

## GeoCad, A PRE- AND POSTPROCESSOR FOR TOUGH2

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### **ABSTRACT**

GeoCad provides pre and post processing facilities for TOUGH2 simulations which simplifies the preparation of models and provide a convenient method to visualize simulation results.

### **INTRODUCTION**

The TOUGH2 (Pruess 1999) family of multiphase flow simulators is a powerful and flexible tool for the simulation of many phenomena associated with the flow of mass and energy in a porous medium. Much of this power and flexibility comes from the approximation of the conservation equations describing porous media flow by integrated finite differences (Narasimhan and Witherspoon and Witherspoon 1976). However this flexibility comes at a cost, and the cost is the need to specify detailed information about the size and connections of every element making up the integrated finite element mesh.

### **REQUIREMENTS OF A PREPROCESSOR**

Input data to TOUGH2 contains no information about the geometry of the domain on which the problem is specified and this is one of the reasons for its flexibility. However any particular problem is defined over a domain and it is generally easier to develop a TOUGH2 model with reference to the geometry of this domain rather than in terms of element volumes, connection areas and distances.

A TOUGH2 model requires the specification of

- Element volumes
- Connection areas
- Source (sink) terms
- Material properties
- Boundary conditions
- Initial conditions
- Run time parameters

Ideally we would like to specify this information in an intuitive way and in a manner that minimizes the likelihood of making an error.

### **DEFINING ELEMENTS**

The GeoCad preprocessor is a computer program that enables the definition of a TOUGH2 model in terms of its geometry. Using a mouse the geometric information defining a TOUGH2 model is drawn onto a computer screen. From this the geometry free input for TOUGH is automatically generated.

GeoCad constructs a TOUGH2 model as one or more layers. A layer is a slice of possibly varying thickness across the domain being modeled. Often this slice is horizontally orientated and is of constant thickness. By altering the gravity we can have vertical layers or even layers orientated at an arbitrary angle to the gravity vector. The number of layers is generally limited to 100 although this number is easily increased.

An example of this element geometry is shown in Figure 1, the layer structure and Figure 2 the element structure of a layer used for a model of the Tauhara geothermal field. This field is located in the Taupo Volcanic Zone, New Zealand.

There are two types of information to define for each layer, material information and element information. Material (or region) information defines the type of material in a particular area where a region is a volume of the domain over which material properties are regarded as constant. Each layer is split into a number of elements where an element is a volume of the model domain over which P, T and S are regarded as constant. The elements defined on a layer become the elements used by TOUGH2.

Typically a model is constructed layer by layer by first defining the areal extent of a layer (Figure 3- Figure 4) as either a rectangle or a polygon and then further subdividing this (Figure 5). There is no requirement that elements be rectangular, the

elements in the mesh shown in Figure 6 were generated outside GeoCad then GeoCad was used to add material information, calculate connection areas and generate TOUGH2 input.

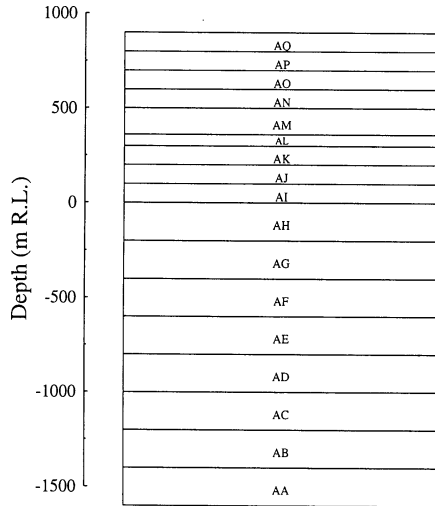


Figure 1. Example of a layer structure used for a geothermal reservoir model

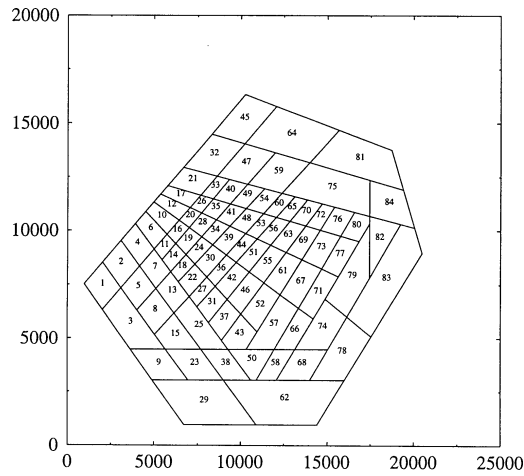


Figure 2. Typical element layout of a layer

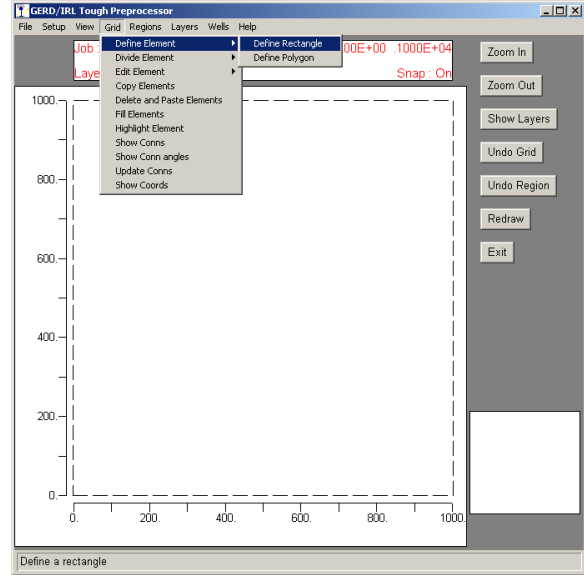


Figure 3. The first step in defining a layers structure

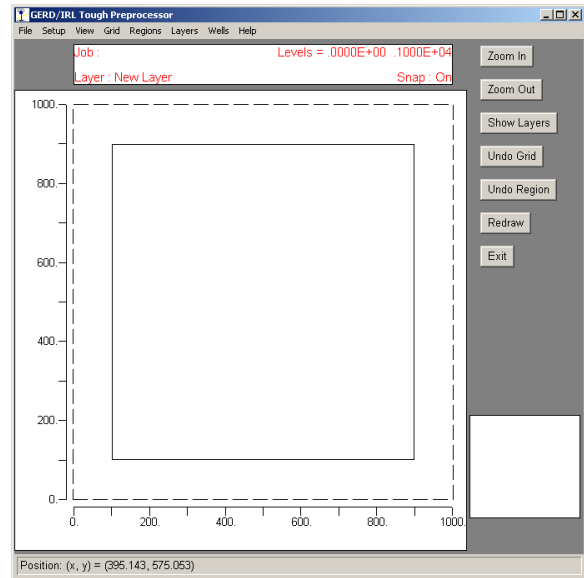


Figure 4. The outer boundary of the layer is rectangular in this example.

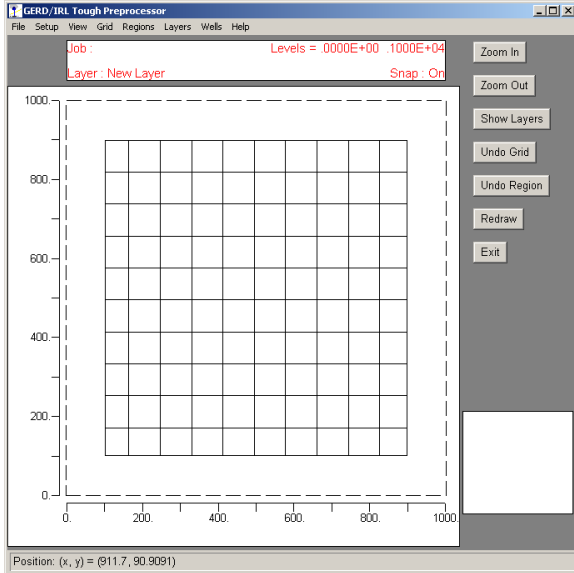


Figure 5. The initial element is subdivided into many elements.

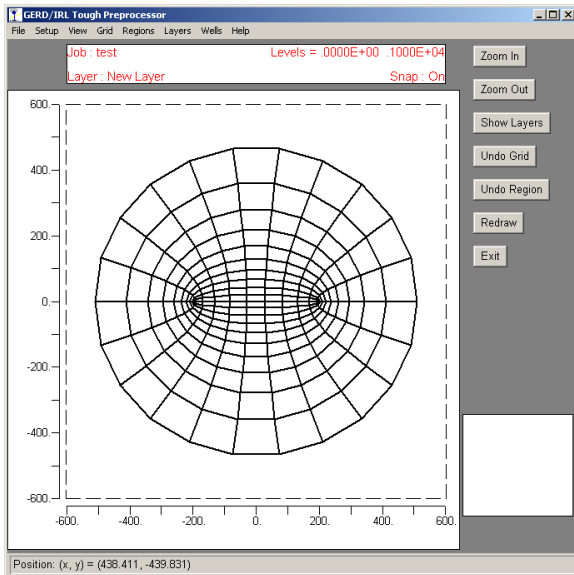


Figure 6. An example of a non-rectangular mesh.

Information on source and sink location may be entered using the mouse or by reading coordinates from a file. Sources (sinks) are defined over a brick shaped volume of the model domain. This volume may encompass several elements and the source or sink will be divided between these elements based on the volume of the well occurring in each element. This allows the definition of not only wells but extended sources like rain over the surface of a model or upflow zones in a geothermal field.

### **BOUNDARY AND INITIAL CONDITIONS**

Boundary conditions are specified on the sides of a rectangular box. Only elements touching the sides of

the box are connected to boundary elements. The sides of the box may be assigned a number of boundary conditions

- Constant pressure or temperature
- Pressure or temperature interpolated from specified spot values
- Hydrostatic Pressure
- Boiling point for depth Temperature and Pressure
- No flow

Initial conditions are assigned by interpolating the values at the boundary of a layer over the whole layer. Figure 7 shows a typical screen used to define boundary conditions on a box enclosing the model domain.

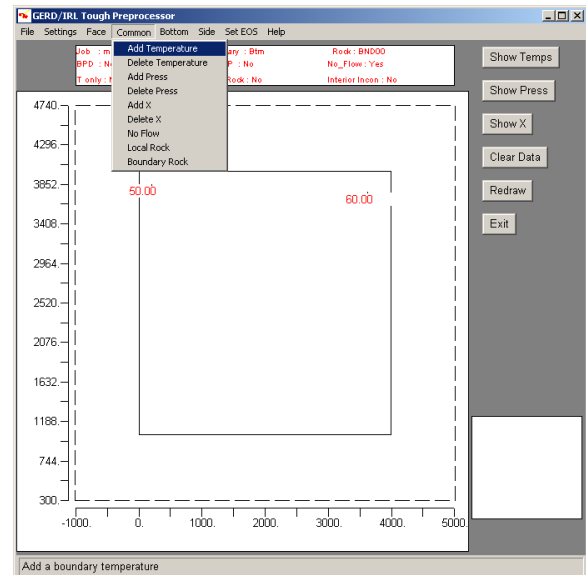


Figure 7. Adding temperature boundary conditions over a face.

### **PARAMETERS**

Parameters for input blocks such as RPCAP, PARAMS and ROCKS are set by filling in a series of forms. Where possible, sensible defaults are assigned so a job may be generated with the minimum of input. An example of a screen defining rock properties is shown in Figure 8.

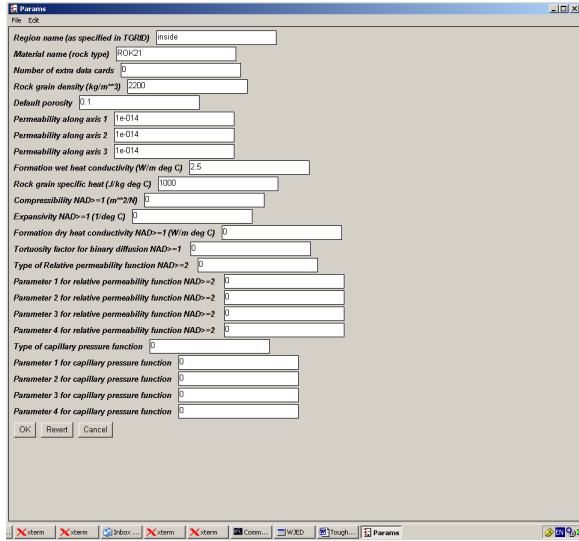


Figure 8. Specifying rock properties.

## REQUIREMENTS OF A POST-PROCESSOR

Analysis of the results of TOUGH2 simulations involves visualising three-dimensional data sets. Useful visualisations are contours plots, line plots, iso-surfaces and time profiles. During model development, generating the plots required to understand model performance, and how it might be improved, is often a time-consuming exercise. For example, to check the temperature distribution at two depths and to check a pressure history at three locations requires:

1. Writing a program to parse the TOUGH2 output file
2. Associating a TOUGH2 element with a point in 3-D space
3. Extracting a data set of (X, Y, Z, P, T, S, X) at each output time
4. Interpolating values from the 3-D data set onto the depths of interest
5. Plotting the contours from these interpolated data sets
6. Extracting data sets (t(ime), P) at each of the three locations
7. Producing t-P plots at each location

This process, while cumbersome, can be automated if the locations of the output are known. For example, when a simulation is testing the impact of a future scenario, results are generally compared at a number of standard locations.

However, during model development, when we are trying to optimise the model structure and parameters to match the field history, it is often necessary to examine the results at many locations – not just a standard set. In this situation it is desirable to have an interactive tool that provides an easy and intuitive way of viewing simulation results. Such a tool would provide:

- Contours of all model variables on horizontal and vertical cross-sections through the model
- Plots of model variables against depth at arbitrary locations
- Plots of model variables against time at arbitrary locations, together with any measured data at that location
- Iso-surfaces of model variables
- Plots of flows across arbitrary planes.

## THE GEOCAD POSTPROCESSOR

The GeoCad postprocessor (GeoView) is a computer program that enables users to interactively display and examine the output from a TOUGH2 simulation. The program provides

- Contours on planes
- Profiles along lines
- Time profiles at a point
- Iso-surfaces
- Flows across planes

The main input for the program is a TOUGH2 output file, a coordinate file assigning a 3D point to the centre of each TOUGH2 element (this is automatically produced by GEOCAD), and a configuration file specifying the format of the TOUGH2 output (for instance file column numbers and names for each variable). Configuration files for the standard EOS modules are provided with the program, and new ones can be easily added.

By way of an example, let us look at some steps in analysing the output from a TOUGH2 simulation. Firstly, we might be interested in examining the temperature distribution in the model. GeoView allows us to view the temperature on a plane or a line through the model, or as an iso-surface. In Figure 9 a horizontal plane at level  $z = -125$  is being defined in the dialog box.

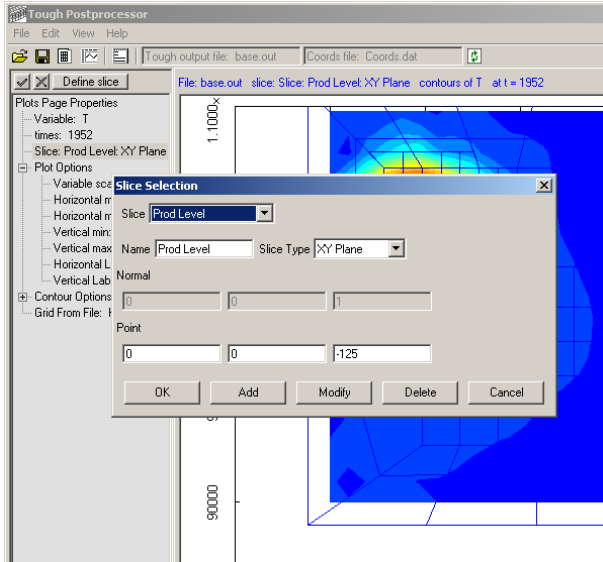


Figure 9. Defining the horizontal plane  $z = -125$  on which to view the temperature contours

Once the plane is defined, the contours of any variables in the simulation can be viewed. Figure 10 shows filled temperature contours at the level  $z = -125$ . New planes can be easily added and the results viewed immediately. There can be a slight delay while the interpolation is undertaken – this will only be a second or so on a modern PC.

In addition to plotting the contours, the GEOCAD grid can be overlaid, to assist with viewing the contours. From the contours in Figure 10, a hot upflow can be seen in the top left of the model. We might then be interested in looking at the vapour saturation underneath this area. This can be achieved using a profile on a line, or contours on a vertical slice. A profile on a line showing the vapour saturation can be seen in Figure 11. The contours and profiles can be viewed for any time at which the simulation results are written.

In addition to looking at the spatial behaviour of the model, we are often interested in examining the behaviour of the model with time, particularly matching model results with measured data. This can also be easily achieved in GeoView, by specifying a point in the model together with a file containing history data at that point. Figure 12 shows a comparison of model pressure with measured at a selected location in the model.

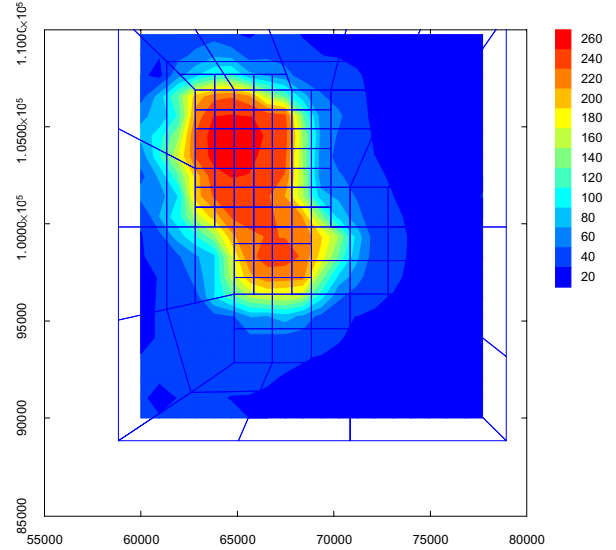


Figure 10. Filled temperature contours on the plane defined in Figure 9. The blue lines show the TOUGH2 grid for the model at that level.

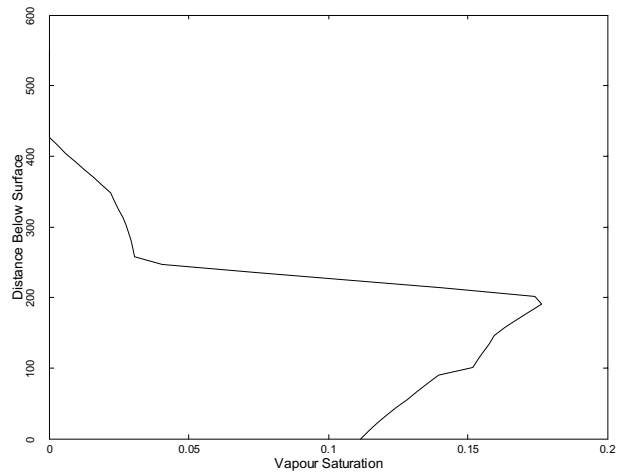


Figure 11. Vapour Saturation on a vertical line through the hot upflow of Figure 10. The vertical axis shows depth below the surface.

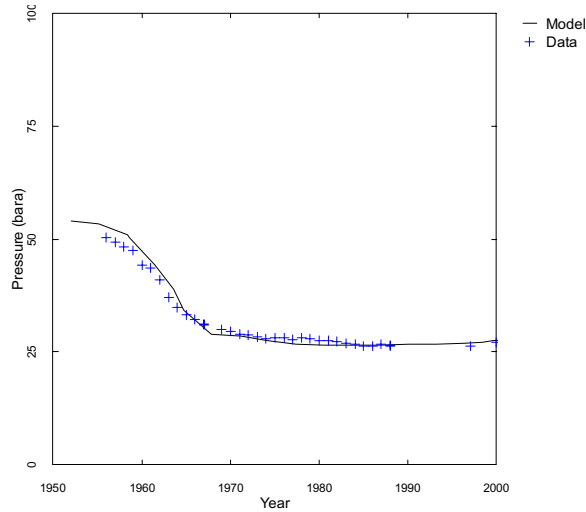


Figure 12 Comparison of model results with history data at a selected location.

One of the major problems involved with the graphical display of data is interpolation onto a grid suitable for generating contours, profiles, and iso-surfaces. Typically, contouring algorithms require that the data be specified on a regular grid of some sort. There are standard algorithms, such as the Kriging Algorithm, for interpolating scattered data. However, great care must be taken especially with pressure data which usually has a linear relationship with depth.

In geothermal systems, the relationship between pressure and depth can be extremely complex where vapour and liquid dominated regions may exist side-by-side. The complexity of these relationships precludes simply subtracting a best-fit trend from the data, but the trend needs to be accounted for otherwise erroneous result may occur. GeoView has user specified options for controlling some aspects of the interpolation process.

### CONCLUSIONS

The GeoCad pre-processor provides a very flexible, user-friendly interface to TOUGH2. It allows users to very rapidly develop rectangular integrated finite difference meshes and also has the flexibility to produce irregular meshes. The Post-processor provides a convenient method of presenting TOUGH2 output in a graphical form and simplifies the process of comparing field measurements with simulation results.

### REFERENCES

- Narasimhan, T.N. and Witherspoon, T.A. An Intergrated Finite Difference Method for Analyzing Fluid Flow in Porous Media, *Water Resour. Res.*, 12(1), 57-64, 1976.
- Pruess, K., C. Oldenburg, and G. Moridis, *TOUGH2 User's Guide, Version 2.0*, Report LBNL-43134, Lawrence Berkeley National Laboratory, Berkeley, Calif., 1999.