

USING PETRASIM TO CREATE, EXECUTE, AND POST-PROCESS TOUGH2 MODELS

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ABSTRACT

PetraSim is an integrated model creation, analysis, and post-processor for the TOUGH2 family of codes, including T2VOC and TMVOC. It gives the analyst a tool to interactively create a grid, define all model properties, run the analysis using the integrated solvers, and then display 3D and time history plot of the results.

Key design decisions used in the development of PetraSim include: (1) high level geometric feature definition of the model, (2) use of Java for the graphical user interface to allow cross-platform execution, (3) automatic writing and execution (using the integrated TOUGH2 executable) of the input file, and (4) translation of the simulator output files to a common visualization format that is used for integrated 3D and time history display.

This paper illustrates the capabilities of PetraSim.

MOTIVATION

Although powerful, the TOUGH2 codes were initially developed as research tools, using a text-based input file. This presents significant hurdles to a new user, who must create an input file that describes a valid mesh and specifies the appropriate solution controls. Possible simulator options are often activated by flags that are confusing and may appear in unrelated locations in the text-based input file

It is hard enough to solve nonisothermal, multicomponent, multiphase problems without the additional difficulty of preparing complex and lengthy input files. While experienced users will have learned the idiosyncrasies of TOUGH2 and will have gathered their own toolkit for its use, even they may need additional help to exploit models with tens of thousands of cells or to enable rapid remeshing for convergence studies.

The solution to this problem has four key features: (1) use of a high level model description based on geometric features of the reservoir (stratigraphy, well coordinates), (2) presentation of the required input options grouped in a logical format with appropriate default options activated, (3) automatic writing and

execution of the input file, and (4) rapid access to visualization of results. Such a program should be interactive, with immediate visual confirmation of any user actions.

PetraSim is a new pre- and post-processor for TOUGH2 that incorporates these features into an integrated program for model creation, analysis, and results display. To allow cross-platform execution, it uses Java for the graphical user interface with native implementation of compute intensive algorithms. In the remainder of this paper, we describe the most significant features of PetraSim and give an example of its use.

PETRASIM FEATURES

Problem Description/Conceptual Model

A significant difference between PetraSim and the input file to a simulator is that PetraSim uses a geometric model to store the problem description rather than a grid-based description. A geometric model is a high-level, geometry-based representation of an object. This representation provides a natural and convenient location to store all of the necessary information associated with a numerical analysis problem, such as material properties and boundary conditions. Combining the geometric model with the parameters of the analysis creates a problem description unique to the problem at hand, but independent of any given analysis method. Conceptually, this also means that the same model description can be used for different simulators.

The advantage of such an approach is clear. When the grid serves as the fundamental carrier of information, any change in geometry, material properties, or initial conditions requires identification of the associated cells and a change to their properties. Refinement of a mesh may require the user to essentially start the analysis over from the beginning, redefining all associated cell conditions.

In contrast, if a high level geometric description is used, the grid may be changed at will and all properties and boundary conditions will automatically be applied when the simulator input file is written. As a particular example, in PetraSim the user can define

material boundaries and then assign properties to the regions created by the boundaries, Figure 1. This description is independent of the mesh. When the grid is created, the cell properties will inherit the proper material values and initial conditions from the region in which they are located.

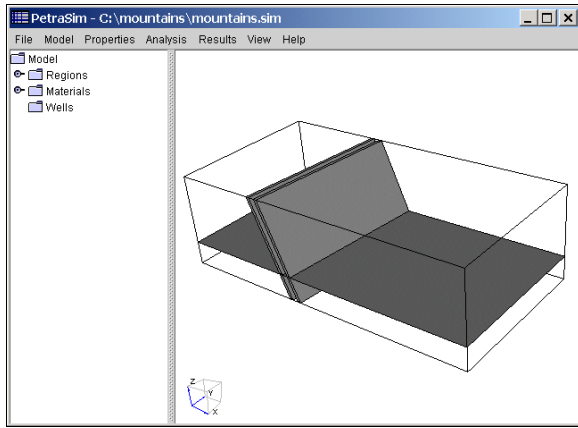


Figure 1. Model with internal material boundaries.

Figure 1 also illustrates several options for high level interaction with the model. On the left of the window is a tree that displays features in the model. Using the tree, the user can select a specific feature. Alternately, the model can be manipulated in the 3D display and features selected with the mouse. In either case, once a feature is selected all associated properties can be modified.

Grid Definition

An appropriate grid for an analysis must satisfy several constraints: (1) it must be able to capture the essential features of the reservoir, such as stratigraphic layers with different material properties, (2) it must be sufficiently refined to accurately represent regions of high gradient in the solution, and (3) it must satisfy the requirements of the simulator for proper convergence of the solution. A prismatic 3D grid is guaranteed to satisfy the convergence requirements of TOUGH2 and is used in PetraSim.

PetraSim gives the option of creating grids by simply specifying the number of cells to be used on each edge (along with an optional size factor for geometrically increasing cell sizes) or the option of using an input similar to the Meshmaker input for TOUGH2. To specify the Meshmaker input, the user fills a table that defines the direction, number of repeated cells, and the cell sizes, Figure 2. There is no limitation on grid size.

In addition, the user can specify contours that define the top and bottom of the grid. This can be used to represent topography, such as mountains and valleys.

Above and below this contour, the cells will be disabled and not included in the analysis. Finally, as will be discussed, a Grid Editor can be used to interactively modify the grid.

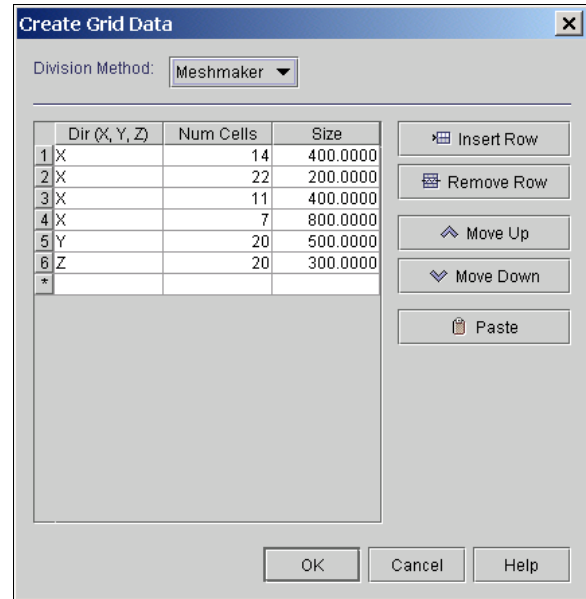


Figure 2. Definition of grid in PetraSim.

A grid created using internal boundaries, non-uniform cell sizes, and a contour to define the surface topography is illustrated in Figure 3. As can be seen, the disabling of cells enables the representation of a valley, while still maintaining the proper convergence properties for TOUGH2.

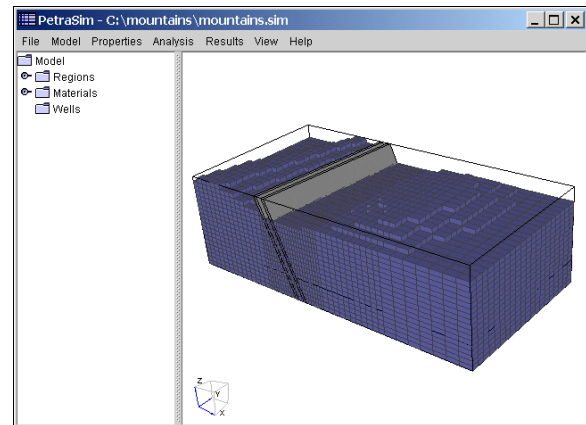


Figure 3. Prismatic grid defined on model.

In the future, more general grids can be added, since TOUGH2 uses the integral finite difference method. However, for convergence to the correct solution, the integral finite difference method requires that the mesh satisfy the Voronoï condition (that is, boundaries of the elements must be formed by planes which

perpendicularly bisect the lines between volume centers). Generation of such grids is relatively simple in 2D, but algorithms are much more complex for a general 3D Voronoi grid.

Gridlines can be edited, deleted, or inserted interactively. This editing is performed in the Grid Editor window. It is important to remember that the model has a grid, but the grid is not the model. The model is a higher level, grid independent, description of the reservoir.

Input of Model Properties

A properly designed user interface can guide the user through the model definition process, organizing into logical groupings input that may appear in many locations in a simulator input file. The interface can ease learning for a beginning user and act as a reminder for an experienced user.

As an example, the TOUGH2 code has the capability to model a fracture bounded by a confining bed that only conducts heat. To activate this option, the user must activate the MOP(15) flag, insert an artificial element at the end of the ELEME data, ensure that it is initialized to the confining bed initial conditions, and insert a material that is referenced by the artificial element to define the confining bed material properties. Finally, each element of the fracture must have its contact area with the confining bed defined as input. Undoubtedly there are historical reasons why the input file is organized in such a way.

The user interface, however, can be much simpler. Figure 4 shows how the required information is presented in PetraSim. A box is checked to indicate that this boundary condition is active, then initial temperature and material properties are specified, with reasonable default values given. When the TOUGH2 input file is written, PetraSim handles the details of creating the artificial element, specifying the contact areas, etc. As a result, there is a much greater chance that the user will actually solve the problem as intended.

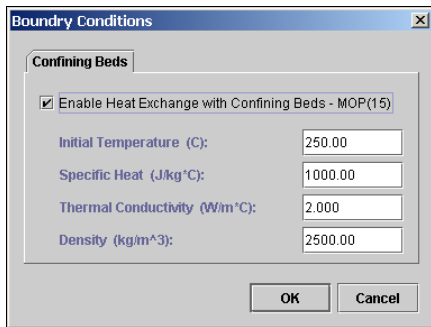


Figure 4. Dialog used to specify TOUGH2 confining bed data.

Two other examples of organizing data will be illustrated. The first is the definition of material properties in TOUGH2. Figure 5 shows the dialog used to input this data. The left pane allows the user to select any existing material or create a new one. In the right pane, the user can edit properties of the selected material. This includes MINC data (only activated if the MINC option has been enabled) and, under the Advanced button, the capability to customize relative permeability and capillary functions.

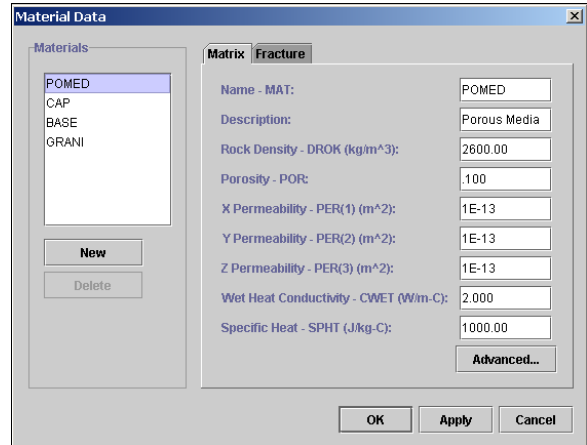


Figure 5. TOUGH2 material definition.

Figure 6 illustrates the organization of the solution parameters of TOUGH2. Again, common parameters have been grouped in an arrangement that helps the user understand and specify all parameters from one location. Similar organization is used for the solver and other solution parameters.

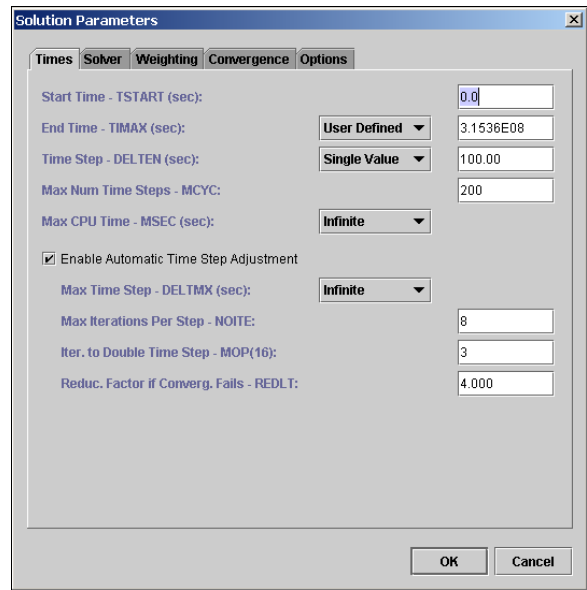


Figure 6. Solution controls dialog.

Editing of Cell Properties

After the grid is defined, cell properties may be edited directly. The goal of PetraSim is not to encourage cell editing. However, there may be times when individual cell editing is required. This is accomplished in the Grid Editor window, which allows the user to select a grid layer and edit any cell in that layer, Figure 7. The user can view the grid on any plane (XY, YZ, XZ) and on any layer in that plane.

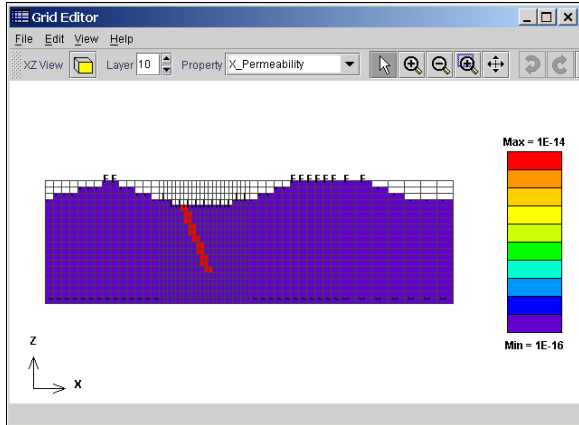


Figure 7. Grid Editor.

To help orient the user to which cells are being edited, PetraSim can highlight the current layer being edited, Figure 8.

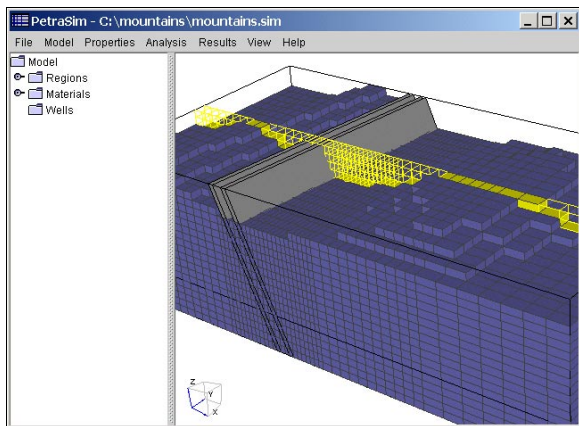


Figure 8. Highlight of the layer being edited in the Grid Editor.

In the Grid Editor the user can display any editable value and then select a cell or group of cells to edit that value. Figure 9 illustrates the plotting of cell temperatures.

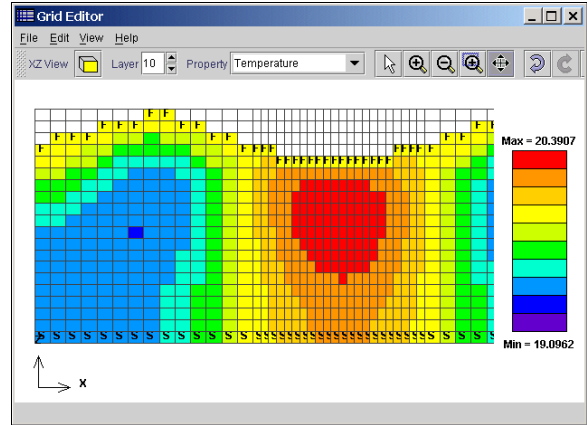


Figure 9. Plot of cell temperatures.

The user can also select cells to define sources and sinks, Figure 10.

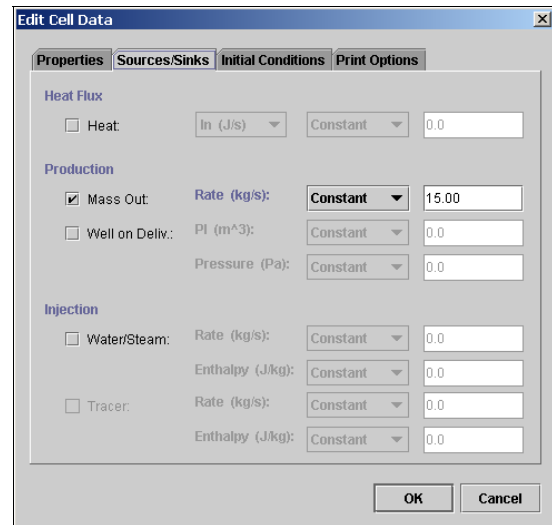


Figure 10. Defining a source or sink in the Grid Editor.

Writing a Simulator Input File

The whole point of a pre-processor is to automatically write the simulator input file in a correct format and without intervention by the user. In PetraSim, this task is performed by a function that accesses the model, the grid, and all other data necessary to write the file.

A portion of an example file is shown in Figure 11. Since the TOUGH2 program has not been modified, the input file written by PetraSim is in standard TOUGH2 format. Because PetraSim is writing the file, there is no need to keep the file small. Each element, connection, and initial condition is written explicitly. It can also be seen that the elements are given sequential numerical names. It is intended that

the user never need to know or examine these names. Any type of data, such as the definition of a source or sink, knows the associated cell and correctly writes the cell name when the simulator input file is written.

The resulting input file is correctly formatted and ready for input to TOUGH2.

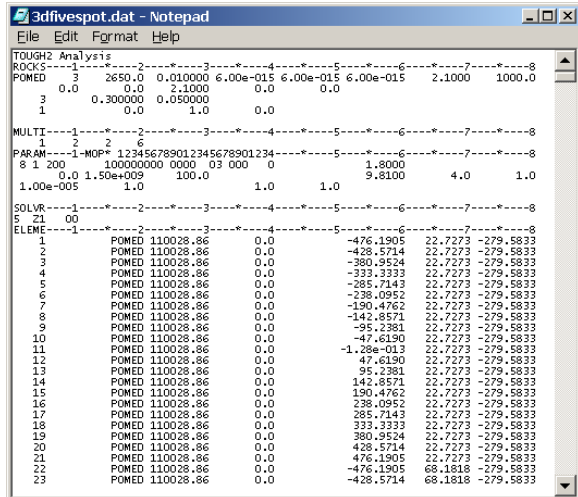


Figure 11. Portion of TOUGH2 input file created by PetraSim.

Integrated Solution

Thunderhead Engineering has received a license from the US Department of Energy that allows the integrated distribution of TOUGH2 executables. Therefore, to run the analysis, all the user needs to do is select Analysis/Run TOUGH2 and the analysis will proceed, using the integrated executable.

If the users own their own license for the TOUGH2 source code (can be obtained separately from the US DOE), PetraSim can be used to write the input file. Then the user can edit the input file to accommodate any specific input changes needed to run their version of TOUGH2.

Visualization

After the solution is completed, either 3D or time history plots of the results may be made. Figure 12 shows an example of an iso-surface plot of temperature. PetraSim uses a common results display component to read the data from the simulator-specific results files. For TOUGH2, the standard printed output file is parsed to extract the cell data.

As shown in Figure 12, once the data is read, the user can select any available variable and time for plotting. The user can rotate, pan, and zoom the image interactively. Image details, such as the number of

iso-surfaces and the data range can be controlled. Also, cutting planes can be defined on which the results are contoured. Finally, the user can export the data in a simple X, Y, Z value format for import into other presentation quality graphics programs, such as TECPLOT. In PetraSim, results are readily accessible to rapidly evaluate the analysis.

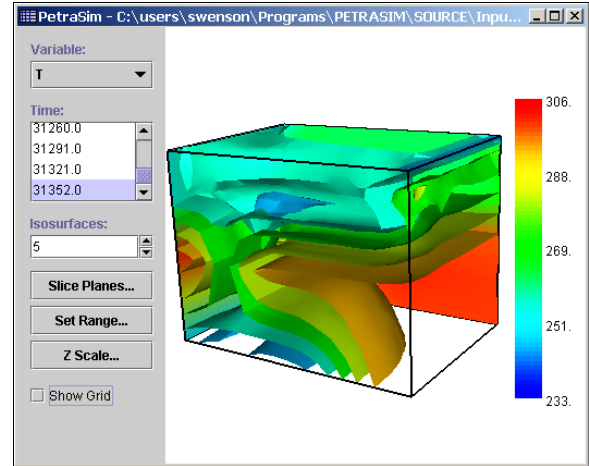


Figure 12. Iso-surface plot of temperatures.

In a similar manner, time history plots of results may be made, Figure 13.

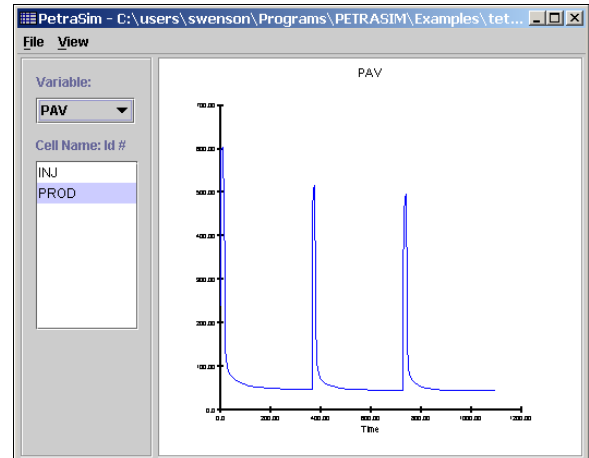


Figure 13. Time history plot (from TOUGH2 FOFT file).

Similar to the 3D plots, a common time history display component is used, with different translators to read the different simulator results files. For TOUGH2, the FOFT file is read.

As illustrated in Figure 13, the user can select any saved data and make a time history plot. If a cell was given a user-defined name, this name will be available for selecting the plot data. Once any plot is made, the data can be exported in a format that can

be read in a spreadsheet or other presentation quality graphics program.

EXAMPLE

To demonstrate PetraSim features, we give instructions to solve a variation on Problem 4 – Five-spot Geothermal Production/Injection (EOS1) described in the TOUGH2 User’s Manual (Pruess et al., 1999). This problem models a five-spot pattern of injection and production from a geothermal reservoir.

The geometry of the problem is shown in Figure 14. Water is injected in the center well and produced at the four corner wells. We use a half-symmetry model.

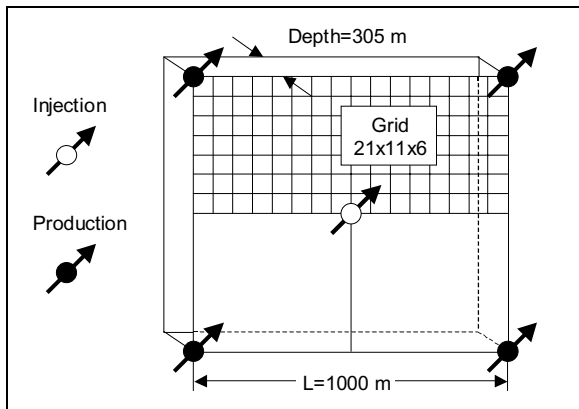


Figure 14. Five-spot well pattern with grid modeling 1/2 symmetry domain.

Model Creation

Start PetraSim by selecting *Start/Programs/PetraSim*. To define the boundary of the model, select *Model/Define Boundary...* and create the model boundary with the values X min = -500, X max = 500.0, Y min = 0.0, Y max = 500.0, Z min = -305.0, and Z max = 0.0. We create the grid on the model by selecting *Model/Create Grid...* and specifying 21 X divisions, 11 Y divisions, and 6 Z divisions. The resulting mesh is displayed in Figure 15.

Solution Controls

We next specify the information that will control the solution by selecting *Properties/Solution Controls...*. The Times tab allows us to specify parameters associated with the start and ending of the analysis and the time steps used for the calculation. In this case, we will start at 0 sec, end at 1. 5E9 sec (approximately 50 years), and specify an initial time step size of 100 sec. We allow a maximum of 200 time steps and select the Automatic Time Step adjustment option.

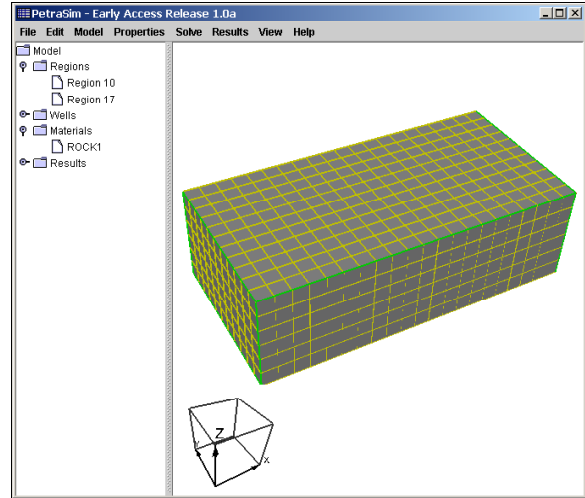


Figure 15. Five spot model after creating the grid.

We will change the solver to the stabilized bi-conjugate gradient solver by selecting the Solver tab, then selecting that solver, Figure 16.

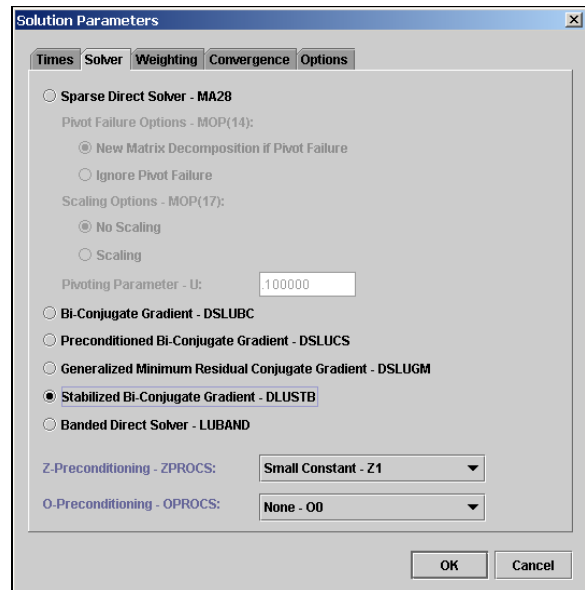


Figure 16. Selecting the solver.

Material Properties

To define the material properties, select *Properties/Materials...*. Change the material name to POMED, the rock density to 2650 kg/m³, the porosity to 0.01, the permeabilities to 6.0E-15 m², the conductivity to 2. 1 W/m-C, and the specific heat to 1000 J/kg-C. We need to specify both the relative permeability data and the capillary pressure data. To do this, select *Advanced* and then the appropriate tabbed pane. Use Corey’s Curves for the relative permeability, with constants of 0.30 and 0.05 and use a Linear

Function for the capillary pressure with constants of 0.0, 1.0, and 0.0.

Initial Conditions

To specify the default initial conditions, select *Properties/Initial Conditions...* Select the Two-Phase (T , S_g) option and then specify the temperature to be 300 °C and the gas saturation to be 0.01.

Sources and Sinks

Sources and sinks are defined by selecting cells individually in the Grid Editor. Select *Model/Edit Grid* to display the Grid Editor. There are a total of 6 layers in the Z direction. We will inject in layer 5 (the second from the top). To define the injection, first click on the layer spin-box on the tool bar to layer 5. Then, right click on the center lower cell and select the *Source/Sink...* menu option. Select the *Injection: Water/Steam* option with a flow rate of 15.0 kg/s and an enthalpy of 5.0E5 J/kg. We will produce from layer 3, so click on the layer spin-box arrow until layer 3 is selected. Next, right click on the top right cell and select the *Source/Sink...* menu option. Select *Production Mass Out*, then specify the mass flow rate at 7.5 kg/s, Figure 14. Repeat this for the top left cell. At this point, we have defined one injection cell and two production cells.

Save PetraSim Model File

We have now completed the input necessary for the solution and can save the PetraSim model by selecting *File/Save...* and giving the file name as 3d_five_spot.sim (the .sim extension will be added automatically if you do not give it).

We will also save a TOUGH2 input file by selecting *File/Write TOUGH2 File...* and giving the name 3d_five_spot.dat (the .dat extension will be automatically added if not specified).

Perform TOUGH2 Analysis

Select *Analysis/Run TOUGH2...* from the menu. This will start the analysis and indicate when the solution is finished.

View Results of the Analysis

Results can be displayed using 3D iso-surfaces, as contours on 3D planes, or as time history plots at the cells selected by the user for time history output. Data for the 3D views are obtained from the output file (in this case 3d_five_spot.out). Data for time history plotting is obtained from the FOFT file.

To view the results in 3D, select *Results/3D Contours...* . This will display a window in which the user can select the display variable, the time, and options on the number of isosurfaces, the grid, the

plot range, and slicing planes. Figure 17 shows a plot of temperature at 1.5E9 sec. This view shows the grid and uses two slice planes on which matching contours are drawn.

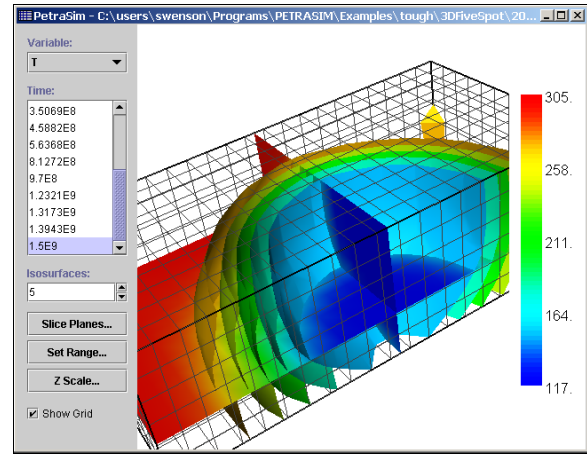


Figure 17. Display of calculated temperatures at $t=1.5E9$ sec.

To view time history plots of cell data, select *Results/Cell Results...*, Figure 18. In this window the user can select the plot parameter and the cell for which results are to be plotted. This plotted data can be written in column format to a file by selecting *File/Export Data...* in the time history menu. This data can then be imported into another program for additional plotting or comparison with data.

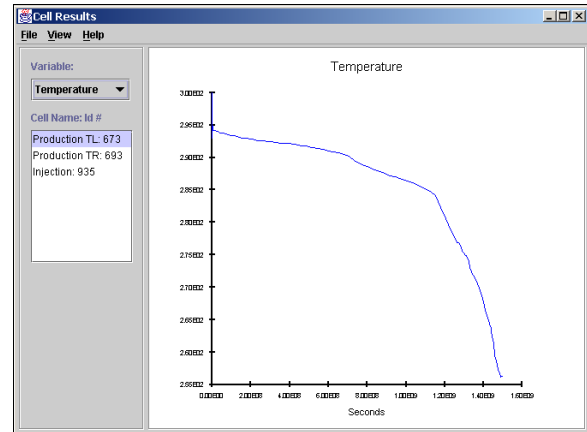


Figure 18. Cell results.

OBTAINING PETRASIM

A 30 day trial version of PetraSim can be downloaded at www.petrasim.com. Licenses are available for education (free, but limited capability), research, and commercial use.

ACKNOWLEDGMENTS

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REFERENCES

Pruess, K., Oldenburg, C., and Moridis, G., TOUGH2 User's Guide, Version 2.0, Earth Sciences Division, Lawrence Berkeley National Laboratory, LBNL-43134, November, 1999.