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# **TOUGH2 Example: Time-Dependent Essential (Dirichlet) 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](mailto:K_Pruess@lbl.gov)>.

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## Time-Dependent Essential (Dirichlet) Boundary Conditions

In this example we demonstrate how to apply time-dependent boundary conditions. The user should refer to the PetraSim manual for further discussion. In this example, we will first illustrate the basic concepts using a single cell model. We will add boundary condition cells to define boundary conditions on the model cell. We will then demonstrate how to apply time-dependent boundary conditions to a more complex model.

### Create a One Cell Model

Following the instructions already presented in previous example problems, make a new model using EOS1 and dimensions of 10x10x10 meters.

1. Edit the default layer to have only one cell in the Z-direction.
2. Create a 1 x 1 regular mesh.
3. Use the default material properties for the model.
4. The initial conditions for the model should be a temperature of 100 °C and a pressure of 1.0E6 Pa (single phase liquid).
5. Print time history data for the model cell

The single cell model is shown below. In the following description, “model” cell means this 10x10x10 cell. We add cells to define the boundary conditions. These will be called “boundary condition” cells.

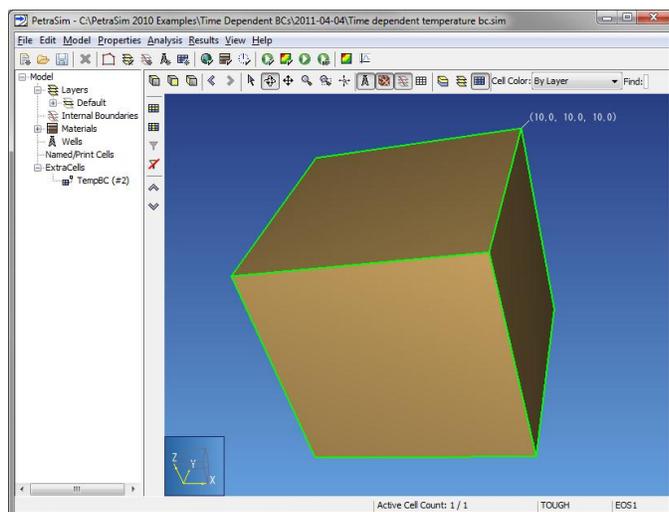


Figure 1: Single cell model

### Material for Temperature Boundary Condition

For the temperature boundary condition cell, we do not want flow into or out of the cell. This can be accomplished by making a special material that has zero permeability and small porosity.

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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*. The cell will be essentially all solid, so 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.
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, time the factor, for a volume of  $1.0E20 \text{ m}^3$ ).
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.

To define the connection between the boundary condition cell and the model cell:

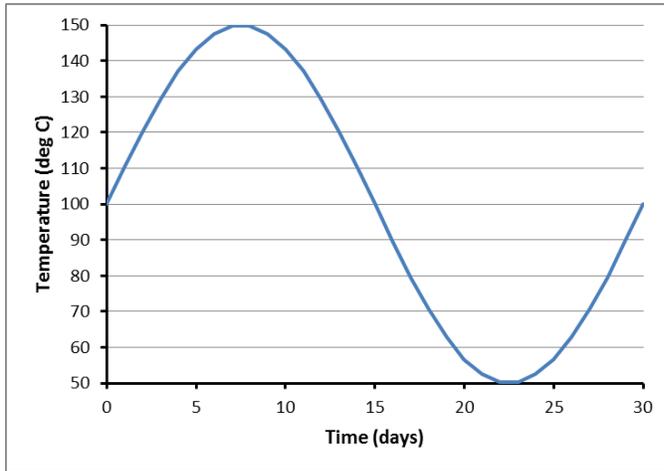
1. Click the **Connected Cells** tab
2. In the **'To' Cell** box, type *1* (this boundary condition cell will be connected to the model cell with ID 1)
3. In the **Orientati...** box, type *1* (use the *TEMP* material X permeability value for this connection)
4. In the **Dist. 'This'** box, type *0.001* (the flow distance in this boundary cell is small so that the temperature boundary condition is applied to the surface of the model cell)
5. In the **Dist. 'To'** box, type *5.0* (the true distance of flow in the model cell)
6. In the **Area** box, type *100* (the true area between the cells)
7. In the **Gravitati...** box, type *1* (the boundary cell is directly above the model cell)
8. In the **Rad. He...** box, type *0.0* (no radiation heat transfer)

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

## Heat Flow into Boundary Condition Cell

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



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

We calculate the heat flux 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.

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**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. In the tree display, expand the **ExtraCells** list and double-click the **TempBC** cell
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.

---

## 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** (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 **Model** 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.

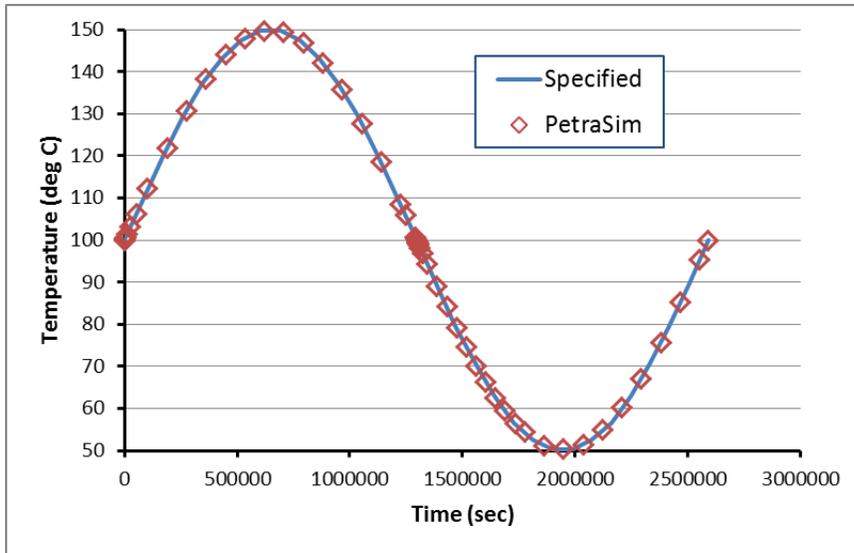


Figure 3: Comparison of calculated and desired boundary condition cell temperatures

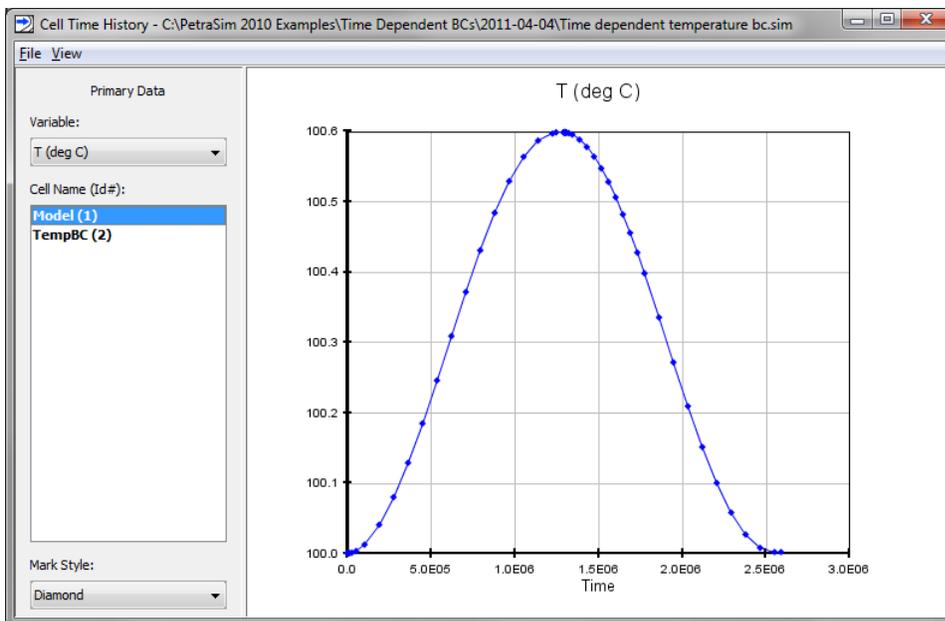


Figure 4: Time history response of model cell

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

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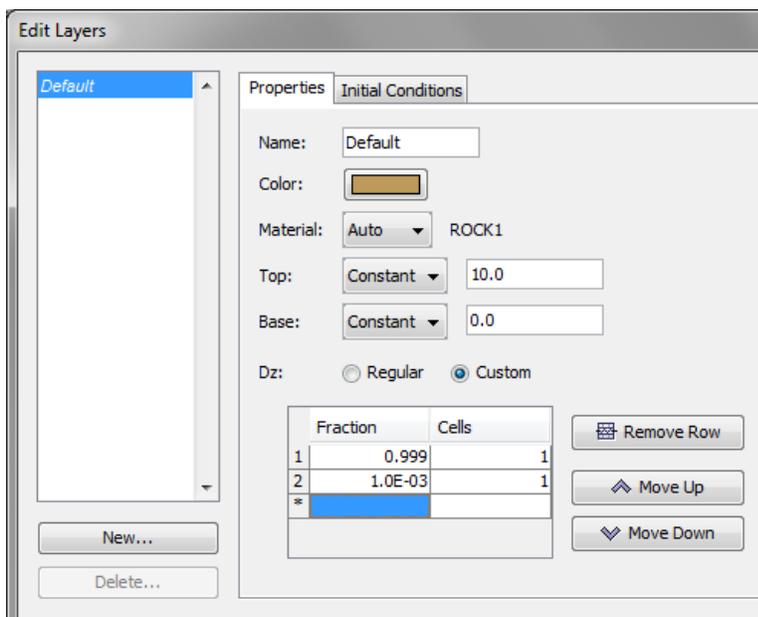
## Boundary Condition using Thin Cell

We now repeat the specifying a temperature boundary condition, but using a thin cell instead of adding an extra cell.

1. Open the previous model
2. Delete the extra cell
3. Save the model under a different name.

To define the thin cell:

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 5)
5. In the second row **Fraction** box type  $0.001$  and in the **Cells** box type  $1$  (Figure 5)
6. Click **OK** to save changes to the default layer



**Figure 5: 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.

We now need to regenerate 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

To set the boundary conditions in the thin top cell:

1. Spin the model and click on the top cell.
2. On the **Edit** menu, click **Properties...**
3. In the **Cell Name** box, type *TempBC*
4. In the **Vol. Factor** box, type *1.0E20* (this factor multiplies the geometric cell volume of  $1 \text{ m}^3$ )
5. In the **Material** list, select *TEMP* (we want to use the special boundary condition material)
6. Click the **Sources/Sinks** tab, Click **Heat In**, and input the same values as described in the previous **Heat Flow into Boundary Condition Cell** section.
7. Click the **Print Options** tab and select both print options
8. Click **OK**

Select the model cell, name it, and select the print options.

Run the analysis and essentially the same results will be obtained.

## 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

To calculate and set the boundary conditions in the top lower left polygonal cell:

1. Spin the model and click on the top cell in the lower left corner top layer cell, Figure 6. Note that the projected area is  $0.4217 \text{ m}^2$  and that the volume is  $4.2169\text{E-}3 \text{ m}^3$ .
2. On the **Edit** menu, click **Properties...**
3. In the **Cell Name** box, type *TempBC*
4. In the **Vol. Factor** box, type *237.137E20* (this factor was chosen to give the cell a volume of  $1.0\text{E}20 \text{ m}^3$ , the same value as in the previous examples)
5. In the **Material** list, select *TEMP* (we want to use the special boundary condition material)
6. Click the **Sources/Sinks** tab
7. Click **Heat In**
8. In the options list, select **Table Flux** and input the values shown in Table 2. These values were calculated to give the same heat flow as in the previous examples, but use an area of  $0.4217 \text{ m}^2$ .

9. Click the **Print Options** tab and select both print options
10. Click **OK**

We now repeat this for all top cells:

1. Spin the model, click the **Select Mesh Layer** tool, and click on the top cell in the lower left corner. This will select the entire top layer .
2. Right-click and select **Edit Cells...**
3. In the **Vol. Factor** box, type  $237.137E20$
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.
8. Click **OK**

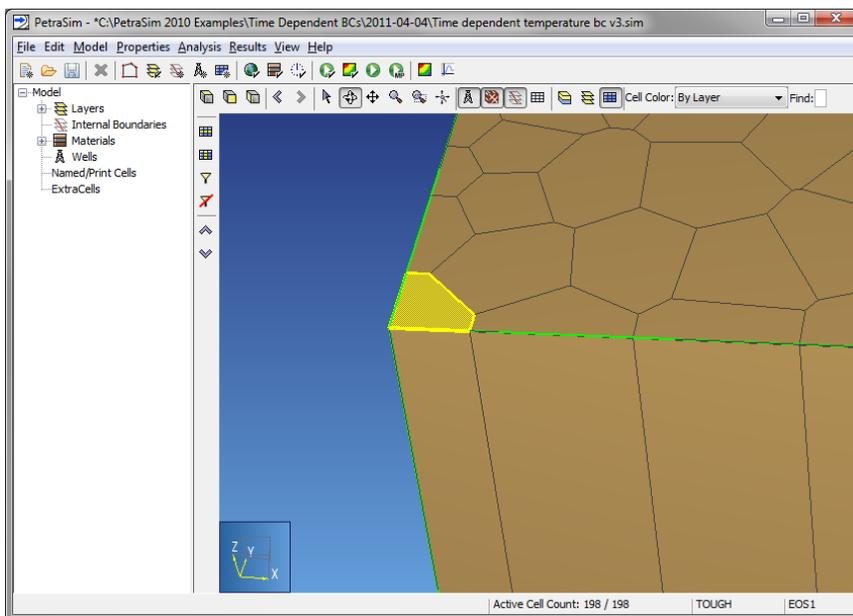


Figure 6: Selection of lower left cell in thin top layer

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

Time	Flux
0	7.41830900E+22
86400	7.09409330E+22
172800	6.45983168E+22
259200	5.54324442E+22
345600	4.38439078E+22
432000	3.03391822E+22
518400	1.55084888E+22
604800	0.00000000E+00
691200	-1.55084888E+22
777600	-3.03391822E+22
864000	-4.38439078E+22
950400	-5.54324442E+22
1036800	-6.45983168E+22
1123200	-7.09409330E+22
1209600	-7.41830900E+22
1296000	-7.41830900E+22
1382400	-7.09409330E+22
1468800	-6.45983168E+22
1555200	-5.54324442E+22
1641600	-4.38439078E+22
1728000	-3.03391822E+22
1814400	-1.55084888E+22
1900800	0.00000000E+00
1987200	1.55084888E+22
2073600	3.03391822E+22
2160000	4.38439078E+22
2246400	5.54324442E+22
2332800	6.45983168E+22
2419200	7.09409330E+22
2505600	7.41830900E+22
2592000	2.37867304E+22

Select the at least two model cells, name them, and select the print options.

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.

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## References

1. **Pruess, Karsten, Oldenburg, Curt and Moridis, George.** *TOUGH2 User's Guide, Version 2.0.* Berkeley, CA, USA : Earth Sciences Division, Lawrence Berkeley National Laboratory, November 1999. LBNL-43134.
2. **Falta, Ronald, et al., et al.** *T2VOC User's Guide.* Berkeley, CA, USA : Earth Sciences Division, Lawrence Berkeley National Laboratory, March 1995. LBNL-36400.
3. **Pruess, Karsten.** *Personal communication.* 2003. email.