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# GEOCAP TRAINING MODUL

## NATURAL STATE

GEOHERMAL MASTER PROGRAM ITB  
EMPOWERING GEOHERMAL COMMUNITY

## NATURAL STATE MODULE

This module demonstrates an initial state calculation. It also demonstrates the use of contour therefore the surface represents both of atmospheric condition and topography. Surface conditions such as bottom and side boundary are also definite. This module will show the steps for make a model of liquid-dominated reservoir with area of 4 x 2 km<sup>2</sup> and the thickness is 3.6 km. The pressure profile is near to hydrostatic pressure. While the component of heat source, reservoir, cap rock and boundary implemented to the synthetic model.

### I. Computer Model

The Computer model in TOUGH2 will use EOS1, the equation of state (EOS) model used for multiphase water and tracer. The dimension of a computer model will be 4000x2000x3600 meters. This information can be entered using the New Dialog (Figure 1 in the ribbon of PetraSim).

To create the model:

1. On the **File** menu, click **New**
2. In the **Simulator Mode** list, Select **TOUGH2**
3. In the **Equation of State (EOS)** list, select **EOS1**
4. In the **X Min, Y Min, Z Min**, types 0, 0, -2500
5. In the **X Max, Y Max, Z Max**, types 4000, 2000, 1100
6. Click **OK** to Close the dialog and create the model

The 'New Model' dialog box contains the following settings:

- Simulator Mode:**
  - ☒ TOUGH2
  - ☐ TOUGHREACT
  - ☐ TMVOC
  - ☐ TOUGH-Fx
- Equation of State (EOS):**
  - ☒ EOS1 MP
  - ☐ EOS2 MP
  - ☐ EOS3 MP
  - ☐ EOS4 MP
  - ☐ EOS5 MP
  - ☐ EOS7 MP
  - ☐ EOS7R MP
  - ☐ EOS9
  - ☐ EWASG MP
  - ☐ ECO2N MP
  - ☐ T2VOC
  - ☐ TMVOC
  - ☐ HYDRATE
- Model Bounds (Default):**
  - X Min: 0.0, X Max: 5000
  - Y Min: 0.0, Y Max: 5000
  - Z Min: -2500, Z Max: 500

Figure 1. New dialog to create model computer size and to choose EOS.

The initial computer model shown in Figure 2.

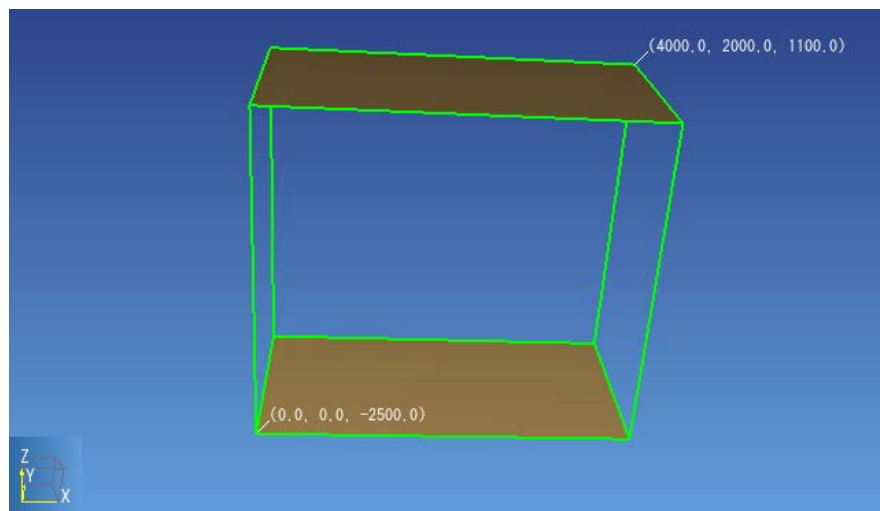


Figure 2. Initial computer model.

## II. Create Materials

The next step is define all the material first. The simulation will use several material to specify properties for the first material before the material data iterates.

1. On the **Properties** menu, click **Edit Materials**
2. In the tab **Matrix** box, fill **Name-MAT**, **Description**, choose **Color**, **Density**, **Porosity**, **XYZ Permeability**, **Wet Heat Permeability**, **Specific Heat** with reasonable data.

For this simulation we will use the default linear data for relative permeability and not include any capillary pressure. These are found by selecting **Additional Material Data**.

Table 1. Material Data.

Name - MAT	Density - DROK (km/m <sup>3</sup> )	Porosity - POR	Permeability (m <sup>2</sup> )			Wet Heat Conductivity - CWET (W/m.C)	Specific Heat - SPHT (J/kg.C)
			X - PER(1)	Y - PER(2)	Z - PER(2)		
ATM	2650	1.00	1.00E-13	1.00E-13	1.00E-13	2.0	10000
BOND	2350	0.22	1.00E-17	1.00E-17	1.00E-17	2.9	10000
CAPR	2700	0.22	1.00E-18	1.00E-18	1.00E-18	3.0	10000
HEAT	2700	0.10	1.00E-15	1.00E-15	1.00E-15	2.0	10000
RES1	2700	0.20	4.00E-14	4.00E-14	2.00E-14	2.0	10000
RES2	2500	0.15	2.00E-14	2.00E-14	1.00E-14	2.0	10000
RES1	2500	0.10	2.00E-15	2.00E-15	1.00E-15	2.0	10000
FAUL	2500	0.10	1.00E-13	1.00E-13	1.00E-13	2.0	10000

Now we will create another material shown in Table 1 that implemented to computer data.

1. In the material data dialog, click **New**
3. Then On the **Properties** menu, click **Edit Materials**
2. In the tab **Matrix** box, fill **Name-MAT**, **Description**, choose **Color**, **Density**, **Porosity**, **XYZ Permeability**, **Wet Heat Permeability**, **Specific Heat** with the data in table 1.
3. Click **OK** to save changes and exit the **Edit Materials** dialog.
4. Repeat all the material data.

### III. Define Top Contour

Before creating the mesh we define the top contours of the model. This is done using an XYZ file listed below. The contour defined by this is shown in Table 2.

Table 2. Top contour of computer model.

Top Contour		
<b>X</b>	<b>Y</b>	<b>Z</b>
0	2000	1100
1800	2000	1300
1400	1600	1300
0	400	1300
2400	2000	1200
2000	1200	1200
1200	400	1200
0	0	1200
2800	2000	1100
2400	1200	1100
1600	400	1100
800	0	1100
4000	0	1100
4000	2000	1100

### IV. Define layers

To define the surface layer geometry:

1. On the **Model** menu, click **Edit Layers**. the Default layer will be selected.
2. In the Name box, type ATM.
3. In the **Top** list, select **From File** and then open the *top.xyz* file.
4. We will subdivide the **Surface** layer with four cells in the Z direction. However, the top cells will be used to define boundary conditions, so we want them to be thin. In the **Dz** options, select **Regular**. The **Dz** table allows us to specify non-uniform grid spacing. This is apportioned by fraction, since the layer does not have a constant thickness. In the first row of the table, type *0.42857* for the **Fraction** and 2 for the **Cells**. (Figure 3 and Table 3).
5. In the **Edit Layers** dialog, click **New**, Repeated all the layer bellow.
6. Click **OK** to close the **Edit Layers** dialog and the output shown in Figure 4.

Name:

Color:

Material:  ATM

Top:

Base:

Dz: ☒ Regular ☐ Custom

Cells:

Factor:

Figure 3. Top Layer.

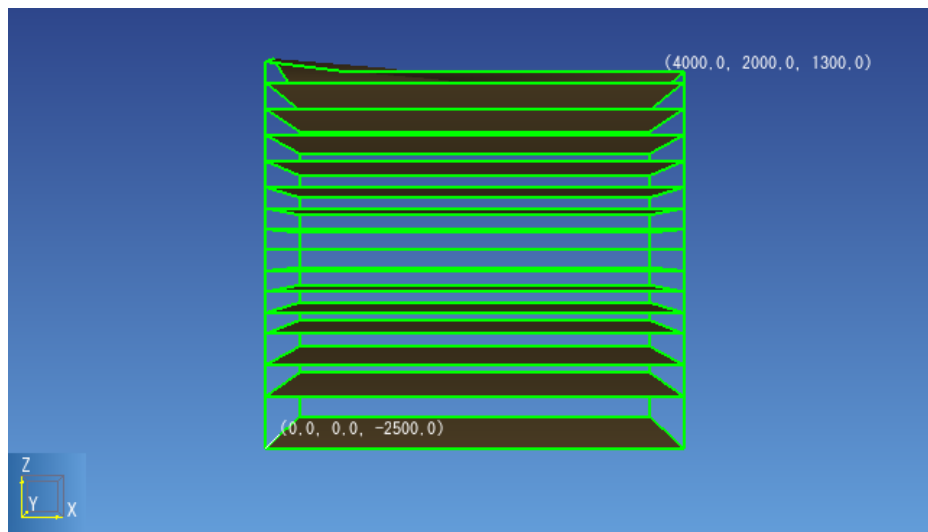


Figure 4. Layers.

Table 3. Layers.

Name	Top	Base	Cells	Factor
ATM	File	1000	2	0.42857
Layer 2	1000	750	1	1
Layer 3	750	500	1	1
Layer 4	500	250	1	1
Layer 5	250	0	1	1
Layer 6	0	-200	1	1
Layer 7	-200	-400	1	1
Layer 8	-400	-600	1	1
Layer 9	-600	-800	1	1
Layer 10	-800	-1000	1	1
Layer 11	-1000	-1200	1	1
Layer 12	-1200	-1400	1	1
Layer 13	-1400	-1700	1	1
Layer 14	-1700	-2000	1	1
Layer 15	-2000	-2500	1	1

## V. Create Mesh

In this model, we also want to specify boundary conditions on the right side (+X), so we want a thin layer of cells. To do this, we will use sotum divisions.

1. On the **Model menu**, click **Create Mesh**.
2. In the **Divisions** options, select **Custom**.
3. Define three rows in the X Direction and one row in the Y direction, as shown below.  
The total length in the X direction is 4000 m and 2000 in the Y Figure 5.
4. Click **OK** to create the mesh.

The following results shown in figure

Divisions: ☐ Regular ☒ Custom

	Dir [X, Y]	Cells	Cell Size
1	X	20	200.0
2	Y	10	200.0
*			

Figure 5. Mesh.

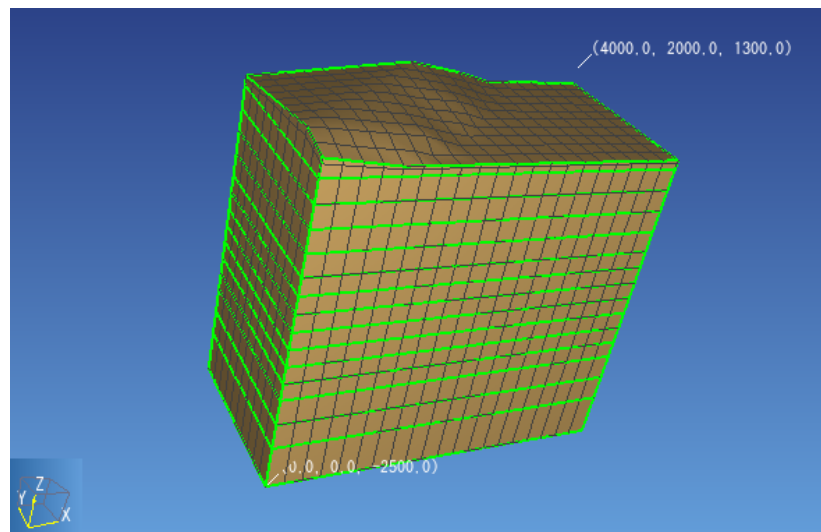


Figure 6. Layers with mesh.

## VI. Assign Materials to Layers

When specifying materials for each cell, PetraSim uses a tiered system that allows cells to inherit values from the containing region, regions from the containing layer and layers from global defaults. In this example, we will assign materials by layer.

To assign the material:

1. On the **Model menu**, click **Edit Layers**. The **Surface** layer will be selected.
2. In the **Material** list, select **ATM**.

- On the side tools, **Select Mesh Layer** and **Select Mesh Column**, then right click to choose **Edit Cells**. Choose the material data **Type**.
- Choose the appropriate material data base on Figure 7.
- Click **Ok** to create computer model.

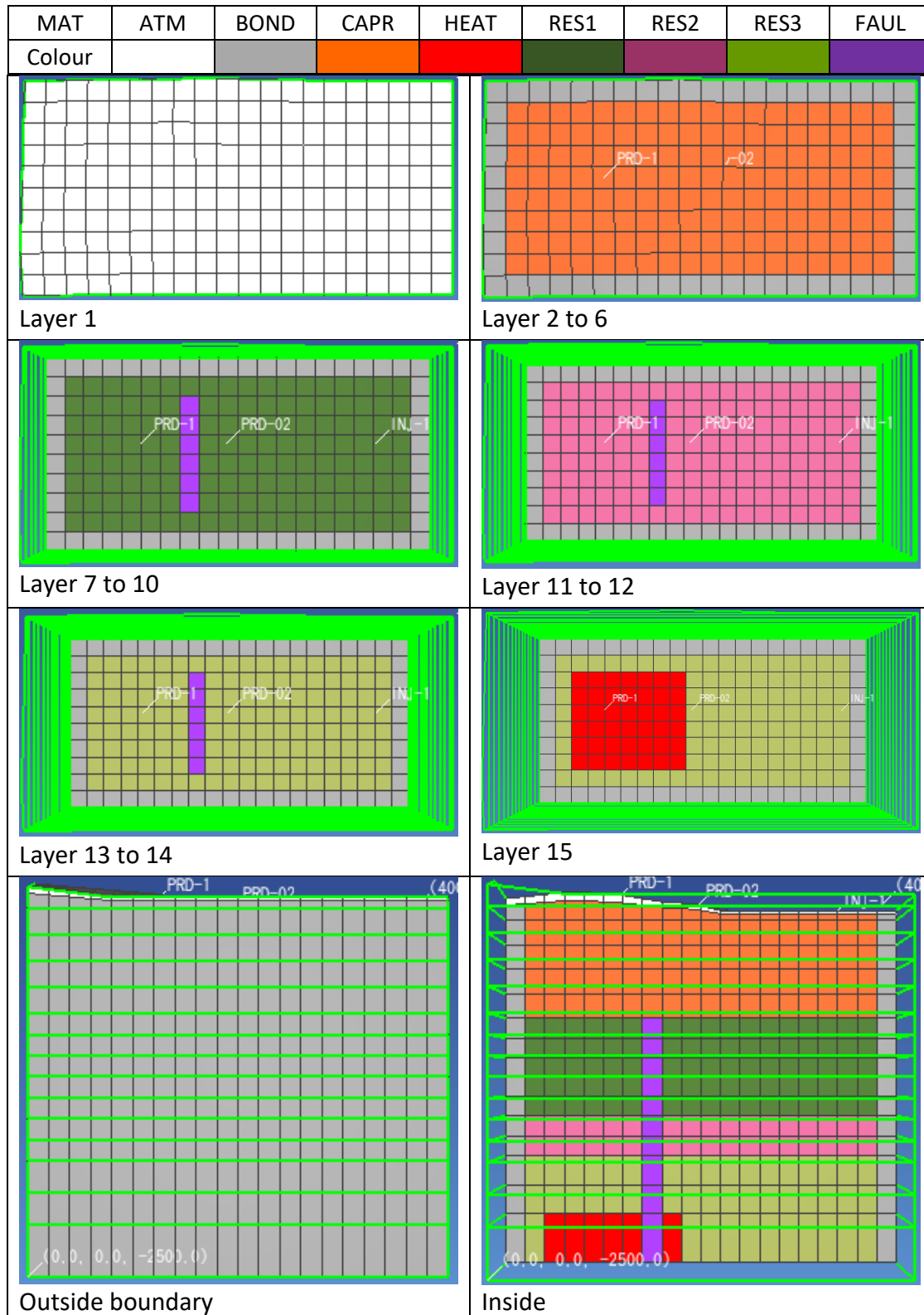


Figure 7. Layers with material data.

## VII. Initial Conditions

When specifying parameters such as initial conditions, PetraSim uses a tiered system that allows cells to inherit values from containing region, regions from the containing layer, and layers from the global defaults. Once we set the default initial conditions, these values will be used by all except those where we have explicitly set values.

In this model, we will use linear pressure and temperature gradients. At the surface (1000 m), the pressure will be 1E5 Pa (1 bar) and the temperature 23 C. at the bottom of the reservoir (-2500 m), the pressure will be approximate hydraulic head Pa and temperature of C. These initial conditions have been chosen to approximate our initial solution. As will be illustrated, the defaults initial conditions can be over-ridden for individual cells.

To set the global initial conditions:

1. On the **Properties** menu, click **Initial Conditions...**
2. In the **EOS1** list, select **Single-Phase (P, T)**
3. In the **Pressure** options list, select *Function*.
4. In the **A** box, type *8.27E06* and in the **D** box, type *-6289.47*
5. In the **Temperature** options list, select *Function*.
6. In the **A** box, type *122.63* and in the **D** box, type *-7.89E-02*
7. Click **OK** to save changes and exit the dialog.

Initial Conditions

EOS1: Water, Non-Isothermal

Single-Phase (P, T)

Pressure (Pa): Function =  $A + Bx + Cy + Dz$  A: 8.27E06 B: 0.0 C: 0.0 D: -6289.47

Temperature (C): Function =  $A + Bx + Cy + Dz$  A: 122.63 B: 0.0 C: 0.0 D: -7.89E-02

Gas Saturation: Constant 0.0

Mass Fraction of Tracer: Constant 0.0

OK Cancel

Figure 8. Initial conditions.

## VIII. Boundary Conditions

We now want to define surface boundary conditions for the model. This will be a pressure. These will be a pressure of 1E5 Pa (1 bar) and a temperature of 25°C. To set the surface conditions:

1. Zoom in to view the top layer in the model.
2. Select the **Select Mesh Layer** tool and then click on the top cell layer in the model. This will select all cells in the top mesh layer (Figure 8).
3. Right-click on the selected cells and click **Edit Cells...**(Figure 9)



4. For the **Type**, click **Fixed State**.
5. Click on the **Initial Conditions** tab and select **Specify Initial Conditions by Cell**.
6. In the **Pressure** box type  $1.0E5$ .
7. In the **Temperature** box type 25
8. Click **OK**.

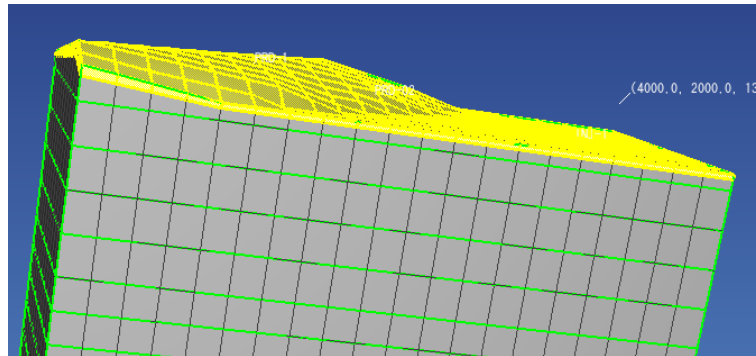


Figure 9. Initial condition for top surface as atmosphere.

After define surface conditions then we should define side boundary conditions. To set side boundary conditions (Figure 10), we use hydrostatic pressure and normal gradient temperature.

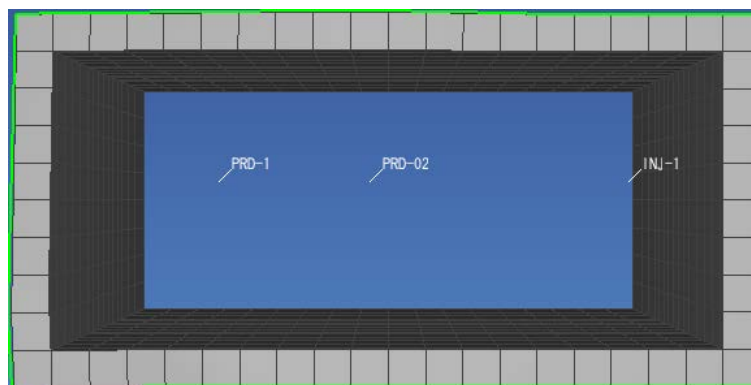


Figure 10. Side boundary.

The least for boundary conditions is heat source. We will assume that there is a heat source at the bottom of the reservoir. This will applied 42 cell (Y = 6 cells, and X = 7 cells) with initial conditions  $2.4E07$  & 320 C and constant flux. We will define at total flow of 21 kg/s. We could just specify 0.5 kg/s for each cell, but will demonstrate using flux. The total projected XY area of these cells is  $42 \times 20000 \text{ m}^2$ , for a flux of  $0.000025 \text{ kg/s.m}^2$ .

1. Using the **Select Mesh Layer** tool, select the bottom mesh layer and right-click to **Show Only Selected Cells**.
2. Click **Top View** on the toolbar.
3. Use the **Select Objects** tool to select the indicated cells.
4. Right-click the selected cells, and click **Edit Cells ...** (Figure 7 – layer 15)
5. Under tab **Properties**, type  $1.0E38$  for **Vol. Vector**.

6. Click the **Initial Conditions** and choose **Single Phase (P,T)** then type 2.4E07 for pressure and 320 for temperature.
7. Click the **Sources/Sinks** tab and under **Injection**, select the **Water/Steam** check box
8. In the option list select **Constant Flux**.
9. In the **Rate** box, type 0.000025
10. In the **Enthalpy** box, type 1.085E6
11. Click **Show All Cells** and then click **OK**.

#### IX. Edit Solutions Control

Parameters relating to the solver and time stepping can be found in the Solution Controls dialog. Because we use a material with zero conductivity, experience has shown that the solution will converge more reliably if the stabilized bi-conjugate gradient solver is used.

1. On the **Analysis** menu, click **Solution Controls**
2. In the **End Time** list, click **Infinite**
3. In the **Max Num Time Steps** box, click **Infinite**
6. Click **OK**

#### X. Save and Run

The input is complete and you can run the simulation. The simulator will generate numerous output files (e.g. FOFT, mesh.csv, etc.). Since these files have the same name for every simulation, it is usually a good idea to create a folder specifically for a particular model.

To save your model:

1. On the **File** menu, click **Save**
2. Create a folder named *Initial*
3. Save the model with the name *initial*
4. Click **Save**

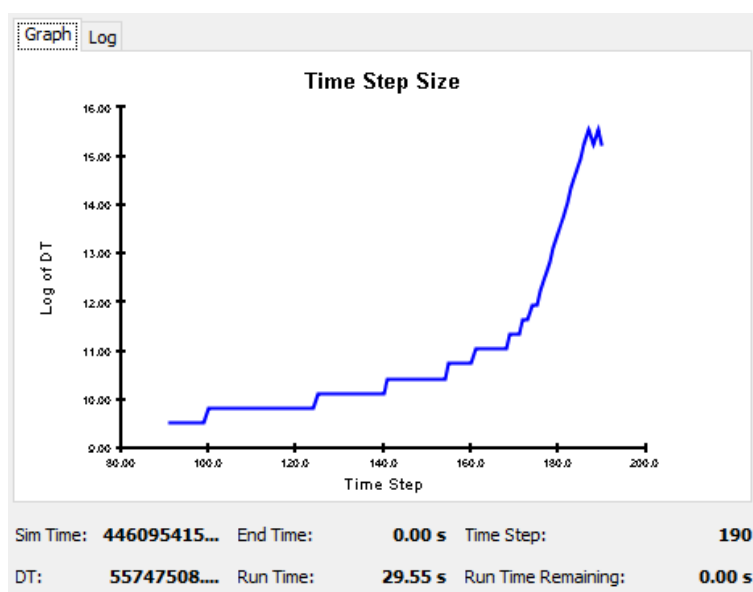


Figure 11. Running of simulation.

To run the simulation, on the **Analysis** menu, click **Run TOUGH2**. You should see a graph showing (Figure 11) the increase in time step size as the simulation converges. If there are any problems, you can view the log. Output that has been identified as errors will appear in red. The **Simulation Complete** dialog will notify you when the end time has been reached. Click **OK** to dismiss the notification and click **Close** to exit the **Running TOUGH2** dialog.

## XI. View 3D Results

To open the **3D Results** dialog:

1. On the **Results** menu, click **3D Results**

By default, the display will show isosurfaces corresponding to pressure for the first output step.

To show temperature isosurfaces for the last time step:

1. In the **Scalar** list, click **T**
2. In the **Time(s)** list, click the last entry ( $t = 6.31139E11$ )

To show scalar data on a slice plane:

1. Click **Slice Planes...**
2. In the **Axis** list, click **Y**
3. In the **Coord** box, type *1000*
4. Click the **Scalar** checkbox
5. To add a display of flow vectors, on the second slice plane in the **Axis** list, click **Y**
6. In the **Coord** box, type *1*
7. Click to remove the **Scalar** checkbox and then click to select the **Vector** checkbox
8. Click **Close**
9. In the **Vector** list, click **FLOF**

The resulting visualization is shown Figure 12. There is fluid down flow from the surface and up flow from the bottom source. When finished, you can close the **3D Results** dialog.

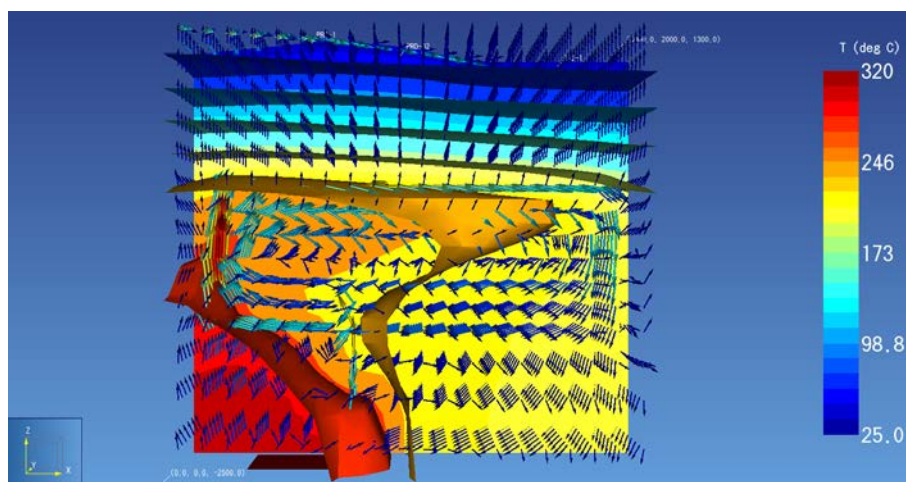


Figure 12. 3D Results.

## XII. References

1. Tunderhead Engineering: PetraSim 5 User Manual, USA.
2. Tunderhead Engineering: TOUGH2 Example Initial State and Production Analyses in a Layered Model, USA.