

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

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ABSTRACT

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 input file. It is hard enough to solve non-isothermal, multi-component, multi-phase problems without the additional difficulty of preparing complex and lengthy input files. In addition, the user must develop their own toolkit to display results. Even experienced users may need additional help to exploit models with tens of thousands of cells or to enable rapid remeshing for convergence studies.

PetraSim – an integrated program for TOUGH2 model creation, analysis, and results display – has undergone continual development since its first release in August, 2002. The latest version includes support for TOUGHREACT and TOUGH-Fx/HYDRATE. New features to be demonstrated in version 3.0 include: support for “extra cells” that are not part of the physical mesh (used for special boundary conditions, etc.), display of a 2D image (such as a map) in the 3D views, improved support for wells, improved 2D editor performance including cell search features, and several other interface enhancements.

Use of PetraSim and the TOUGH2 programs will be demonstrated in the poster session.

PETRASIM FEATURES

PetraSim provides four key features that help speed and simplify the use of the TOUGH2 and TOUGH-Fx family of codes: (1) use of a high level model description based on geometric features of the reservoir, (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. PetraSim is interactive, with immediate visual confirmation of any user actions.

Problem Description/Conceptual Model

PetraSim allows the user to define regions and wells as high level geometric entities, independent of the grid. For example, Figure 1 shows a model in which internal material boundaries have been defined and can then be used to assign properties to the regions created by the boundaries. 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.

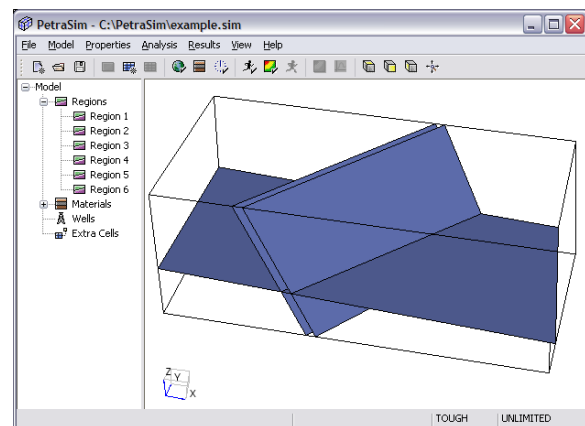


Figure 1: Model with internal material boundaries

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. 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. A grid created using internal boundaries, non-uniform cell sizes, and a contour to define the surface topography is illustrated in Figure 2. As can be seen, the disabling of cells enables the representation of a valley, while still maintaining the proper convergence properties for TOUGH2.

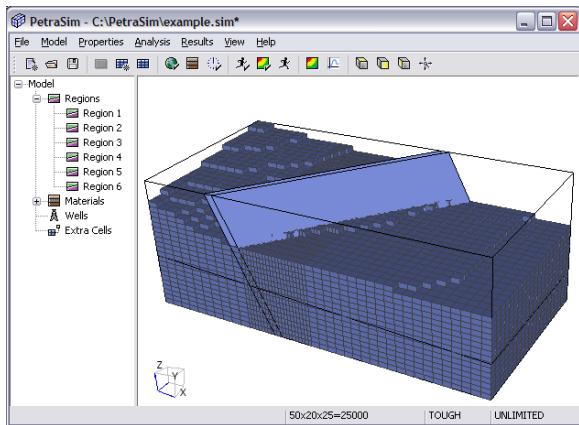


Figure 2: Prismatic grid defined on model

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 Voronoi 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.

The definition of material properties in TOUGH2 is shown in Figure 3. 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 Relative Perm..., the capability to select and preview relative permeability and capillary functions, Figure 4.

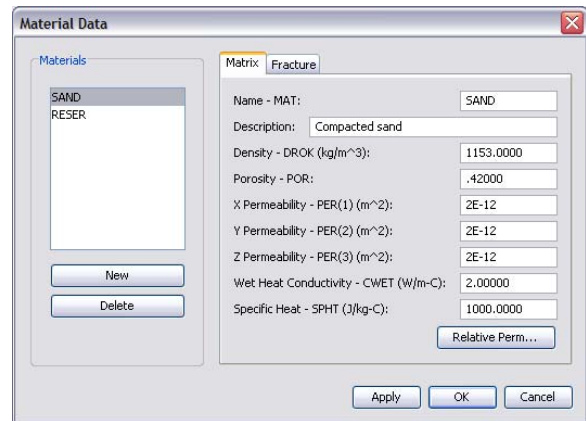


Figure 3: TOUGH2 material definition

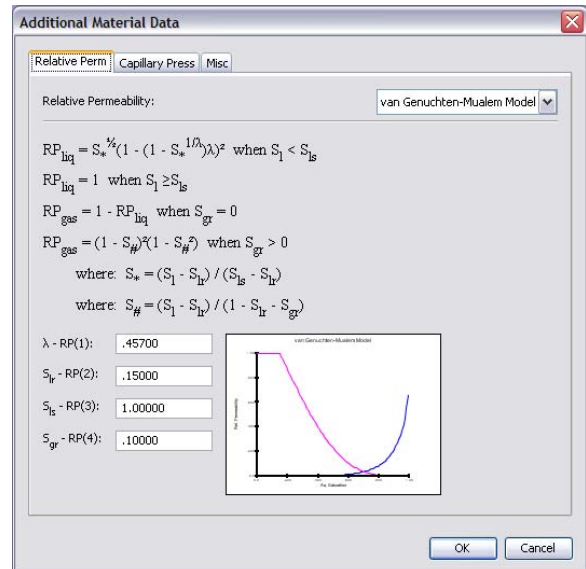


Figure 4: Selection and preview of relative permeability functions

Figure 5 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.

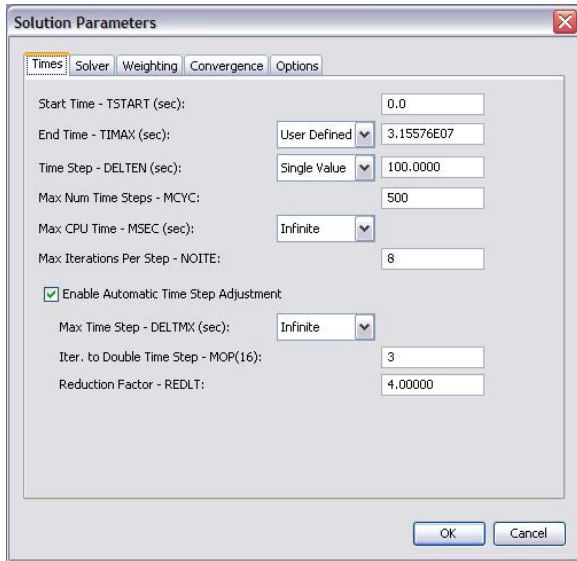


Figure 5: Solution controls dialog

Editing of Cell Properties

After the grid is defined, cell properties may be edited directly. 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 6. The user can view the grid on any plane (XY, YZ, XZ) and on any layer in that plane.

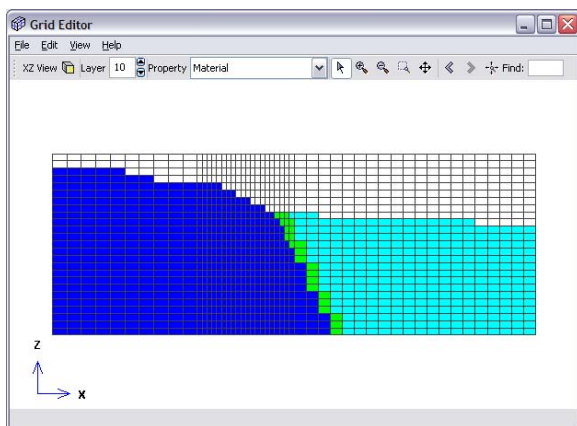


Figure 6: Grid editor

To help orient the user to which cells are being edited, PetraSim can highlight the current layer being edited, Figure 7.

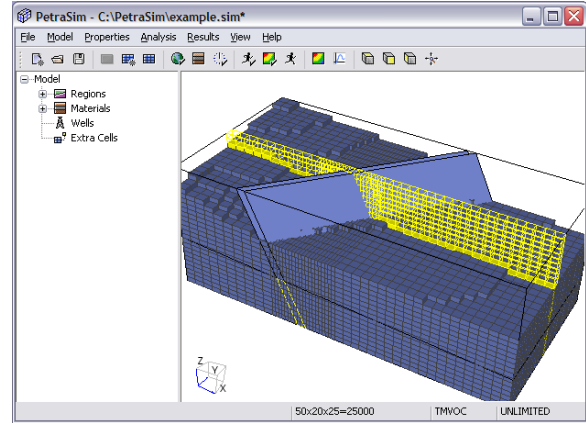


Figure 7: Highlight of the layer being edited in the Grid Editor

In the Grid Editor, the user can also select cells to define sources and sinks, Figure 8.

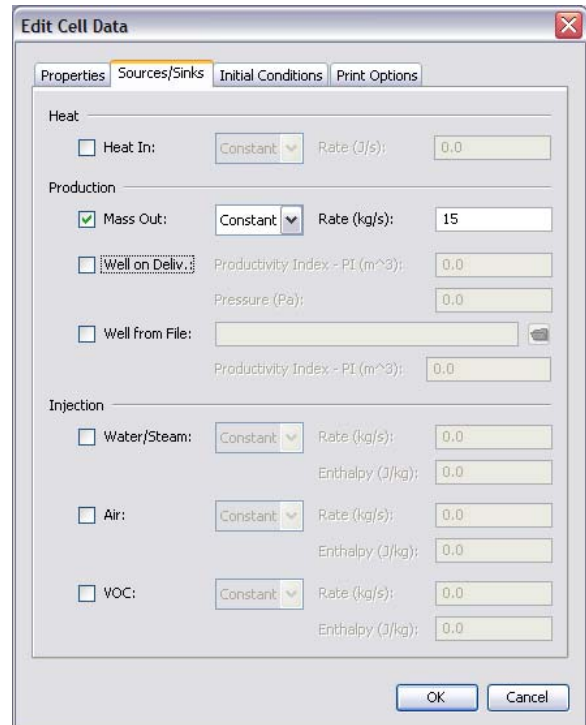


Figure 8: Defining a source or sink in the Grid Editor

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 9. 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.

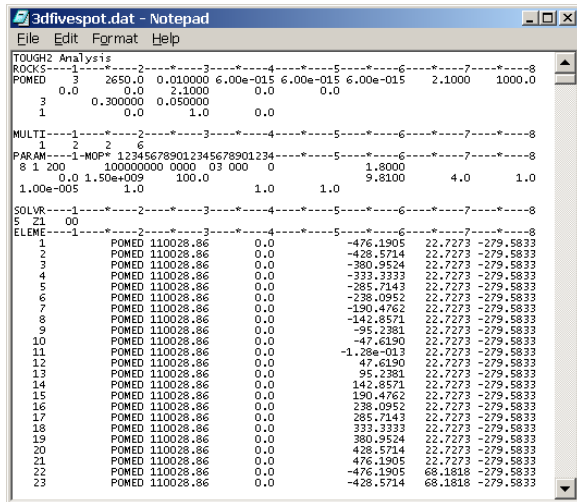


Figure 9: Portion of TOUGH2 input file created by PetraSim

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 user owns 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 10 shows an example of an iso-surface plot of temperature. PetraSim uses a common results display component for all simulators, with different translators 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 10, 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. Vectors can be used to display items such as fluid flow. 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.

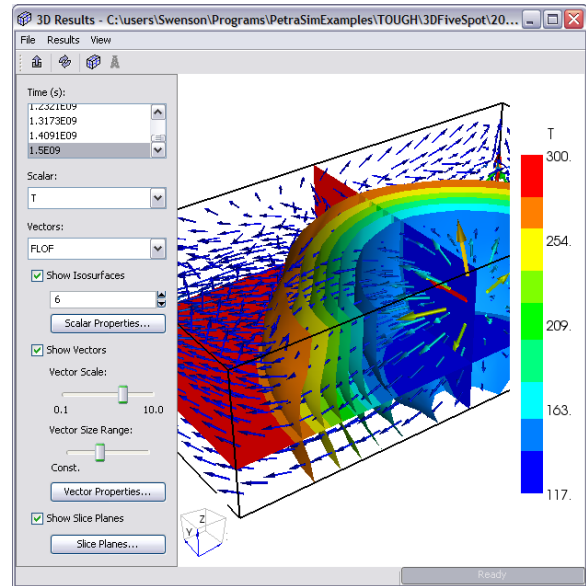


Figure 10: Iso-surface plot of temperatures

In a similar manner, time history plots of results may be made, Figure 11. 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.

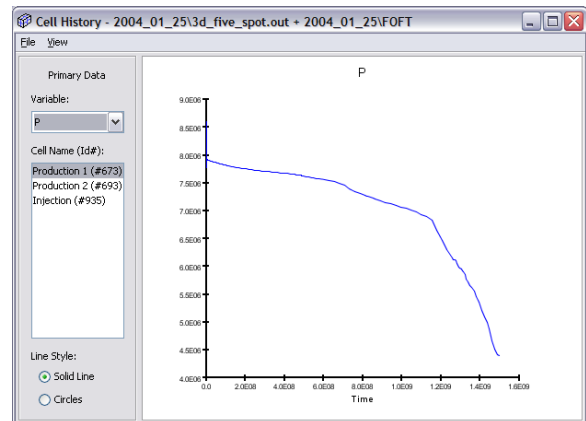


Figure 11: Time history plot (from TOUGH2 FOFT file)

As illustrated in Figure 11, 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.

NEW FEATURES IN VERSION 3.0

Version 3.0 of PetraSim is in testing and scheduled for release in June, 2006. Some of the new features include:

- Support for ECO2N, the new TOUGH2 equation of state designed for studies of CO₂ storage in saline aquifers.
- Support for non-geometric “extra cells” in the model, Figure 12. Many modelers use non-geometric cells to represent special boundary conditions. The user can now input a table of cells, defining the connections to existing cells in the model.

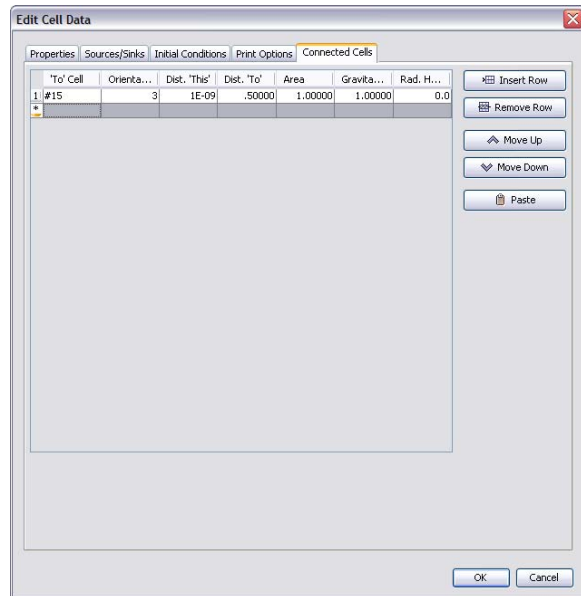


Figure 12: Adding extra (non-geometric) cells using a table

- User-defined labels in the 3D views, Figure 13. The user can edit a table of labels and locations.
- The ability to add an image, such as a map, in the 3D view, Figure 13.
- A graphical progress monitor during TOUGH execution, Figure 14.
- High quality graphics output from the 3D views.
- A find cell feature in the 2D grid editor that allows the user to search for a cell by cell ID.

- Added axis scaling (3D view & Results view) so that long/tall models can be scaled for attractive display.
- User can save favorite views in 3D view for comparison plotting of different model results.
- Prompts user to save a modified model before opening a new file or exiting PetraSim.

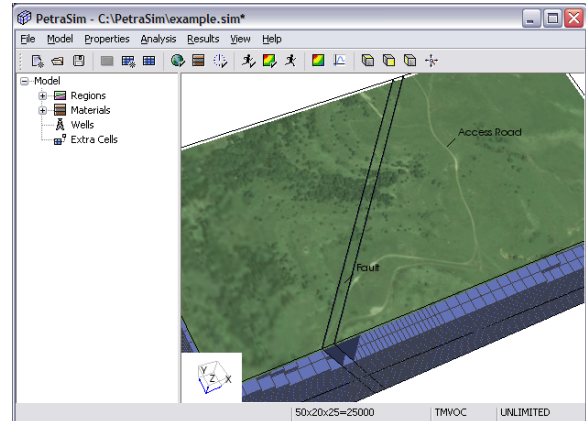


Figure 13: Graphic image superimposed on model with labels

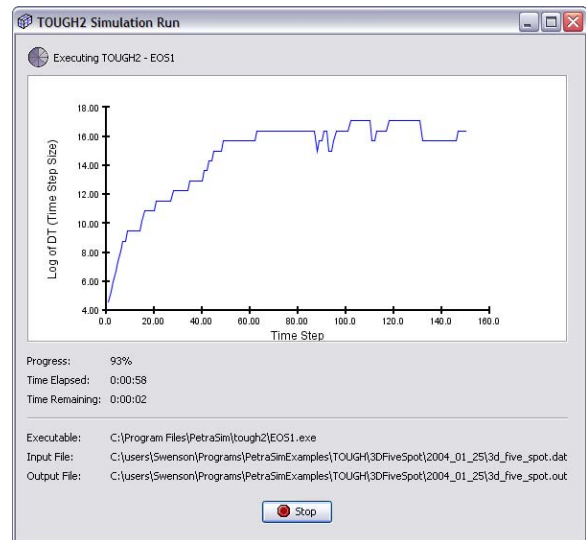


Figure 14: Graphical display of solution progress and time step size

- Improved editing and manipulation of wells.
- Equations and graphs added to the capillary pressure dialogs

Significant effort has also been put into writing a new PetraSim User Manual and in updating the Examples Manual.

OBTAINING PETRASIM

A 30 day trial version of PetraSim can be downloaded at www.petrasim.com. Sales are through RockWare (www.rockware.com). Licenses

are available for education (free, but limited capability), research, and commercial use.

ACKNOWLEDGEMENTS

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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.