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# TOUGH2 Example:

## Setting Single-Phase, Time-Dependent, Essential (Direchlet) Boundary Conditions

PetraSim 5

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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 http://www.petrasim.com. More information about the TOUGH family of codes can be found at: http://www-esd.lbl.gov/TOUGH2/. Printed copies of the user manuals may be obtained from Karsten Pruess at <K_Pruess@lbl.gov>.

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We most sincerely thank our users for their feedback and support.

# Setting Multi-Phase, Time Dependent, Essential (Dirichlet) Boundary Conditions

In this example we demonstrate how to apply time-dependent temperature boundary conditions for single phase problems. The user should refer to the PetraSim manual and the corresponding multi-phase example for further discussion.

In this description, we use a thin layer to define the boundary conditions. An alternate is to use "extra cells", as illustrated in the multi-phase example. We first illustrate the basic concepts using a simple cube. We then demonstrate how to apply time-dependent boundary conditions to a more complex model.

## Create a Simple Model

Following the instructions already presented in previous example problems, make a new model using EOS1 and dimensions of 10x10x10 meters. To define a thin layer on the top of the model:

1. In the **Tree View**, expand the **Layers** node and click **Default**
2. On the **Edit** menu, click **Properties...**
3. In **Dz** click **Custom**
4. In the first row **Fraction** box type *0.999* and in the **Cells** box type *1* (Figure 1)
5. In the second row **Fraction** box type *0.001* and in the **Cells** box type *1* (Figure 1)
6. Click **OK** to save changes to the default layer

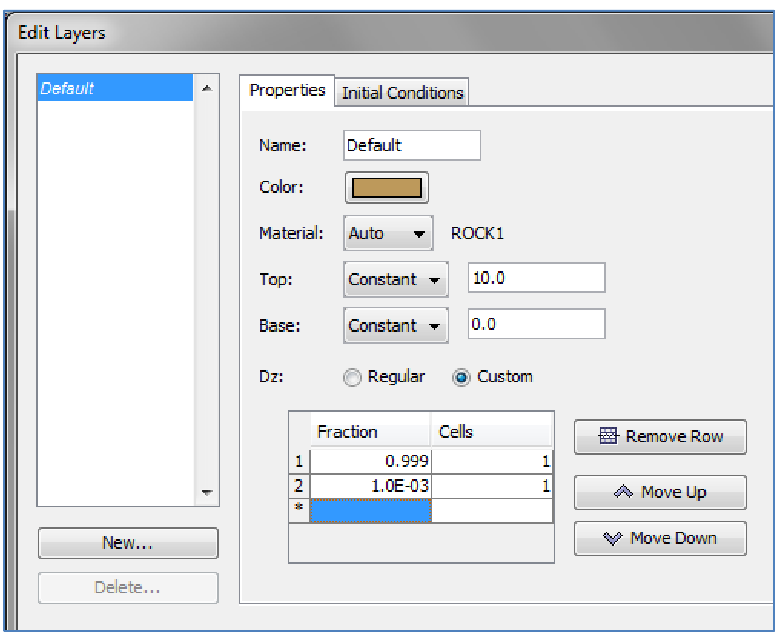


**Figure 1: Input of cell sizes**

If you close and reopen the **Edit Layers** dialog, you will notice that **Dz** has been changed to a **Regular** mesh with a **Factor** of *1.001E-03*. This is an alternate way to describe the same sizes for two elements.

## Generate the Mesh

We now need to generate the mesh:

1. On the **Model** menu, click **Create Mesh**
2. For **Mesh Type**, select *Regular*
3. In the **X Cells** box, type *1*
4. In the **Y Cells** box, type *1*
5. Click **OK** to create the mesh

## Material Properties

The large model cell uses the default material properties. However, for the temperature boundary condition cell, we want only heat to flow into or out of the cell, not any fluid. This can be accomplished by making a special material that has zero permeability. In addition, we specify a small porosity so that we can use the solid properties for our heat capacity calculations and neglect the heat capacity of the small amount of fluid in the cell.

To make a new material to use in applying the temperature boundary conditions:

1. On the **Properties** menu, click **Edit Materials...**
2. In the Material Data dialog, click **New**
3. In the **Name** box, type *TEMP*
4. Click **OK** to create the new material, by default, the new material data will be based on theROCK1 data
5. For the *TEMP* material, change the value in the **Porosity** box to *0.001*.
6. For the *TEMP* material, in all three **Permeability** boxes (X, Y, and Z), type *0.0*. There will be no flow into the cell.

Click **OK** to save changes and exit the **Edit Materials** dialog.

## Define Temperature Boundary Condition in Thin Cell

To modify the thin cell so that it defines a temperature boundary condition:

1. Spin the model and click on the top. This should select only the thin cell.
2. Right-click and select **Edit Cells…**
3. In the **Cell Name** box, type *TempBC*
4. In the **Vol. Factor** box, type *1.0E20* (the volume of the cell will be the actual volume, 1, times the factor, for a volume of 1.0E20 $m^3$.
5. In the **Material** list, select *TEMP* (we want to use the special boundary condition material)

We will return to define sources /sinks in the extra cell. We use the default initial conditions in the boundary condition cell. To turn on detailed printing of time history data:

1. Click the **Print Options** tab
2. Click to select both print options.

## Heat Flow into Boundary Condition Cell

We have now created a boundary condition cell that has a volume of 1.0E20 $m^3$, a density of 2600 $kg/m^3$, a porosity of 0.001, and a specific heat of 1000 J/kg-C. For this example, we will specify a sinusoidal temperature history with an average of 100 ˚C, an amplitude of 50 ˚C, and a period of 30 days, Figure 2.

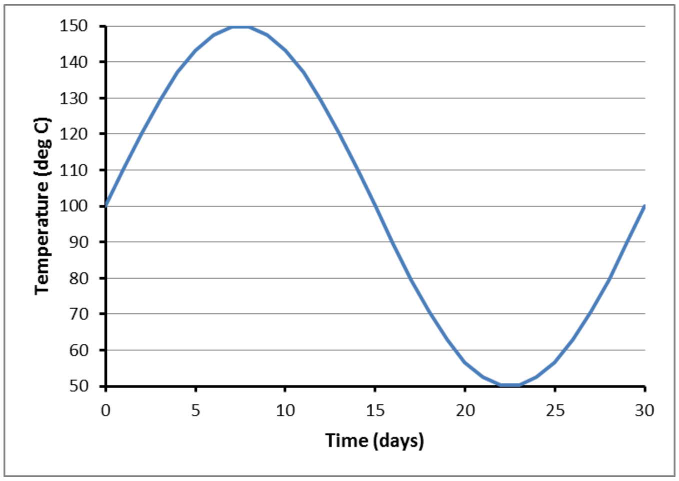


**Figure 2: Desired boundary condition temperature history**

We calculate the heat flow as follows:

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

where $\dot{Q}$ is the heat flow, $V$ 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 heat flows to obtain the desired temperature time history are shown in Table 1.

**Table 1: Calculated heat flow to change boundary cell to desired temperature**

| Time | | Temp (C) | Heat Flow |
|---|---|---|---|
| Day | Sec | | |
| 0 | 0 | 100 | 3.12830090E+22 |
| 1 | 86400 | 110.3956 | 2.99157914E+22 |
| 2 | 172800 | 120.3368 | 2.72411102E+22 |
| 3 | 259200 | 129.3893 | 2.33758617E+22 |
| 4 | 345600 | 137.1572 | 1.84889759E+22 |
| 5 | 432000 | 143.3013 | 1.27940331E+22 |
| 6 | 518400 | 147.5528 | 6.53992972E+21 |
| 7 | 604800 | 149.7261 | 0.00000000E+00 |
| 8 | 691200 | 149.7261 | -6.53992972E+21 |
| 9 | 777600 | 147.5528 | -1.27940331E+22 |
| 10 | 864000 | 143.3013 | -1.84889759E+22 |
| 11 | 950400 | 137.1572 | -2.33758617E+22 |
| 12 | 1036800 | 129.3893 | -2.72411102E+22 |
| 13 | 1123200 | 120.3368 | -2.99157914E+22 |
| 14 | 1209600 | 110.3956 | -3.12830090E+22 |
| 15 | 1296000 | 100 | -3.12830090E+22 |
| 16 | 1382400 | 89.60442 | -2.99157914E+22 |
| 17 | 1468800 | 79.66317 | -2.72411102E+22 |
| 18 | 1555200 | 70.61074 | -2.33758617E+22 |
| 19 | 1641600 | 62.84276 | -1.84889759E+22 |
| 20 | 1728000 | 56.69873 | -1.27940331E+22 |
| 21 | 1814400 | 52.44717 | -6.53992972E+21 |
| 22 | 1900800 | 50.27391 | 0.00000000E+00 |
| 23 | 1987200 | 50.27391 | 6.53992972E+21 |
| 24 | 2073600 | 52.44717 | 1.27940331E+22 |
| 25 | 2160000 | 56.69873 | 1.84889759E+22 |
| 26 | 2246400 | 62.84276 | 2.33758617E+22 |
| 27 | 2332800 | 70.61074 | 2.72411102E+22 |
| 28 | 2419200 | 79.66317 | 2.99157914E+22 |
| 29 | 2505600 | 89.60442 | 3.12830090E+22 |
| 30 | 2592000 | 100 | 1.00308642E+22 |

To specify this heat flow into the boundary cell:

1. Double-click the thin top cell to edit it.
2. Click the **Sources/Sinks** tab
3. Click **Heat In**
4. In the options list, select **Table**
5. Click the **Edit** button and type (or paste) the values shown Table 1
6. Click **OK** to save changes and exit the **Heat Rates** dialog

Click **OK** to save changes and exit the **Edit Cell Data** dialog.

## Initial Conditions

The initial conditions for the model should be a single phase temperature of 100 ˚C and a pressure of 1.0E6 Pa.

## Edit Solution Controls

Parameters relating to the solver and time stepping can be found in the Solution Controls dialog.

To specify the simulation end time:

1. On the **Analysis** menu, click **Solution Controls**
2. In the **End Time** list, click **User Defined** and type *30 days*
3. In the **Max Time Step** list, click **User Defined** and type *1 days*
4. Click the **Weighting** tab
5. For **Permeability at Interface** list, click **Harmonic Weighted**. This will ensure that the permeability at the interface for fluid flow into and out of the boundary will be zero (see the PetraSim user manual and the TOUGH2 user manual for a supporting discussion)
6. Click the **Options** tab
7. For **Boundary condition Interpolation**, click **Rigorous Step**
8. Click **OK**

## Edit Output Controls

By default, the simulation will print output every 100 time steps. For this simulation, we will specify output every time step.

To specify the output frequency:

1. On the **Analysis** menu, click **Output Controls**
2. In the **Print and Plot Every # Steps** box, type *1*
3. Click **OK**

## Save and Run

The input is complete and you can run the simulation.

## View Time History Plots

To view time history plots:

1. On the PetraSim **Results** menu, click **Cell History Plots**
2. In the **Variable** list, click **T (deg C)**
3. In the **Cell Name** list, click **TempBC**
4. In the Cell Time History window, on the **File** menu, click **Export Data…** and save the data.
5. You can then import the data and compare the calculated boundary condition temperatures to the desired values, as shown in Figure 3.

6. In the **Cell Name** list, click **Cell 1** (the large cell) to view the time history of the temperature in the model cell. This response shows a temperature change from 100 ˚C to a maximum of 100.5983 ˚C, Figure 4. A hand calculation gives an analytic value of 100.597 ˚C.

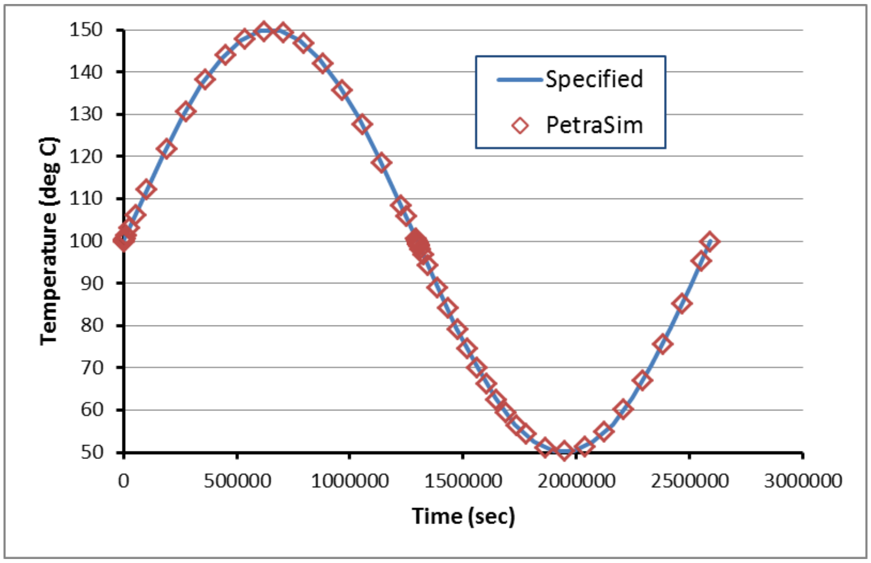


**Figure 3: Comparison of calculated and desired boundary condition cell temperatures**

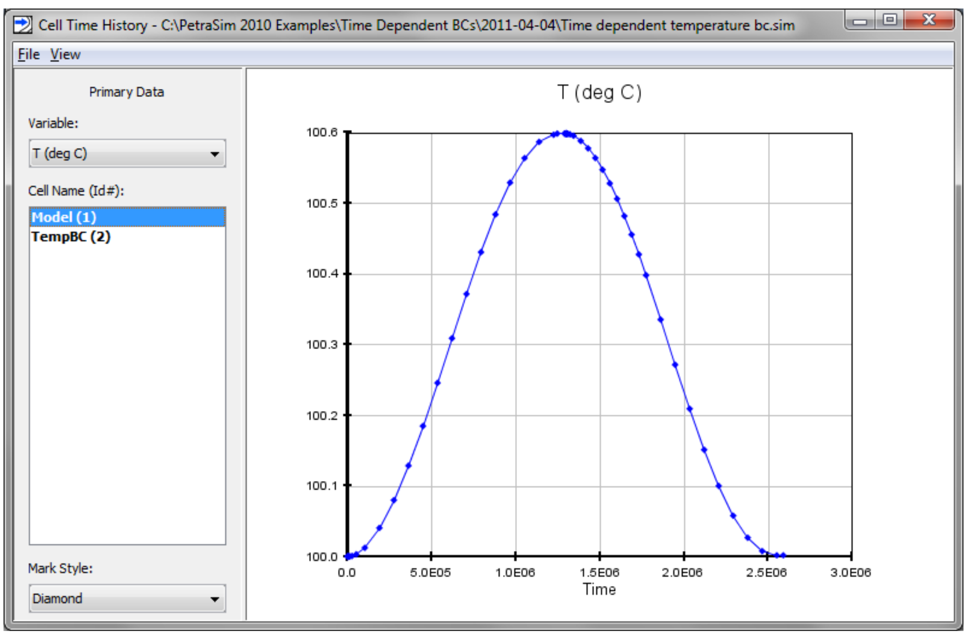


**Figure 4: Time history response of model cell**

When finished, you can close the **Cell History** dialog.

## Boundary Condition using Thin Cell and Polygonal Mesh

We now repeat the specifying a temperature boundary condition, but using a polygonal mesh.

1. Open the previous model
2. Save the model under a different name.

We have already defined the spacing for the thin cell, so that does not need to be modified.

To regenerate the mesh:

1. On the **Model** menu, click **Create Mesh**
2. For **Mesh Type**, select *Polygonal*
3. Click **OK** to create the mesh

We now set the boundary conditions for the top layer. To calculate and set the boundary conditions in the top lower left polygonal cell:

1. Click the **Select Mesh Layer** tool, then select the top thin layer. This will select all the cells in that layer, Figure 5.

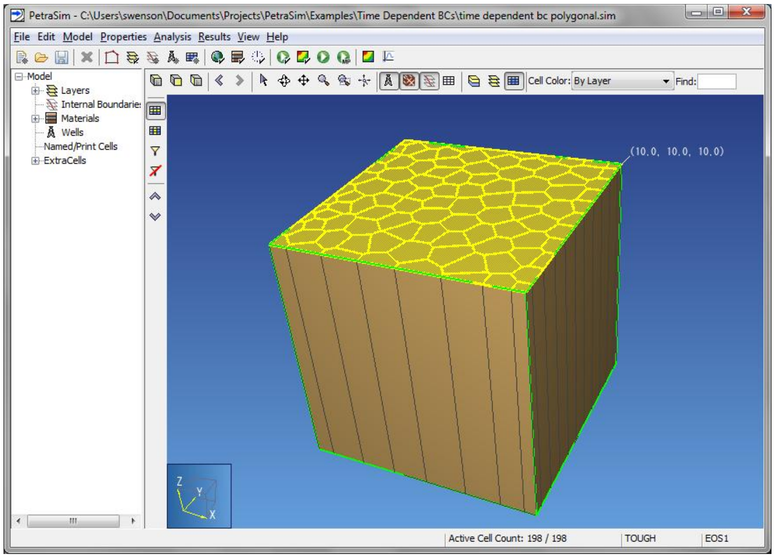


**Figure 5: Select all cells in the top layer**

2. On the **Edit** menu, click **Properties...**
3. In the **Vol. Factor** box, type *1E20* (the entire top layer will have the same volume as the previous example)
4. In the **Material** list, select *TEMP* (we want to use the special boundary condition material)
5. Click the **Sources/Sinks** tab
6. Click **Heat In**

7. In the options list, select **Table Flux** and input the values shown in Table 2. This is the same information as in Table 1, but the heat flow has been divided by the XY area (100 $m^2$) to give the flux.
8. Click **OK**

**Table 2: Specification of heat flow using flux**

| Time | Flux |
|---:|---:|
| 0 | 3.12830000E+20 |
| 86400 | 2.99158000E+20 |
| 172800 | 2.72411000E+20 |
| 259200 | 2.33759000E+20 |
| 345600 | 1.84890000E+20 |
| 432000 | 1.27940000E+20 |
| 518400 | 6.53993000E+19 |
| 604800 | 0.00000000E+00 |
| 691200 | -6.53993000E+19 |
| 777600 | -1.27940000E+20 |
| 864000 | -1.84890000E+20 |
| 950400 | -2.33759000E+20 |
| 1036800 | -2.72411000E+20 |
| 1123200 | -2.99158000E+20 |
| 1209600 | -3.12830000E+20 |
| 1296000 | -3.12830000E+20 |
| 1382400 | -2.99158000E+20 |
| 1468800 | -2.72411000E+20 |
| 1555200 | -2.33759000E+20 |
| 1641600 | -1.84890000E+20 |
| 1728000 | -1.27940000E+20 |
| 1814400 | -6.53993000E+19 |
| 1900800 | 0.00000000E+00 |
| 1987200 | 6.53993000E+19 |
| 2073600 | 1.27940000E+20 |
| 2160000 | 1.84890000E+20 |
| 2246400 | 2.33759000E+20 |
| 2332800 | 2.72411000E+20 |
| 2419200 | 2.99158000E+20 |
| 2505600 | 3.12830000E+20 |
| 2592000 | 1.00309000E+20 |

Select at least one cell in the thin layer and on in the thick layer to print time history data.

Run the analysis and essentially the same results will be obtained in the model cells.

## Summary

This has illustrated how to apply temperature-only boundary conditions in a PetraSim/TOUGH2 model. Other combinations of boundary conditions are discussed in the PetraSim User Manual. The principles are the same.