403 Poyntz Avenue, Suite B
Manhattan, KS 66502
USA
+1.785.770.8511
www.thunderheadeng.com

TMVOC Buckley-Leverett Flow

PetraSim 2016.1

Table of Contents

Disclaimer

Thunderhead Engineering makes no warranty, expressed or implied, to users of PetraSim, and accepts no responsibility for its use. Users of PetraSim assume sole responsibility under Federal law for determining the appropriateness of its use in any particular application; for any conclusions drawn from the results of its use; and for any actions taken or not taken as a result of analyses performed using these tools.

Users are warned that PetraSim is intended for use only by those competent in the field of multi-phase, multi-component fluid flow in porous and fractured media. PetraSim is intended only to supplement the informed judgment of the qualified user. The software package is a computer model that may or may not have predictive capability when applied to a specific set of factual circumstances. Lack of accurate predictions by the model could lead to erroneous conclusions. All results should be evaluated by an informed user.

Throughout this document, the mention of computer hardware or commercial software does not constitute endorsement by Thunderhead Engineering, nor does it indicate that the products are necessarily those best suited for the intended purpose.

1. Buckley-Leverett Flow

Description

This example is Problem No. 2 (*rblm*) - "1-D Buckley-Leverett Flow" - as described in "TMVOC, A Numerical Simulator for Three-Phase Non-Isothermal Flows of Multicomponent Hydrocarbon Mixtures in Saturated-Unsaturated Heterogeneous Media", Pruess and Battistelli, LBNL-49375, 2002.

The geometry of the problem is given below. A horizontal column, 304.8 m long is divided into 40 elements. The column is filled with an initial mixture of NAPL and water. Water is injected at one end and, at the other end, a single cell is used to define a constant boundary condition.

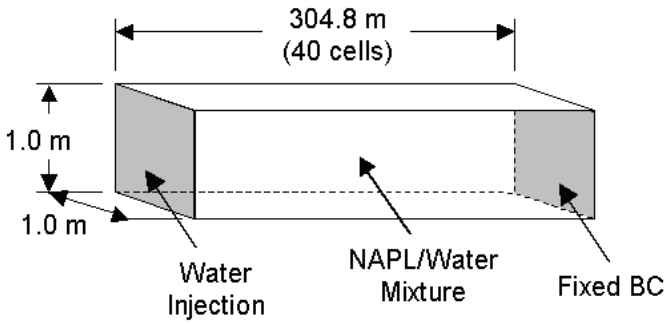

Figure 1.1: Problem geometry

Create a New Model

1. On the **File** menu, click **New**.
2. For both the **Simulator Mode** and **EOS** choose **TMVOC**.
3. For the **Model Bounds** enter the coordinates as shown in Table 1.1.
4. Click **OK**.

Table 1.1: Model bounds

Axis	Min (m)	Max (m)
X	0.0	304.8
Y	0.0	1.0
Z	-1.0	0.0

Default Units

By default, PetraSim uses the TOUGH2 metric unit system (for example, the TOUGH2 system specifies permeability in units of m^2). We will use the default system. To change the default units:

1. On the **View** menu, click **Unit System.**
2. Select the units you wish to use for each parameter.

Note that even if using the default TOUGH2 system, you can enter values in any of the optional units supported by PetraSim. For example, you can type **10 years** for time or **5 mD** for permeability. PetraSim will convert to the units being used in the model.

Save the Model

It is good practice to save the model initially. Some of the files created by TOUGH have the same name for every simulation, so it is good practice to create a separate folder for simulation.

To save your model:

1. On the **File** menu, click **Save.**
2. Create a new folder named **TMVOC Prob 2** and in the **File Name** box, type **TMVOC_prob2.**
3. Click **Save.**

Specify the Solution Mesh

For this simulation, we only want one cell in the (Z) direction. This is the default value, so we do not need to edit this value in the layers. However, we do need to define the mesh in the X and Y directions:

1. On the **Model** menu, click **Create Mesh**.
2. In the **X Cells** box, type **40**.
3. In the **Y Cells** box, type **1**.
4. Click **OK** to create the mesh.

Global Properties

1. On the **Properties** menu, click **Global Properties**.
2. In the **Name** box, type **TMVOC Problem 2**.
3. Click the **EOS** TAB.
4. Select the **Isothermal Mode** check box.
5. Click the **Edit Options** button to edit thermophysical options.
6. In the **Air Solubility Correlation** list, select **K_H=10^{10}(Pa) Independent of Temperature**.
7. Click **OK** to close the **Thermophysical Properties** dialog.

Edit VOC Data

The VOC (NAPL) used in this example is not chemically active, so it is necessary to create a new VOC with some modifications. Note: When you create a new VOC, the data is saved to the voc.dat file usually located in the C:\ProgramData\PetraSim folder.

To create a new VOC:

1. Click the **Edit VOC Data** button.
2. Click **New**.
3. In the **Name** box, type **Chlorobenzene Modified**.
4. In the **Based On** list, select **Chlorobenzene (STD)**.

5. Click **OK**. If you receive a message that the name **Chlorobenzene Modified** is already being used, then do not create a new VOC. Instead, cancel and open the existing **Chlorobenzene Modified** to edit the input data.

Change CHEMP.6 Data

1. Click the **CHEMP.6** tab near the top of the **Edit VOC Data** dialog.
2. In the **Reference Density for NAPL** box, type **998.3**.
3. In the **Reference Temperature for NAPL** box, type **292.15**.
4. In the **Reference Binary Diffusivity of VOC in Air** box, type **8.0E-6**.
5. In the **Reference Temperature for Gas Diffusivity** box, type **273.15**.
6. In the **Chemical Diffusivity Exponent** box, type **1.0**.

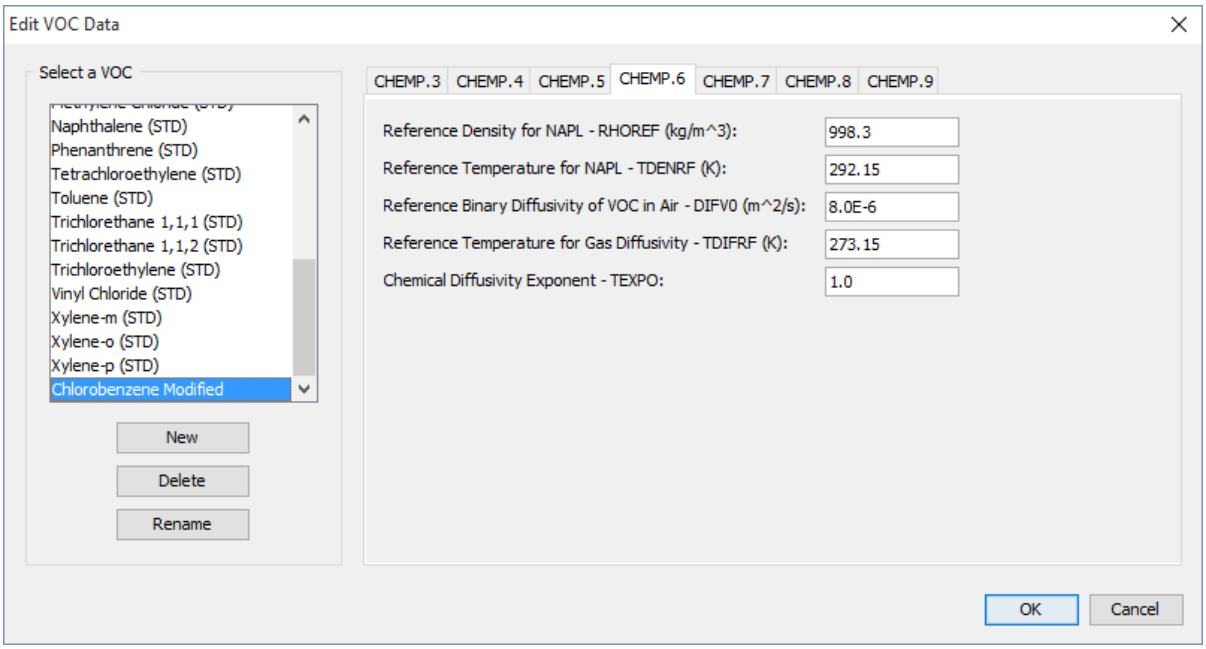

Figure 1.2: Edit CHEMP.6 Data

Change CHEMP.7 Data

1. Click the **CHEMP.7** tab**.**
2. In the **VLOA** box, type **0.0**.
3. In the **VLOB** box, type **0.0**.
4. In the **VLOC** box, type **1.0**.
5. In the **VLOD** box, type **292.15**.

Change CHEMP.8 Data

1. Click the **CHEMP.8** tab.
2. In the **SOLA** box, type **1.06E-7**.

Change CHEMP.9 Data

1. Click the **CHEMP.9** tab.
2. In the **Chemical Organic Carbon Partition Coef.** Box, type **0.0**.
3. In the **Default Fraction of Organic Compound in Soil** box, type **0.0**.
4. Click **OK** to close the **Edit VOC Data** dialog.

Add to Active VOC List

1. Select **Chlorobenzene Modified** in the **VOC Library** list.
2. Click the right arrow (-->) to move the selection to the **Active Simulation VOCs** list.
3. Click **OK** to close the **Global Properties** dialog.

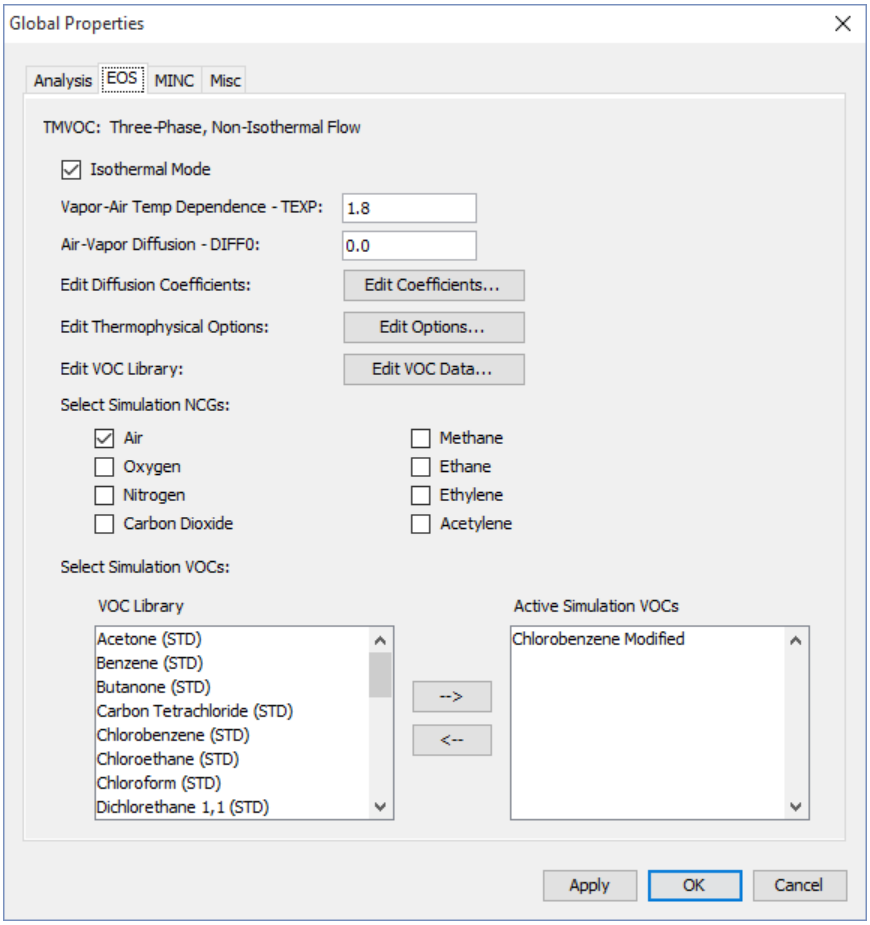

Figure 1.3: Global Properties

Material Properties

1. On the **Properties** menu, click **Edit Materials**.
2. In the **Name** box, type **DIRT1**.
3. In the **Porosity** box, type **0.2**.
4. In the **X, Y, Z Permeability** boxes, type **2.96E-13**.
5. In the **Wet Heat Conductivity** box, type **3.1**.

Define Additional Material Data

1. Click the **Additional Material Data** button.
2. In the **Relative Permeability** box, select **Faust (1985)**. The default properties are correct.
3. Click the **Misc** tab.
4. In the **Pore Compressibility** box, type **1.0E-8**.
5. Click **OK** to close the **Additional Material Data** dialog.
6. Click **OK** to close the **Material Data** dialog.

Initial Conditions

1. On the **Properties** menu, click **Initial Conditions**.
2. In the **Phase** list, select **6 - Water and NAPL**.
3. In the **Pressure** box, type **6.895E5**.
4. In the **Temperature** box, type **19.0**.
5. In the **Water Saturation** box, type **0.159**.
6. In the **Mole Fraction** box for Chlorobenzene Modified, type **1.0**.
7. Click **OK**.

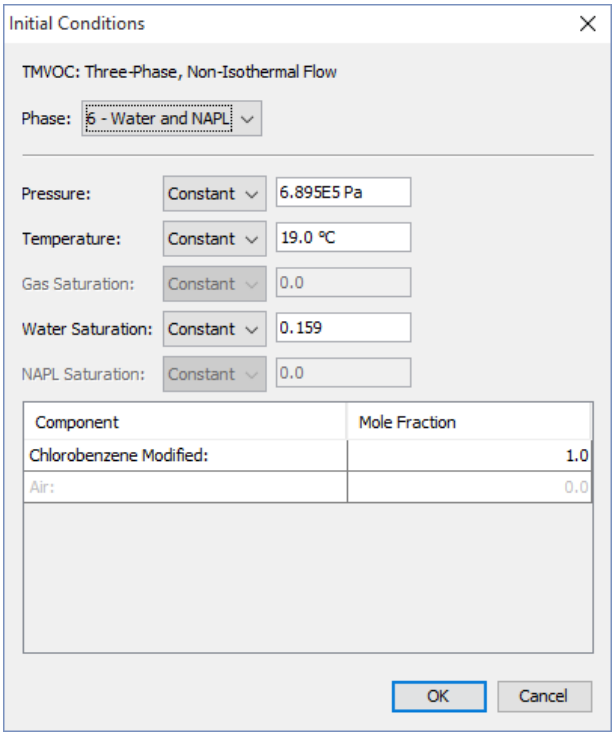

Figure 1.4: Initial Conditions

Edit Mesh

To make it easier to work with this 1D problem, you can scale the Y or Z axes. To scale the Y axis:

1. On the **View** menu, click **Scale Axes**.
2. In the **Y Factor** box, type 10.

3. Click **OK**.

At X=0, water is injected at a constant rate of 150.6E-6 kg/s. To name this cell, specify the water injection, and mark the cell for additional time history output:

1. Click to select the left-most cell (or search for cell 1 in the **Find** box).
2. On the **Edit** menu, click **Properties**.
3. In the **Cell Name** box, type **Injection**.
4. Click the **Sources/Sinks** tab.
5. In the **Available Components** list, select **Water/Steam**.
6. Select the **Component is a Source** check box.
7. In the **Rate** box, type **1.506E-04**.
8. In the **Enthalpy** box, type **8.0E4**.
9. Click the **Print Options** tab.
10. Select the **Print Time Dependent Flow and Generation (BC) Data** check box.
11. Click **OK** to exit out of the **Edit Cell Data** dialog.

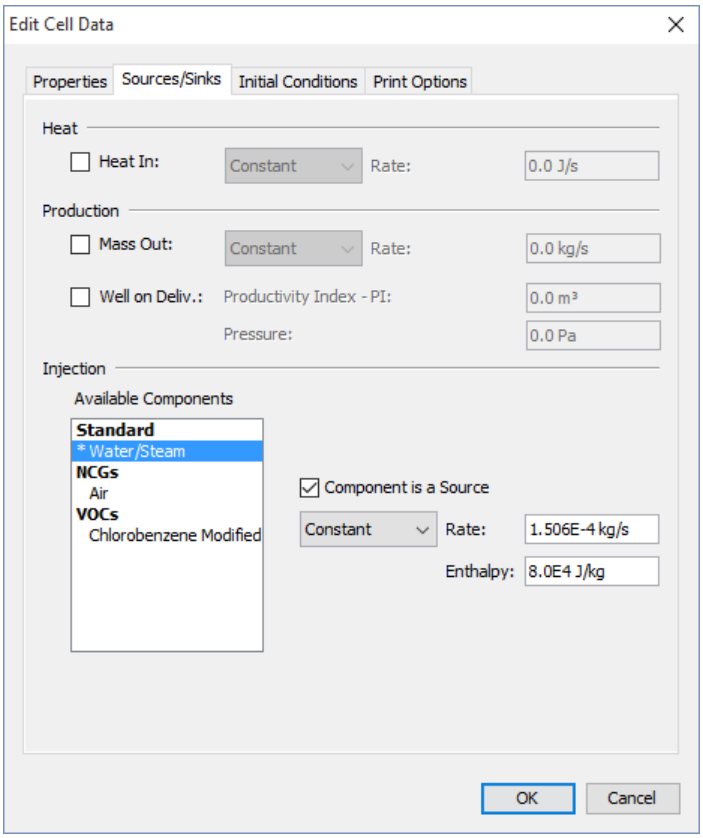

Figure 1.5: Edit Cell Data dialog

At X=304.8, a fixed state is defined.

1. Click to select the right-most cell (or search for cell 40 in the **Find** box).

2. On the **Edit** menu, select **Properties**.
3. In the **Cell Name** box, type **Fixed**.
4. In the **Type** box, select **Fixed State**.
5. Click the **Print Options** tab.
6. Select the **Print Time Dependent Flow and Generation (BC) Data** check box.
7. Click **OK** to exit out of the **Edit Cell Data** dialog.

To generate additional time history output at the center cell:

1. Click to select a cell near the center (or search for cell 19 in the **Find** box).
2. On the **Edit** menu, click **Properties**.
3. In the **Cell Name** box, type **Center**.
4. Click the **Print Options** tab.
5. Select the **Print Time Dependent Flow and Generation (BC) Data** check box.
6. Click **OK** to exit out of the **Edit Cell Data** dialog.

Solution Controls

1. On the **Analysis** menu, click **Solution Controls**.
2. In the **End Time** box, type **1500 days**.
3. In the **Max Time Step** dropbox, select **User Defined**.
4. In the **Max Time Step** box, type **10 days**.
5. Click **OK**.

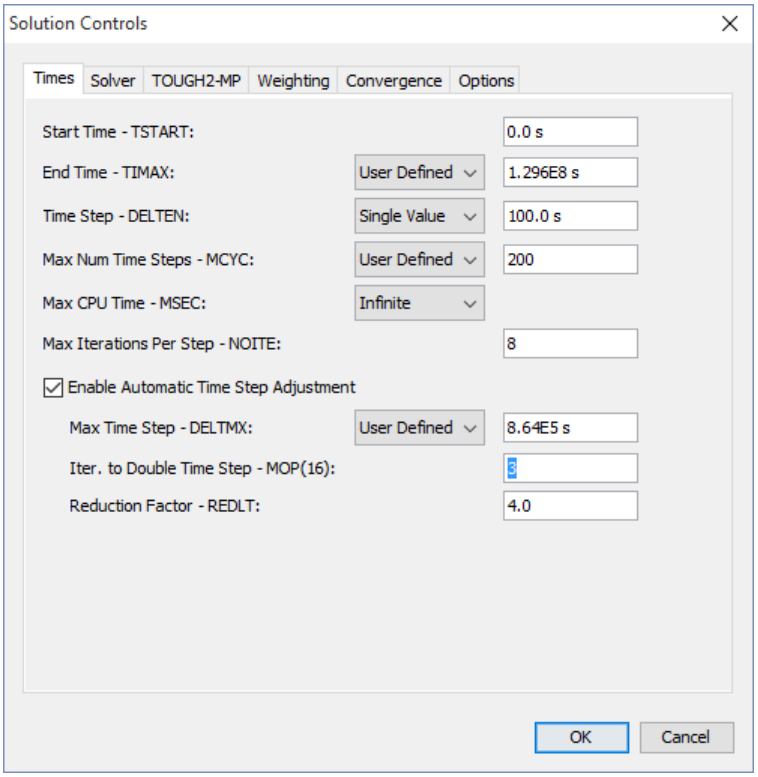

Figure 1.6: Solution Controls

Output Controls

1. On the **Analysis** menu, click **Output Controls**.
2. In the **Print and Plot Every # Steps** box, type **20**.
3. Click the **Relative Permeability, Viscosity, and Enthalpies** check box.
4. Click **OK**.

Save and Run

1. On the **File** menu, click **Save**.
2. On the **Analysis** menu, click **Run TOUGH2**.

View Results

You can view 3D results using the **3D Results** dialog. To view 3D results, on the **Results** menu, click **3D Results**. To scale the Z-axis for better visualization:

1. On the **Results** menu, click **3D Results**.
2. On the **View** menu, click **Scale Axes**.
3. In the **Y Factor** box, type **50.0**.
4. Click **OK**.

To show slice planes for oil saturation:

1. In the left-hand navigation pane, click **Slice Planes**.
2. In the **Axis** list, select **Z**.
3. In the **Coord** box, type **-0.5**.
4. Click **Close**.
5. In the **Time** list, select the last entry (**1.296E08**).
6. In the **Scalar** list, select **SO**.

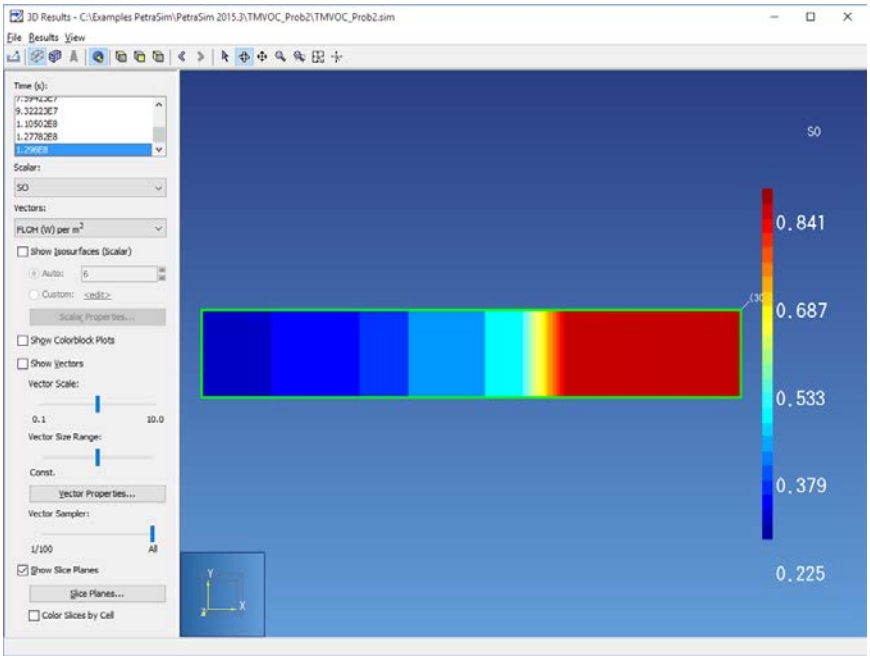

Figure 1.7: 3D Results

When finished, you can close the **3D Results** dialog.

View Cell Time History Plots

To view 2D time history plots for oil saturation:

1. On the **Results** menu, select **Cell History Plots**.
2. In the **Variable** list, select **Soil**.
3. In the **Cell Name** list, select **Center (19)**.

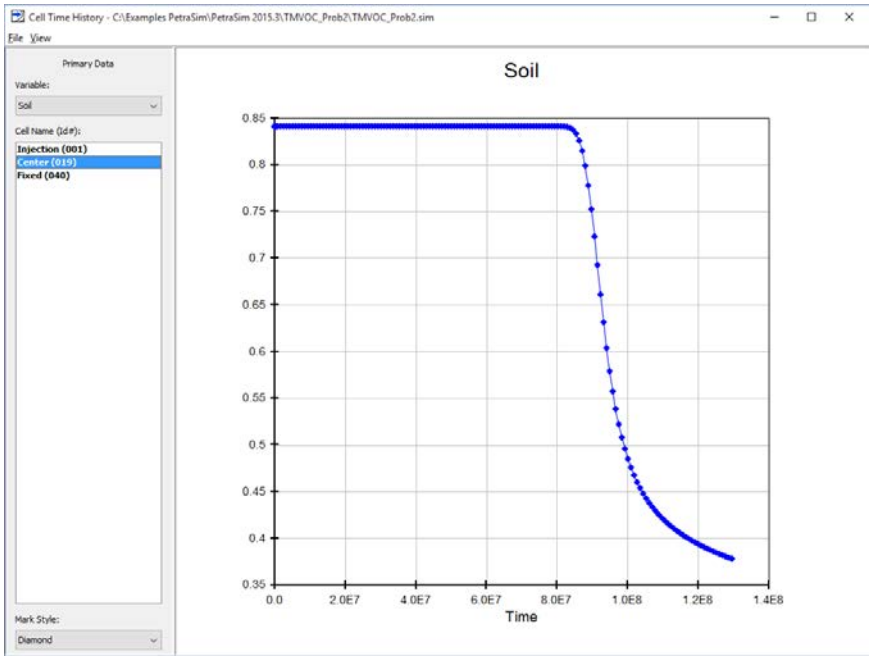

Figure 1.8: Time history plot of oil saturation in center cell

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