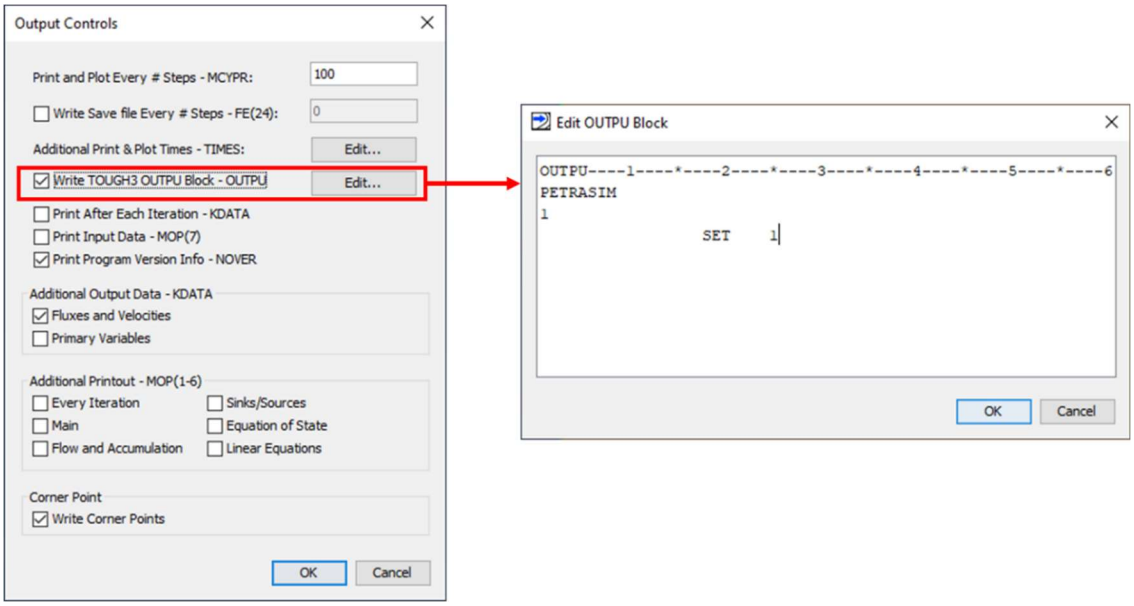



**Figure 14-2: Access the OUTPU block settings through Analysis | Output Controls**

## TOUGH3 MOMOP Block

The MOMOP (MOP2) block can be written to the input file if the user would like to take advantage of a number of new simulator settings available in TOUGH3. This can be accessed through the **Analysis |Solution Controls** menu item under the **MOMOP** tab. It is the user's responsibility to be sure that the MOMOP input is in the correct format and that each parameter is assigned an appropriate number of spaces.

## Running a TOUGH3 Simulation

TOUGH3 simulations cannot currently be run directly through the interface. The TOUGH3 input file (called INFILE) can be created through the **File | Write TOUGH3 File** menu item. Once the file is created, the user can run the simulation through a command line. This is most easily done by placing the TOUGH3 executable in the same directory as the INFILE and PetraSim SIM file. The simulation can then be run through a command line that simply lists the location and name of the TOUGH3 executable. As the simulation runs, output files will be written to the directory where the INFILE is located.

Note that not all of the new features implemented in TOUGH3 are supported in the PetraSim interface. If the user would like to create a TOUGH3 simulation that uses unsupported features, it will be necessary to make modifications to the INFILE before running the simulation.

## Plotting Results from a TOUGH3 Simulation

If the OUTPU block is set up to output data in a PetraSim format, the simulator will output a number of different CSV files:

- OUTPUT_ELEME.csv – cell-based data that is plotted through the Results menu
- OUTPUT_CONNE.csv – connection-based data that is plotted the Results menu
- Other cell or connection-based CSV files (FOFT, COFT, etc.) The time series data for individual cells and connections is not currently supported in the PetraSim interface and should be viewed and plotted through Excel or a similar program.

To display these results, select the **Results** menu and choose the appropriate 2D or 3D option.

# 15. TOUGHREACT v3.32 and 2.0 Simulations

PetraSim is installed with TOUGHREACT v1.2 executables that were optimized to work with PetraSim, licensed through a contract with the US DOE. PetraSim also supports TOUGHREACT v2.0, which is no longer distributed or supported by LBL. PetraSim includes limited support for TOUGHREACT v3.32, including input file creation and 2D and 3D display of cell-based data. Note that PetraSim currently supports the following EOS modules within TOUGHREACT v3.32: EOS1, EOS2, EOS3, EOS4, EOS7, EOS9 and ECO2N.

## TOUGHREACT v2.0 Support

TOUGHREACT v2 is no longer available or supported by LBL. If a customer purchased TOUGHREACT v2.0 through RockWare or LBL in the past, RockWare can provide TOUGHREACT v2.0 executables that are designed to work with PetraSim.

## Acquiring TOUGHREACT v3.32

TOUGHREACT v3.32 can be acquired through Lawrence Berkely National Lab. Pricing and licensing information can be found at: https://tough.lbl.gov/. At the time this documentation was being written, TOUGHREACT v4.13 had just been released by LBL. If you are using TOUGHREACT v4.13 and would like information on compatibility with PetraSim, please contact tech@rockware.com. We hope to incorporate some support for TOUGHREACT v4.13 later in 2022.

## Setting up a TOUGHREACT v3.32 Simulation

TOUGHREACT v3.32 simulations can be created using the TOUGHREACT v3.32 Simulator Mode. Many users prefer to experiment with the TOUGHREACT v1.2 simulator initially, and then transfer the TOUGHREACT v1.2 simulation to TOUGHREACT v3.32. This can be done by going to **File | Import TOUGHREACT as 3.32**.

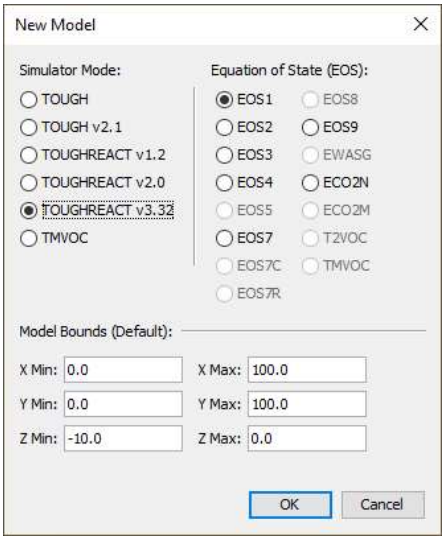



**Figure 15-1: Select the TOUGHREACT v3.32 Simulator Mode and EOS Module**

## Outputting Data in a TecPlot Format

If you would like to visualize the results of the TOUGHREACT v3.32 simulation in PetraSim, the **Output in TecPlot Format** option should be checked on in the **Output Controls Window** (access through the **Analysis | Output Controls** menu item). PetraSim now includes a tool that will convert the TecPlot output files to CSV files that can be displayed within the PetraSim interface.

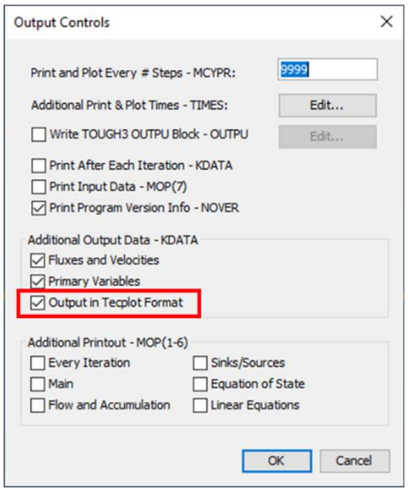



**Figure 15-2: Output in Tecplot Format option in the Output Controls window**

## Running a TOUGHREACT v3.32 Simulation Through the Interface

TOUGHREACT v3.32 simulations can be run through the interface, or can be run from a command line. If the user would like to run the simulation through the interface, the TOUGHREACT v3.32 files will need to be placed in the following directory and named appropriately:

C:\Program Files\PetraSim 2022\tough64\treact_v3.

See Appendix B for a list of executable locations and names. In addition to this, the following DLLs, included with the TOUGHREACT source code/executable, should be placed in this directory:

- libifcoremd.dll
- libiomp5md.dll
- libmmd.dll
- svml_dispmd.dll

Here is a screen shot of this directory set up to run a TOUGHREACT v3.32 ECO2N simulation. Note that the CO2TAB file should be placed in the same directory.

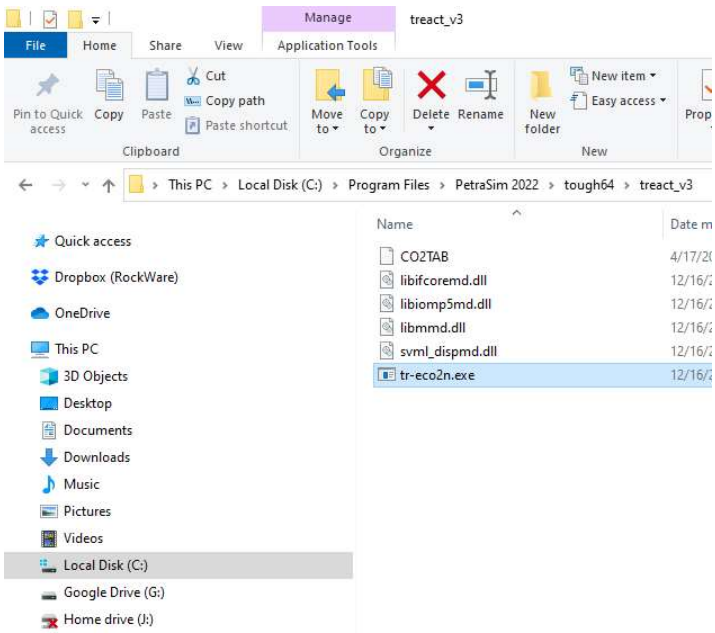



**Figure 15-3: File required to run TOUGHREACT v3.32 ECO2N through the PetraSim Interface**

## Running a TOUGHREACT v3.32 Simulation Through a Command Line

Some users prefer to run the simulation through a Command Line. The TOUGHREACT input files can be created through the **File | Write REACT files** menu item. The following input files will be created:

1. Flow.inp
2. Chemical.inp
3. Solute.inp
4. thermodb.txt (this is a copy of the thermodynamic database referenced in the SIM file)
5. CO2TAB file (for ECO2N simulations only)

The TOUGHREACT v3.32 executable and supported DLL files should be placed in the same directory as the input files. The command to run the simulation is simply the name of the executable, for example, to run the EOS3 TOUGHREACT executable, the command would be: **treact_eos3.exe**

## Using the CSV Converter

PetraSim 2022 includes a new tool called the CSV Converter, which can be used to convert TOUGHREACT v3.32 data in a TecPlot format to CSV files that can be plotted through the Results menu.

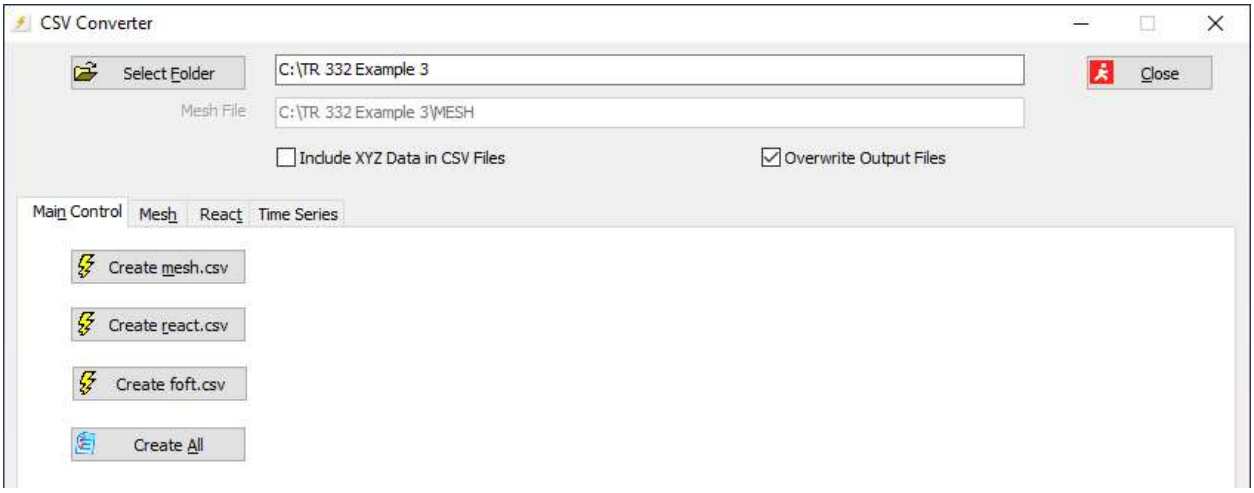



**Figure 15-4: The CSV Converter tool used for TOUGHREACT v3.32 Simulations**

The CSV Converter is used to create the following PetraSim CSV files:

- mesh.csv – composed of cell-based data from the "flow" portion of the simulation.
- react.csv – composed of cell-based data from the "reaction" portion of the simulation. This data can be pulled from one or more files output by a TOUGHREACT simulator.
- foft.csv – composed of cell-based data for cells marked as **Print** cells in the PetraSim model. This is typically output every time step or at a shorter output interval than the other output files.

It is important to note that the CSV Converter needs to be used each time a model is rerun. The window can stay open while models are run so that settings do not need to be reset.

**Selecting a Folder**

When the CSV Converter is opened through the PetraSim program (using the **Results | CSV Converter** menu item), the program automatically selects the directory where the currently opened SIM file is located. The program also searches for and identifies the MESH file that contains element names within the simulation. The user would typically not need to make adjustments to these settings.

**mesh.csv File Creation**

The CSV Converter will automatically use the flowdata.tec file that is output by the TOUGHREACT simulation to create the mesh.csv file. Note that it is important that the **Output in TecPlot Format** option is selected under the **Analysis | Output Options** menu so that the file is output in the correct format. The flowvectors.tec file, which contains flow vector information, is not currently supported in PetraSim.

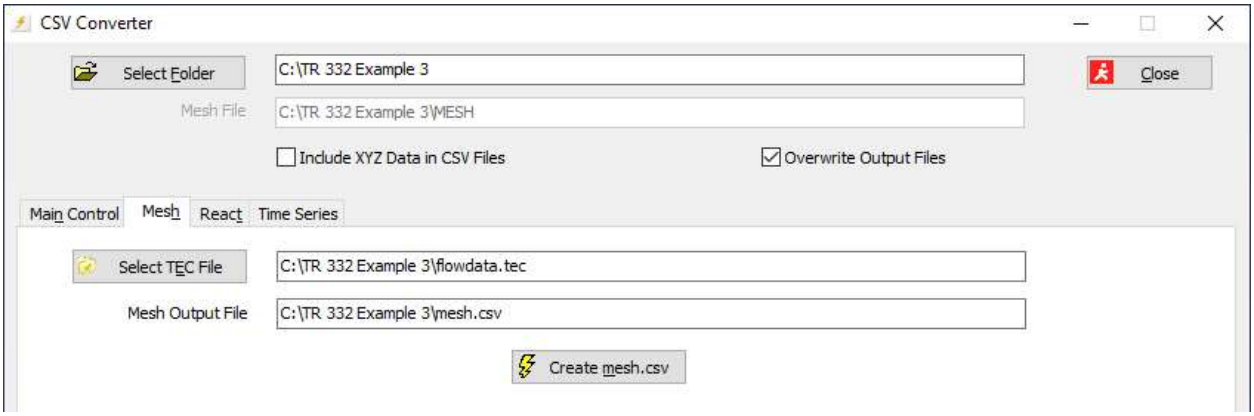



**Figure 15-5: The Mesh tab in the CSV Converter**

The location of the flowdata.tec and mesh.csv file can be viewed through the Mesh tab and the mesh.csv file can be created by clicking the **Create mesh.csv** button in the Main Control and Mesh tabs.

**react.csv File Creation**

The PetraSim react.csv file can include data from one or more file output by the simulator.

File that are typically output by a TOUGHREACT simulation and are automatically loaded into the CSV Converter include:

- plot.tec - Aqueous Concentrations
- solid.tec - Mineral Data
- gas.tec - Gas Data

Other files that are output in a TecPlot format and could be added to the react.csv file include:

- min_SI.tec
- rctn_rate.tec
- rct_sfarea.tec
- thermalparam.tec

Note that the files listed above are only created if MOPR(8) is set correctly in the flow.inp file. These settings are accessed in PetraSim through the **TOUGHREACT | Output Options** menu item in the **Debug** tab.

Click the React tab to see the options for the react.csv file creation. By default, the program will select the gas, plot and solid file and put them in the Order panel. The user can drag the files up and down to adjust the order that the data will fall in the react.csv file, and can also remove files by selecting the file and clicking the **Remove** button.

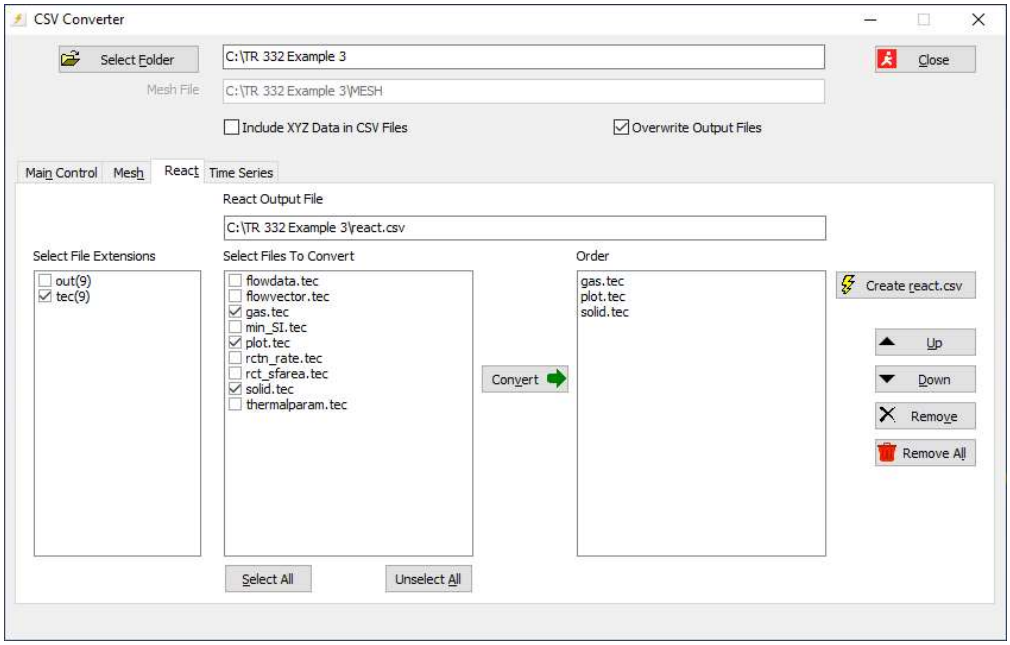



**Figure 15-6: The React Tab in the CSV Converter**

To add a different file to the Order panel, click the **Unselect All** button, select the files that should be transfer to the Order panel and then click the Convert button. It is recommended that the user not include more than a few of the .tec files in the react.csv file, as many of the files include the same column titles, which could cause confusion in the 3D viewer.

The react.csv file can be created by clicking the **Create react.csv** button in the Main Control and React tabs

**foft.csv File Creation**

The Time.out file that is created by the TOUGHREACT simulator is converted to a foft.csv file for display as Cell History data in PetraSim. The foft.csv file can be created by clicking the **Create foft.csv** button in the Main Control and Time Series tabs.

## Plotting Results from a TOUGHREACT v3.32 Simulation

To display the mesh, react or foft CSV files created using the CSV Converter, select the **Results** menu and choose the appropriate 2D or 3D option.

# 16. Command Line Execution of TOUGH2

There may be times that the user wants to execute TOUGH2 from the command line using the TOUGH2 executables shipped with PetraSim. One case would be when a user wants to perform a sensitivity study requiring the simulation of varying models with slightly varied parameters. Because the TOUGH2 executables shipped with PetraSim are secured so that they cannot be executed with a PetraSim license, special procedures must be implemented.

## Single PetraSim Licenses

If the user is working with a single license of PetraSim they will need to place the PetraSim *.lic file and rlm922.dll in the same directory as the simulation executable to be run. It is recommended that the input file is placed in this directory as well.

## Network PetraSim Licenses

The floating license server is needed to authorize the simulator use before running the model. After opening the command prompt, an environment variable needs to be set. This will be something like:

**c:\>set theng_license=52100@servername**

In this case, the correct server name and port number should be substituted into the line. After setting the environment variable, the executables can be run from the command line (below) and will pick up and use the floating license.

## TOUGH2, T2VOC, TMVOC

For TOUGH2, T2VOC, and TMVOC, the command line call will be of the form:

**Executable name <input file> output file**

For example, to run a model called heat_pipe.dat using EOS3, the command line would look like:

**eos3.exe <heat_pipe.dat> heat_pipe.out**

## TOUGHREACT

To manually run a TOUGHREACT model, the user should place the following files in the directory with the executable:

6. **Flow.inp**
7. **Chemical.inp**
8. **Solute.inp**
9. **thermodb.txt** (this is a copy of the thermXu4.dat file stored under **C:\Program Files\PetraSim 2022**)

The command to run the simulation is simply the name of the executable, for example, to run the EOS3 TOUGHREACT executable, the command would be: **treact_eos3.exe**

## TOUGH2-MP

TOUGH2-MP cannot be run from a single command outside of the PetraSim software. If a need for doing so arises, the user can contact support to acquire a batch file.

## Restarting TOUGH2

Another case where it is useful to run TOUGH2 from the command line is restarting a MINC analysis, initializing both the fracture and matrix cells to the end states of the previous analysis. To restart an analysis and run from the command line:

1. Copy the original folder to a new folder named Restart (or whatever name you want). The reason to do this is that TOUGH2 writes to files (**SAVE**, **INCON**, etc.) whose names cannot be changed. Using a different folder prevents loss of the old data from over-writing of files.
2. Optionally, rename the *.sim and *.dat files in the new Restart folder to new names (for example, rename **bubble.sim** to **restart.sim** and **bubble.dat** to **restart.dat**). This just helps to make clear which analysis you are performing.
3. Make a copy of the **SAVE** file. Name it something like **SAVE Copy**. This preserves your original **SAVE** data.
4. Delete the **INCON** file and rename the **SAVE** file to **INCON**. The **INCON** file now contains the data that will be applied as initial conditions in the new analysis.
5. Use a text editor (such as Notepad) to remove all INCON data in the *.dat file. If this data is not removed, it will take precedence over the data in the **INCON** file, and the correct restart data will not be used.

```
 7676 7736                    3       5.0       5.0      10.0      -1.0
 7677 7737                    3       5.0       5.0      10.0      -1.0
 7678 7738                    3       5.0       5.0      10.0      -1.0
 7679 7739                    3       5.0       5.0      10.0      -1.0
 7680 7740                    3       5.0       5.0      10.0      -1.0

GENER----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8

INCON----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    1
          12658100.0                 0.0                 0.0                35.7
    2
          12658100.0                 0.0                 0.0                35.7
    3
          12658100.0                 0.0                 0.0                35.7
    4
          12658100.0                 0.0                 0.0                35.7
    5
          12658100.0                 0.0                 0.0                35.7
    6
          12658100.0                 0.0                 0.0                35.7
    7
          12658100.0                 0.0                 0.0                35.7
    8
          12658100.0                 0.0                 0.0                35.7
    9
          12658100.0                 0.0                 0.0                35.7
   10
          12658100.0                 0.0                 0.0                35.7
   11
          12658100.0                 0.0                 0.0                35.7
```

**Figure 16-1: *.dat file before removing INCON data**

```
 7676 7736                    3       5.0       5.0      10.0      -1.0
 7677 7737                    3       5.0       5.0      10.0      -1.0
 7678 7738                    3       5.0       5.0      10.0      -1.0
 7679 7739                    3       5.0       5.0      10.0      -1.0
 7680 7740                    3       5.0       5.0      10.0      -1.0

GENER----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8

FOFT ----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
  796
  797
  798
  799
  8 0
  8 1
  8 2
  8 3
  8 4
  8 5
 11 0
 14 0
 20 0
 23 0
 26 0

MESHM----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
MINC
PART THRED     MMALL
  3  2OUT       10.0      10.0      10.0
      0.01       0.1

ENDCY
```

**Figure 16-2: *.dat file after removing INCON data**

6. Copy your license file (or files if there are more than one) from your license folder into your restart folder. For more information on how to do this, see above discussion above.
7. Identify the location of the EOS executable that you want to run. For example, if you are using EOS1, it will be located in **C:\Program Files (x86)\PetraSim 2015\tough2.**
8. Start a Command Prompt window, go to the restart folder, and type:

   **"C:\Program Files (x86)\PetraSim 2015\tough2\eos1.exe" <restart.dat >restart.out**

   Note that the quotes are required and that this assumes you are using EOS1 and that your *.dat file is named **restart.dat**. More information about calling the executable can be found in the above section.

9. Execution should now proceed and you should be able to open the **restart.sim** model and display the restart results.

# 17. Miscellaneous

## Finding TOUGH2 Options in PetraSim

This map provides a listing of where TOUGH2 variables are accessed in PetraSim. Italics are used to indicate a menu item. The map is organized following the TOUGH2 User's Guide format. In addition, one each dialog, the TOUGH name for each input variable is provided.

### TITLE

- TITLE - **Properties->Global Properties…** in Tough Global Data dialog on Analysis tab.

### MESHM

This is only used with the MINC option. MINC data is given in **Properties->Global Properties…** in the Tough Global Data dialog on the MINC tab.

### ROCKS

#### *ROCKS.1 Record*

- MAT - *Properties->Materials* in Material Data dialog.
- NAD - Automatically determined based on user input.
- DROK - *Properties->Materials* in Material Data dialog.
- POR - *Properties->Materials* in Material Data dialog.
- PER(I) **-** *Properties->Materials* in Material Data dialog.
- CWET - *Properties->Materials* in Material Data dialog.
- SPHT **-** *Properties->Materials* in Material Data dialog.

#### *ROCKS.1.1 Record*

- COM - *Properties->Materials* Select **Relative Perm...** button in Material Data dialog. On Misc tab Additional Material Data dialog.
- EXPAN - *Properties->Materials* Select **Relative Perm...** button in Material Data dialog. On Misc tab Additional Material Data dialog.
- CDRY - *Properties->Materials* Select **Relative Perm...** button in Material Data dialog. On Misc tab Additional Material Data dialog.
- TORTX - *Properties->Materials* Select **Relative Perm...** button in Material Data dialog. On Misc tab Additional Material Data dialog.
- GK - *Properties->Materials* Select **Relative Perm...** button in Material Data dialog. On Misc tab Additional Material Data dialog.
- XKD3 - *Properties->Materials* Select **Relative Perm...** button in Material Data dialog. On Misc tab Additional Material Data dialog. Only shown for EOS7R.
- XKD4 - *Properties->Materials* Select **Relative Perm...** button in Material Data dialog. On Misc tab Additional Material Data dialog. Only shown for EOS7R.
- FOC - *Properties->Materials* Select **Relative Perm...** button in Material Data dialog. On Misc tab Additional Material Data dialog. Only shown for T2VOC.

### *ROCKS.1.2 Record*

- IRP - *Properties->Materials* Select **Relative Perm...** button in Material Data dialog. Automatically determined from selection on Relative Perm tab of Additional Material Data dialog.
- RP(I) - *Properties->Materials* Select **Relative Perm...** button in Material Data dialog. On Relative Perm tab of Additional Material Data dialog.

### *ROCKS.1.3. Record*

- ICP - *Properties->Materials* Select **Relative Perm...** button in Material Data dialog. Automatically determined from selection on Capillary Press tab of Additional Material Data dialog.
- CP(I) - *Properties->Materials* Select **Relative Perm...** button in Material Data dialog. On Capillary Press tab of Additional Material Data dialog.

### *ROCKS.2 Record*

- Automatically written.

## MULTI

Automatically written based on EOS type and EOS options selected on *Properties->Global Properties* in Tough Global Data dialog on EOS tab.

## START Record

Written automatically.

## CHEMP (T2VOC only)

Automatically written for T2VOC based on VOC data specified in *Properties->Global Properties* in Tough Global Data dialog on EOS tab.

## PARAM

### *PARAM.1 Record*

- NOITE - *Analysis->Solution Controls* in Solution Parameters dialog on Times tab.
- KDATA - Automatically determined from selections on *Analysis->Solution Controls* in the Print and Plot Options dialog.
- MCYC - *Analysis->Solution Controls* in Solution Parameters dialog on Times tab.
- MSEC - *Analysis->Solution Controls* in Solution Parameters dialog on Times tab.
- MCYPR - *Analysis->Solution Controls* in the Print and Plot Options dialog.
- MOP(1) through MOP(7) - Automatically determined from selections on *Analysis->Solution Controls* in the Print and Plot Options dialog.
- MOP(9) *Analysis->Solution Controls* in Solution Parameters dialog on Options tab.
- MOP(10) - *Analysis->Solution Controls* in Solution Parameters dialog on Options tab.
- MOP(11) - *Analysis->Solution Controls* in Solution Parameters dialog on Weighting tab.
- MOP(12) - *Analysis->Solution Controls* in Solution Parameters dialog on Options tab.
- MOP(13) - Not implemented. Used only by T2DM option.
- MOP(14) - *Analysis->Solution Controls* in Solution Parameters dialog on Solver tab.

- MOP(16) - *Analysis->Solution Controls* in Solution Parameters dialog on Times tab.
- MOP(17) - *Analysis->Solution Controls* in Solution Parameters dialog on Solver tab.
- MOP(18) - *Analysis->Solution Controls* in Solution Parameters dialog on Weighting tab.
- MOP(19) - *Properties->Global Properties* in Tough Global Data dialog on EOS tab, as appropriate.
- MOP(20) - Not implemented. Used only by EOS4 option.
- MOP(21) - Not used. Instead the alternate SOLVR record is used to select the solver. Select the solver in *Analysis->Solution Controls* in Solution Parameters dialog on Solver tab.
- MOP(22) - Not implemented. Used only by T2DM option.
- MOP(23) - Not implemented. Used only by T2DM option.
- MOP(24) - *Analysis->Solution Controls* in Solution Parameters dialog on Weighting tab.
- TEXP - *Properties->Global Properties* in Tough Global Data dialog on EOS tab. Select Molecular Diffusion and specify on Edit Coefficients dialog. For T2VOC on EOS tab.
- BE - *Properties->Global Properties* in Tough Global Data dialog on EOS tab. Select Molecular Diffusion and specify on Edit Coefficients dialog.
- DIFF0 - *Properties->Global Properties* in Tough Global Data dialog on EOS tab. Only for T2VOC.

### *PARAM.2 Record*

- TSTART - *Analysis->Solution Controls* in Solution Parameters dialog on Times tab.
- TIMAX - *Analysis->Solution Controls* in Solution Parameters dialog on Times tab.
- DELTEN - Automatically determined based on options selected in *Analysis->Solution Controls* in Solution Parameters dialog on Times tab. You can edit the table of time steps.
- DELTMX - *Analysis->Solution Controls* in Solution Parameters dialog on Times tab.
- ELST - Not implemented, instead select cell for printing in **Edit Cells** dialog.
- GF - *Properties->Global Properties* in Tough Global Data dialog on Misc tab.
- REDLT - *Analysis->Solution Controls* in Solution Parameters dialog on Times tab.
- SCALE - *Properties->Global Properties* in Tough Global Data dialog on Misc tab.

### *PARAM.2.1, 2.2, etc. Record*

- Automatically written if table is used to give time steps in *Analysis->Solution Controls* in Solution Parameters dialog on Times tab.

### *PARAM.3 Record*

- RE1 - *Analysis->Solution Controls* in Solution Parameters dialog on Convergence tab.
- RE2 - *Analysis->Solution Controls* in Solution Parameters dialog on Convergence tab.
- U - *Analysis->Solution Controls* in Solution Parameters dialog on Solver tab.
- WUP - *Analysis->Solution Controls* in Solution Parameters dialog on Weighting tab.
- WNR - *Analysis->Solution Controls* in Solution Parameters dialog on Weighting tab.
- DFAC - *Analysis->Solution Controls* in Solution Parameters dialog on Options tab.

### *PARAM.4 Record*

- This record is not used. Instead, initial conditions for each element are written using the INCON record, see below.

### INDOM

This record is not used. Instead, initial conditions for each element are written using the INCON record, see below.

### INCON

These records are created for each element based on initial condition data. The appropriate data is EOS dependent. See the Initial Conditions chapter for help with defining initial conditions.

### SOLVR

This record is written based on options selected in *Analysis->Solution Controls* in the Solution Parameters dialog on the Solver tab.

### FOFT

The FOFT record defines a list of cells for which output data will be written to a file every time step. This record is written automatically by PetraSim, based on the cells that have been selected for detailed printing.

To select a cell for output, open the **Edit Cells** dialog (see Editing Cells). Go to the Print Options tab. Use the check box to turn on printing. In the Properties tab, you can give the cell a name that will be displayed in the plot. After the analysis is completed and a time history plot made, the data can be written to a file for import into a spreadsheet.

### GOFT

Automatically written for all sources and sinks.

### NOVER

#### *NOVERsion Record*

- *Analysis->Output Controls* in Output Controls dialog.

### DIFFU

#### *DIFFUsion Record*

- All diffusion data is input from *Properties->Global Properties* in the Tough Global Data dialog on the EOS tab. Select Molecular Diffusion and then the Edit Coefficients button and dialog. Not valid for T2VOC.

### SELEC

#### *SELECtion Record*

- Automatically written from data input on *Properties->Global Properties* in the Tough Global Data dialog on the EOS tab.

### RPCAP

This record is not used. Instead, all data is written as part of ROCKS record.

## TIMES

### *TIMES Record*

- A table of output times can be specified in *Analysis->Output Controls* in the Output Controls dialog. These times are then written to the TIMES record.

## ELEME

All element (cell) data is written based on the grid defined by the user.

## CONNE

All connection data is written based on the grid defined by the user.

## GENER

The GENER record defines a list of cells with source or sink boundary conditions. See 0.

# 18. Troubleshooting

## Convergence Problems

It is inevitable that some of the analyses you run will stop execution before your specified end time. Usually this is because of convergence problems during the solution.

Diagnosing TOUGH2 convergence problems is not a trivial task. It requires that you view TOUGH2's output file directly and understand the relationship between the printed output and the solver over time. When problems can't execute a single time step, this process is a bit easier because there is usually some indication of the erroneous input. However, when the simulation runs for several time steps before failing to converge (usually following a rapid sequence of time step size reductions) it is necessary to understand what transient change caused the problem.

Following is the step-by-step process used to look at one user's convergence problems. The user was learning about PetraSim and TOUGH2, so was developing the skills needed to run analyses.

STEP 1: Open the OUT file and look for messages printed before the data for the last time step. This will be before the text "THE TIME IS", so you can search for that text. A sample is copied below. DT is the time step and you can see that it has gotten very small -- 0.0488 sec. We also see that it cannot find the parameters for element 11126 and the problem is that the TEMPERATURE is out of range in SAT. The TEMPERATURE value is 0.999, so it looks like something is cooling down to freezing and TOUGH2 cannot handle that (the new TOUGH-FX version can handle freezing). Jump to step 2.

```
QQQQQQQQQQ SUBROUTINE QU QQQQQQQQQQQQQQQQQQQQ --- [KCYC,ITER] = [ 144,  1]
  TEMPERATURE = 0.999981E+00  OUT OF RANGE IN SAT
  +++++++++   CANNOT FIND PARAMETERS AT ELEMENT *11126* IND = 4
  +++++++++   XX(M) = 0.118536E+06 0.549628E+00 0.999981E+00
  +++++++++ REDUCE TIME STEP AT ( 144,  1) ++++++  NEW DELT = 0.488281E-01

  QQQQQQQQQQ SUBROUTINE QU QQQQQQQQQQQQQQQQQQQQ --- [KCYC,ITER] = [ 144,  1]
  11126( 144,  1) ST = 0.176848E+05 DT = 0.488281E-01 DX1= 0.000000E+00 ...

  QQQQQQQQQQ SUBROUTINE QU QQQQQQQQQQQQQQQQQQQQ --- [KCYC,ITER] = [ 145,  1]
  TEMPERATURE = 0.999996E+00  OUT OF RANGE IN SAT
  +++++++++   CANNOT FIND PARAMETERS AT ELEMENT *11126* IND = 4
  +++++++++   XX(M) = 0.118536E+06 0.549627E+00 0.999996E+00
  +++++++++ REDUCE TIME STEP AT ( 145,  1) +++++   NEW DELT = 0.244141E-01

  QQQQQQQQQQ SUBROUTINE QU QQQQQQQQQQQQQQQQQQQQ --- [KCYC,ITER] = [ 145,  1]
  11126( 145,  1) ST = 0.176848E+05 DT = 0.244141E-01 DX1= 0.000000E+00 ...

  QQQQQQQQQQ SUBROUTINE QU QQQQQQQQQQQQQQQQQQQQ --- [KCYC,ITER] = [ 146,  1]
  11126( 146,  1) ST = 0.176849E+05 DT = 0.488281E-01 DX1= 0.000000E+00 ...

  QQQQQQQQQQ SUBROUTINE QU QQQQQQQQQQQQQQQQQQQQ --- [KCYC,ITER] = [ 147,  1]
  TEMPERATURE = 0.999996E+00  OUT OF RANGE IN SAT
  +++++   CANNOT FIND PARAMETERS AT ELEMENT *11126* IND = 4
  +++++   XX(M) = 0.118536E+06 0.549627E+00 0.999996E+00

  +++++ CONVERGENCE FAILURE ON TIME STEP # 147 WITH DT = 0.976562E-01 SECONDS,
       FOLLOWING TWO STEPS THAT CONVERGED ON ITER = 1
       STOP EXECUTION AFTER NEXT TIME STEP
  +++++ REDUCE TIME STEP AT ( 147,  1) +++++++++++   NEW DELT = 0.244141E-01
```

```
QQQQQQQQQQ SUBROUTINE QU QQQQQQQQQQQQQQQQQQQQ --- [KCYC,ITER] = [ 147,  1]
11126( 147,  1) ST = 0.176849E+05 DT = 0.244141E-01 DX1= 0.000000E+00 ...

TOUGH2 Analysis

OUTPUT DATA AFTER ( 147,  1)-2-TIME STEPS    THE TIME IS  0.20469E+00 DAYS
@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@

TOTAL TIME     KCYC   ITER  ITERC   KON
0.17685E+05    147      1    689     2
   DX1M        DX2M        DX3M        DX4M        DX5M        DX6M
0.00000E+00 0.00000E+00 0.00000E+00
@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@

ELEM.  INDEX     P           T          SG          SW        SO
               (PA)      (DEG-C)

   1    1 0.42499E+06 0.20003E+02 0.00000E+00 0.10000E+01 0.00000E+00
   2    2 0.42344E+06 0.20003E+02 0.00000E+00 0.10000E+01 0.00000E+00
   3    3 0.42299E+06 0.20003E+02 0.00000E+00 0.10000E+01 0.00000E+00
```

STEP 2. Go to the bottom of the OUT file and do an upward search for 11126 with the intent of finding out the current state of that cell. However, the first hit is at the source/sink output and is listed below. So knowing that cell 11126 is a source/sink with a generation rate, the first guess is that the generation rate is larger than can be supported by the flow into the cell and as a result pressure and temperature are dropping in that cell. Go to step 3.

```
@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@

        TOUGH2 Analysis

        KCYC =  147  -  ITER =    1  -  TIME = 0.17685E+05

ELEMENT SOURCE INDEX TYPE GENERATION RATE  ENTHALPY    FF(GAS)     FF(AQ)
                         (MOLE/S) OR (W)  (J/MOLE)

11126       1    1  COM1   0.22003E+03  0.00000E+00
@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@
```

STEP 3: Continue the search for 11126 to get the state of the cell until we find the P, T, etc data, as given below (the last line is for cell 11126). This confirms that the temperature is dropping. The saturation of gas is also lower in this cell. So now let us go and look at the cell in more detail. Go to step 4.

```
ELEM.  INDEX     P           T          SG          SW        SO
                (PA)      (DEG-C)
111 4 8995 0.10102E+06 0.19999E+02 0.87874E+00 0.12126E+00 0.00000E+00
111 5 8996 0.10102E+06 0.19999E+02 0.87874E+00 0.12126E+00 0.00000E+00
111 6 8997 0.10102E+06 0.19999E+02 0.87874E+00 0.12126E+00 0.00000E+00
111 7 8998 0.10102E+06 0.19999E+02 0.87874E+00 0.12126E+00 0.00000E+00
111 8 8999 0.10102E+06 0.19999E+02 0.87874E+00 0.12126E+00 0.00000E+00
111 9 9000 0.10102E+06 0.19999E+02 0.87874E+00 0.12126E+00 0.00000E+00
11110 9001 0.10102E+06 0.19999E+02 0.87874E+00 0.12126E+00 0.00000E+00
11111 9002 0.10102E+06 0.19999E+02 0.87874E+00 0.12126E+00 0.00000E+00
11112 9003 0.10102E+06 0.19999E+02 0.87874E+00 0.12126E+00 0.00000E+00
11113 9004 0.10102E+06 0.19999E+02 0.87874E+00 0.12126E+00 0.00000E+00
11114 9005 0.10102E+06 0.19999E+02 0.87874E+00 0.12126E+00 0.00000E+00
11115 9006 0.10102E+06 0.19999E+02 0.87874E+00 0.12126E+00 0.00000E+00
11116 9007 0.10102E+06 0.19999E+02 0.87874E+00 0.12126E+00 0.00000E+00
11125 9008 0.10102E+06 0.19987E+02 0.87838E+00 0.12162E+00 0.00000E+00
11126 9009 0.11854E+06 0.10000E+01 0.45037E+00 0.54963E+00 0.00000E+00
```

STEP 4: Now we need to find the cell in the model. Cells are numbered in X,Y, Z order starting at the bottom layer. This example model has 36 cells in the X directly and 39 in the Y, so each layer has 36*39=1404 cells. If we divide 11126 by 1404, we get 7.9, which means this cell is in layer 8. We now go to layer 8 in the Grid Editor and see the cell with the Source/Sink in the upper left corner. Zoom in and right-click on the cell. Under Properties the cell ID is 11126, so this is the problem cell. Under Sources/Sinks we see that the user is injecting Water/Steam into this cell at a rate of 3.9 kg/s but with 0.0 enthalpy. BINGO! - zero enthalpy corresponds to water at absolute zero, so the cell is being cooled by very cold injection. We need to change the enthalpy to a realistic value. This means getting out the steam tables. You can either get out the old thermodynamics text or you can download an Excel spreadsheet from the Tools section of Help at our website at:

https://www.rockware.com/petrasim-tools/

Below is the steam table data for a temperature of 250 C and pressure of 2MPa (482 F and 290 psia). The enthalpy is 2901869.965 J/kg and the quality is pure vapor. So doing the calculation with this enthalpy would represent steam injection. Go to step 5.

```
Input Data Here                 English Units
Input (Do not change)
Temperature, C    250.00        Temperature, F  482.00
Pressure, Pa (abs)  2.00E+06    Pressure, psia  290.08
Quality, 0=L, 100=V             Quality, 0=L, 100=V 0
Spec volume, m3/kg              Spec volume, ft3/lb
Enthalpy, J/kg                  Enthalpy, btu/lb  0
Entropy, J/kg/C                 Entropy, btu/lb/f 0

Output                          Output
Temperature, C  250.00          Temperature, F  482.000
Pressure, Pa  2.00E+06          Pressure, psia  290.08
Quality, 0=L, 100=V 100.00      Quality, 0=L, 100=V 100.00
Spec volume, m3/kg  0.111450802 Spec volume, ft3/lb 1.7852
Enthalpy, J/kg  2901869.965     Enthalpy, btu/lb  1247.79
Entropy, J/kg/C 6544.287025     Entropy, btu/lb/f 1.5633
Tsat, C 212.38                  Tsat, F 414.3
Psat, Pa  3.98E+07              Psat, psia  576.90
Deg superheat, C  19.85         Deg superheat, F  67.7
Deg subcool, C  -17.78          Deg subcool, F  0.0
Viscosity, Pa-s 1.79E-05        Viscosity, lb-sec/ft2 3.74E-07
Crit velocity                   Crit velocity 1480.67
Density, kg/m3  8.972568916     Density, lb/ft3 0.5602
SG  0.009                       SG  0.009
Viscosity, poise (P)  1.79E-04
```

STEP 5: Change the enthalpy to an appropriate value, then try to run again. This might not fix everything. For example, maybe the rate you are using for injection will be larger than can be supported by flow to the adjacent cells and the pressure may become too large in the injection cell. This will again be an indication of an unrealistic problem.

## Licensing/Registration Problems

If you experience trouble registering PetraSim, please contact tech@rockware.com.

## Contacting Technical Support

Questions and suggestions should be sent to tech@rockware.com.

# Appendix A. Working with Well Data Files

## File Format Overview

The file format used to represent well data in PetraSim is geared primarily towards usability, and based loosely on the Windows initialization (INI) file. Well variables are represented by a name and a value, separated by a space, a comma, or an equals (=) sign.

In order for a key to be properly parsed, it must be placed in the correct section of the data file. Section names appear in square brackets ([ and ]) on a line by themselves. Sections end when another begins.

### WELL

This section contains general data associated with the well.

```
[well]
name
top
bottom
print_bc_data
…
```

**Table A- 1. WELL Parameters**

| | | |
|---|---|---|
| Name | String | The name of the well. Should be surrounded by quotes if using any delimiting characters. |
| Top | Double | The maximum completion depth |
| Bottom | Double | The minimum completion depth |
| Print_BC_Data | Integer | Specifies if cell data should be printed. “1” is interpreted as TRUE, and “0” is interpreted as FALSE. |

### COORDINATES

This section is used to specify the 3D geometry associated with the well. This section does not use keyed values like in other sections, but instead parses values in an expected, space or comma delimited ordering. There is no limit to the number of coordinates specified, with each coordinate point being defined on a new line.

```
[coordinates]
x y z
…
```

**Table A- 2. COORDINATES Parfameters**

| | | |
|---|---|---|
| X | Double | The x-coordinate of the point |
| Y | Double | The y-coordinate of the point |
| Z | Double | The z-coordinate of the point |

## PRODUCTION

Multiple production sections can be used for a single well. The key "type" can be used to specify the particular type of boundary condition being defined. Support for reading time-rate tables is also available.

[production]
type
apportion
pi
pressure
gradient
rate
…

**Table A- 3. PRODUCTION Parameters**

| | | |
|---|---|---|
| Type | String | The type of boundary condition, specified according to the EOS in use. |
| Apportion | String | The flow in / out of the cells. Can be specified as either "kh" or "uniform". |
| PI | Double | The productivity index. |
| Pressure | Double | The pressure associated with the well. |
| Gradient | Double | If specified, represents the gradient for the well. If not, the model uses the Well Model option detailed in **Error! Reference source not found.**. |
| Rate | Double | If using the MASS production type, this can be specified as a double. If not defined, it is expected that a [time_rate_table] section immediately follows this one. |

## INJECTION

Like production, multiple injections sections can be specified per well. Type more things. Do more stuff.

[injection]
type
apportion
rate
enthalpy

**Table A- 4. INJECTION Parameters**

| | | |
|---|---|---|
| Type | String | The type of boundary condition, specified according to the EOS in use. |
| Apportion | String | The flow in / out of the cells. Can be specified as either “kh” or “uniform”. |
| Rate | Double | A double representing the rate (in kg/s) that mass flows through the cells. If not specified, it is expected that a [time_rate_enthalpy_table] section immediately follows this one. |
| Enthlapy | Double | A double representing the enthalpy of the well. If not specified, it is expected that a [time_rate_enthalpy_table] section immediately follows this one. |

## TIME-RATE Tables

[time_rate_table]
time rate
…

**Table A- 5. TIME-RATE Parameters**

| | | |
|---|---|---|
| Time | Double | The time at which associated rate changes occur. |
| Rate | Double | The time sensitive flow rate value. |

### TIME-RATE-ENTHALPY Tables

[time_rate_enthalpy_table]
time rate enthalpy
…

**Table A- 6. TIME-RATE-ENTHALPY Parameters**

| | | |
|---|---|---|
| Time | Double | The time at which associated rate and enthalpy changes occur. |
| Rate | Double | The time sensitive flow rate value. |
| Enthalpy | Double | The time sensitive enthalpy value. |

# Appendix B. PetraSim Simulator EXE Locations

The following tables show where PetraSim expects to find simulator EXEs. The location of these folders is relative to the PetraSim install location.

For example, when using the default install location, a 32-bit PetraSim installation will expect to find the simulator EXE for TOUGH, EOS1 in the following location:

```
C:\Program Files (x86)\PetraSim 2015\tough64\tough2\EOS1.exe
```

Locations are listed for the 32-bit version of PetraSim only. For the 64-bit version of PetraSim, it is necessary to add files to a folder named "tough64" instead of "tough64".

For example, when using the default install location, a 64-bit PetraSim installation will expect to find the simulator EXE for TOUGH, EOS1 in the following location:

```
C:\Program Files\PetraSim 2015\tough64\tough2\EOS1.exe
```

When attempting to start a simulation, if PetraSim is unable to find the EXE associated with the selected simulation mode, an error dialog will display the correct location for that simulator EXE. Some simulators, such as TOUGHREACT, ECO2 require additional files (CO2TAB, in the case of ECO2). These files should be added to the same folder as the corresponding simulator.

### TOUGH Simulator Mode

| | | |
|---|---|---|
| TOUGH (included) | ECO2N | tough64\tough2\ECO2N.exe |
| TOUGH (included) | EOS1 | tough64\tough2\EOS1.exe |
| TOUGH (included) | EOS2 | tough64\tough2\EOS2.exe |
| TOUGH (included) | EOS3 | tough64\tough2\EOS3.exe |
| TOUGH (included) | EOS4 | tough64\tough2\eos4.exe |
| TOUGH (included) | EOS5 | tough64\tough2\EOS5.exe |
| TOUGH (included) | EOS7 | tough64\tough2\EOS7.exe |
| TOUGH (included) | EOS7R | tough64\tough2\EOS7R.exe |
| TOUGH (included) | EOS8 | tough64\tough2\EOS8.exe |
| TOUGH (included) | EOS9 | tough64\tough2\EOS9.exe |
| TOUGH (included) | EWASG | tough64\tough2\EWASG.exe |
| TOUGH (included) | T2VOC | tough64\tough2\T2VOC.exe |
| | | |
| TOUGH2-MP* | ECO2N | tough64\tough2mp\tough2-mp-eco2n.exe |
| TOUGH2-MP* | EOS1 | tough64\tough2mp\tough2-mp-eos1.exe |
| TOUGH2-MP* | EOS2 | tough64\tough2mp\tough2-mp-eos2.exe |
| TOUGH2-MP* | EOS3 | tough64\tough2mp\tough2-mp-eos3.exe |
| TOUGH2-MP* | EOS4 | tough64\tough2mp\tough2-mp-eos4.exe |
| TOUGH2-MP* | EOS5 | tough64\tough2mp\tough2-mp-eos5.exe |

| | | |
|---|---|---|
| TOUGH2-MP* | EOS7 | tough64\tough2mp\tough2-mp-eos7.exe |
| TOUGH2-MP* | EOS7R | tough64\tough2mp\tough2-mp-eos7r.exe |
| TOUGH2-MP* | EOS8 | tough64\tough2mp\tough2-mp-eos8.exe |
| TOUGH2-MP* | EWASG | tough64\tough2mp\tough2-mp-ewasg.exe |
| | | |
| *via **Run TOUGH2-MP** on the **Analysis** menu. | | |

## TOUGH v2.1 Simulator Mode

| | | |
|---|---|---|
| TOUGH v2.1 | ECO2M | tough64\tough2_v21\eco2m.exe |
| TOUGH v2.1 | ECO2N | tough64\tough2_v21\eco2n.exe |
| TOUGH v2.1 | EOS1 | tough64\tough2_v21\eos1.exe |
| TOUGH v2.1 | EOS2 | tough64\tough2_v21\eos2.exe |
| TOUGH v2.1 | EOS3 | tough64\tough2_v21\eos3.exe |
| TOUGH v2.1 | EOS4 | tough64\tough2_v21\eos4.exe |
| TOUGH v2.1 | EOS5 | tough64\tough2_v21\eos5.exe |
| TOUGH v2.1 | EOS7 | tough64\tough2_v21\eos7.exe |
| TOUGH v2.1 | EOS7R | tough64\tough2_v21\eos7r.exe |
| TOUGH v2.1 | EOS8 | tough64\tough2_v21\eos8.exe |
| TOUGH v2.1 | EOS9 | tough64\tough2_v21\eos9.exe |
| TOUGH v2.1 | EWASG | tough64\tough2_v21\ewasg.exe |
| TOUGH v2.1 | T2VOC | tough64\tough2_v21\t2voc.exe |

## TOUGHREACT v1.2 Simulator Mode

| | | |
|---|---|---|
| TOUGHREACT v1.0† | eco2 | tough64\t2react_v10\treact_eco2.exe |
| | | tough64\t2react_v10\CO2TAB |
| TOUGHREACT v1.0† | eos1 | tough64\t2react_v10\treact_eos1.exe |
| TOUGHREACT v1.0† | eos2 | tough64\t2react_v10\treact_eos2.exe |
| TOUGHREACT v1.0† | eos3 | tough64\t2react_v10\treact_eos3.exe |
| TOUGHREACT v1.0† | eos4 | tough64\t2react_v10\treact_eos4.exe |
| TOUGHREACT v1.0† | eos9 | tough64\t2react_v10\treact_eos9.exe |
| | | |
| TOUGHREACT v1.2 (included) | eco2n | tough64\t2react\treact_eco2n.exe |
| | | tough64\t2react\CO2TAB |
| TOUGHREACT v1.2 (included) | eos1 | tough64\t2react\treact_eos1.exe |
| TOUGHREACT v1.2 (included) | eos2 | tough64\t2react\treact_eos2.exe |
| TOUGHREACT v1.2 (included) | eos3 | tough64\t2react\treact_eos3.exe |
| TOUGHREACT v1.2 (included) | eos4 | tough64\t2react\treact_eos4.exe |
| TOUGHREACT v1.2 (included) | eos9 | tough64\t2react\treact_eos9.exe |
| | | |

| | | |
|---|---|---|
| TOUGHREACT-Pitzer v1.21† | eos1 | tough64\treactPit\eos1p.exe |
| TOUGHREACT-Pitzer v1.21† | eos2 | tough64\treactPit\eos2p.exe |
| TOUGHREACT-Pitzer v1.21† | eos3 | tough64\treactPit\eos3p.exe |
| TOUGHREACT-Pitzer v1.21† | eos4 | tough64\treactPit\eos4p.exe |
| TOUGHREACT-Pitzer v1.21† | eos9 | tough64\treactPit\eos9p.exe |
| | | |
| †Via the **Simulator Version** option in the **Advanced** pane of the **Solution Parameters** dialog. | | |

## TOUGHREACT v2.0 Simulator Mode

| | | |
|---|---|---|
| TOUGHREACT v2.0 | eco2n | tough64\treact_v2\tr-eco2n.exe |
| | | tough64\treact_v2\CO2TAB |
| TOUGHREACT v2.0 | eos1 | tough64\treact_v2\tr-eos1.exe |
| TOUGHREACT v2.0 | eos2 | tough64\treact_v2\tr-eos2.exe |
| TOUGHREACT v2.0 | eos3 | tough64\treact_v2\tr-eos3.exe |
| TOUGHREACT v2.0 | eos4 | tough64\treact_v2\tr-eos4.exe |
| TOUGHREACT v2.0 | eos7 | tough64\treact_v2\tr-eos7.exe |
| TOUGHREACT v2.0 | eos9 | tough64\treact_v2\tr-eos9.exe |

## TOUGHREACT v3.32 Simulator Mode

| | | |
|---|---|---|
| TOUGHREACT v3.32 | eco2n | tough64\treact_v3\tr-eco2n.exe |
| | | tough64\treact_v3\CO2TAB |
| TOUGHREACT v3.32 | eos1 | tough64\treact_v3\tr-eos1.exe |
| TOUGHREACT v3.32 | eos2 | tough64\treact_v3\tr-eos2.exe |
| TOUGHREACT v3.32 | eos3 | tough64\treact_v3\tr-eos3.exe |
| TOUGHREACT v3.32 | eos4 | tough64\treact_v3\tr-eos4.exe |
| TOUGHREACT v3.32 | eos7 | tough64\treact_v3\tr-eos7.exe |
| TOUGHREACT v3.32 | eos9 | tough64\treact_v3\tr-eos9.exe |

## TMVOC Simulator Mode

| | | |
|---|---|---|
| TMVOC | TMVOC | tough64\tough2\TMVOC.exe |

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