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PetraSim Example Manual

July 2007

TMVOC Example Guide

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Chapter 1. Buckley-Leverett Flow

Description

This example is Problem No. 2 (*rblm*) - "1-3 Buckley-Leverette 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.

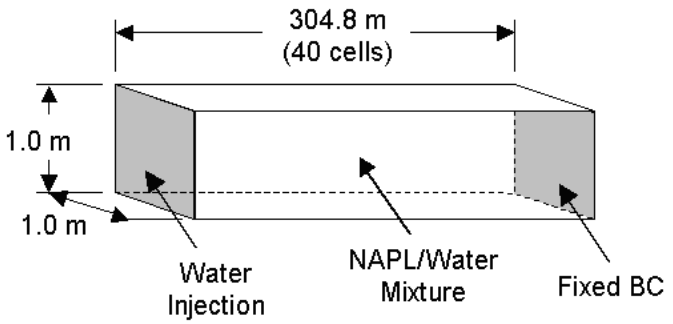

Figure 1.1. Insert title here

Specify the Simulator Mode

1. On the **File** menu, click **Preferences...**.
2. On the **Simulator Mode** list, select **TMVOC**.
3. Click **OK**
4. On the **File** menu, click **New...** to create a new TMVOC model.

Create the Model Boundary

1. On the **Model** menu, click **Define Boundary...**.
2. In the **X max** box, type `304.8`.
3. In the **Y max** box, type `1.0`.
4. In the **Z min** box, type `-1.0`, and in the **Z max** box, type `0.0`.

5. Click **OK**.

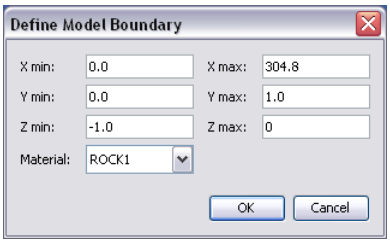

Figure 1.2. Model Boundary

Create the Grid

1. On the **Model** menu, click **Create Grid...**.
2. In the **X cells** box, type `40`.
3. In the **Y cells** box, type `1`.
4. In the **Z cells** box, type `1`.
5. Click **OK**.

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 **Edit 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.

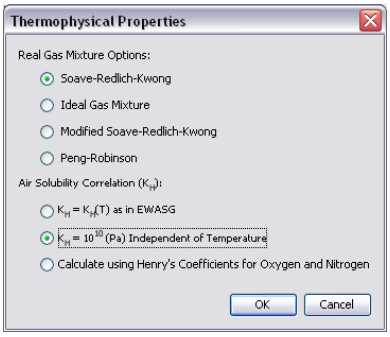

Figure 1.3. Thermophysical Properties

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. To create a new VOC:

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

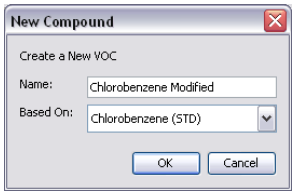

Figure 1.4. New Compound

Change CHEMP.4 Data

1. Click the **CHEMP.4** 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 Binary Temperature for Gas Diffusivity** box, type `273.15`.
6. In the **Chemical Diffusivity** box, type `1.0`.

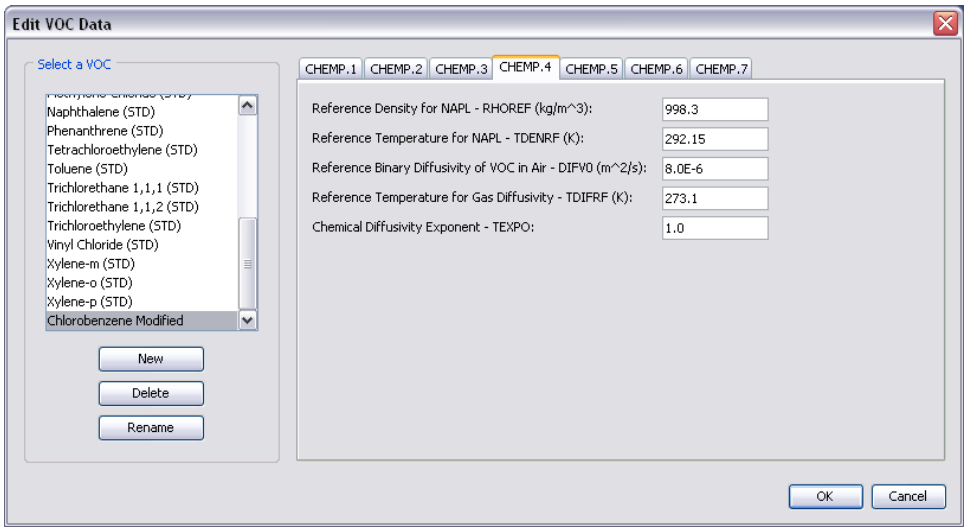

Figure 1.5. Edit CHEMP.4 Data

Change CHEMP.5 Data

1. Click the **CHEMP.5** 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.6 Data

1. Click the **CHEMP.6** tab.
2. In the **SOLA** box, type `1.06E-7`.

Change CHEMP.7 Data

1. Click the **CHEMP.7** 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.

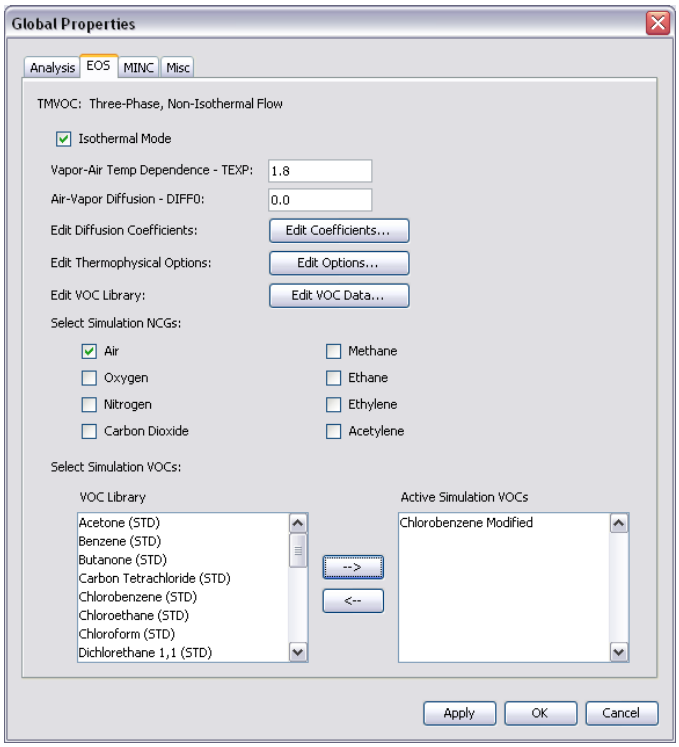

Figure 1.6. Global Properties

Material Properties

1. On the **Properties** menu, click **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`.

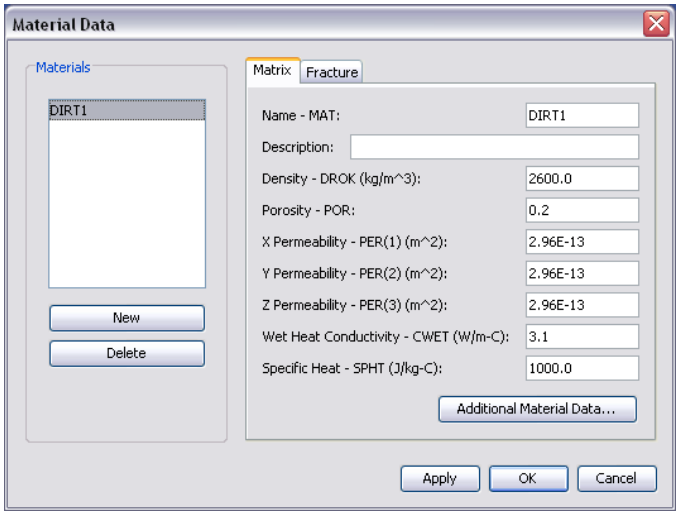

Figure 1.7. Material Data

Define Additional Material Data

1. Click the **Additional Material Data** button.
2. In the **Relative Permeability** box, select **Faust (1985)**.
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 **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**.

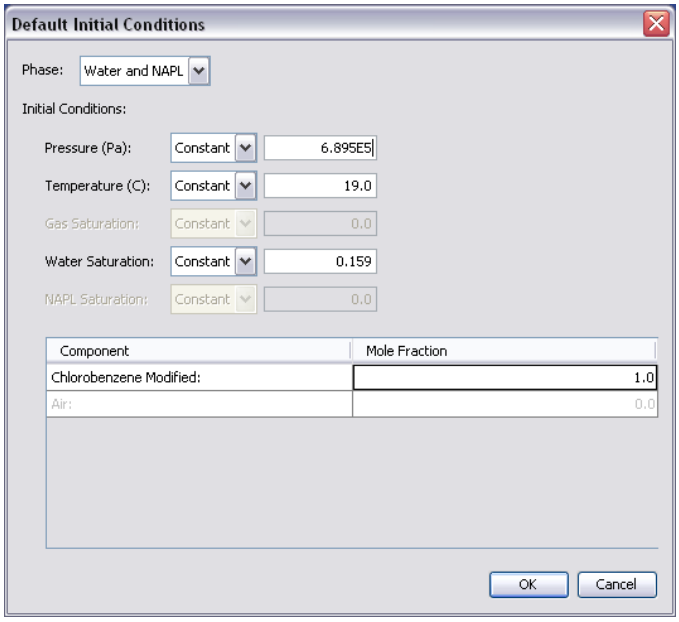

Figure 1.8. Initial Conditions

Edit Grid

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 **Model** menu, click **Edit Grid**.
2. On the **View** menu, click **Scale Axes**.
3. In the **Y Factor** box, type `10`.
4. 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 (id=1).
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-4`.
8. In the **Enthalpy** box, type `8.0E4`.
9. Click the **Print Options** tab.
10. Select the **Print Cell Time Dependent Data** check box.
11. Click **OK** to exit out of the **Edit Cell Data** dialog.

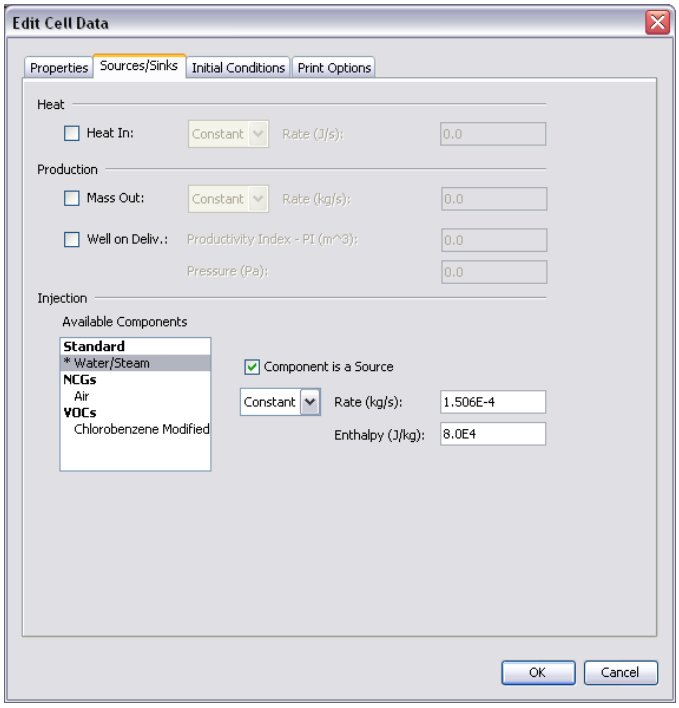

Figure 1.9. Edit Cell Data

At X=340.8, a fixed state is defined.

1. Click to select the right most cell (id=40).
2. Select **Edit 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 Cell Time Dependent 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 (id=19).
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 Cell Time Dependent Data** check box.
6. Click **OK** to exit out of the **Edit Cell Data** dialog.

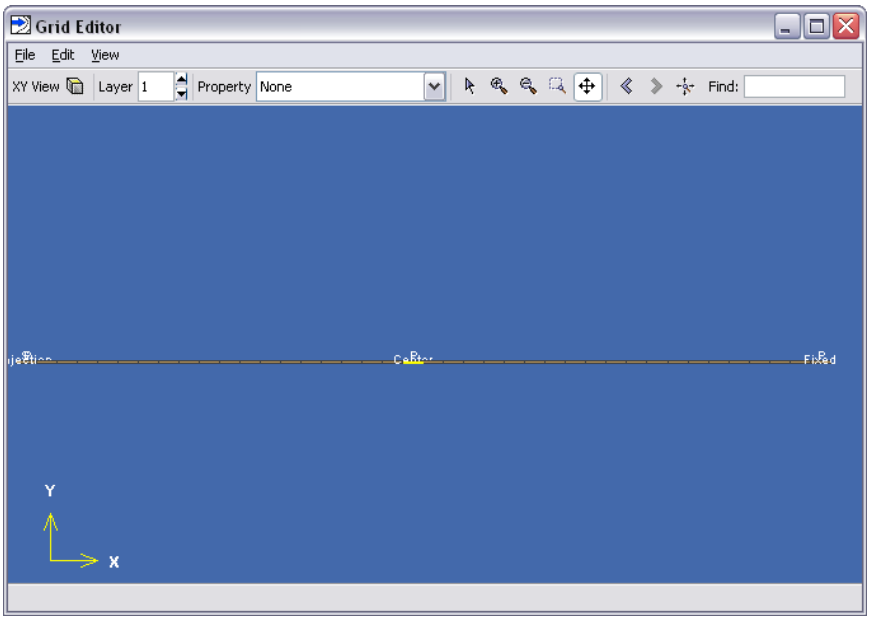

Figure 1.10. Grid Editor

Solution Controls

1. On the **Analysis** menu, click **Solution Controls**.
2. In the **End Time** box, type `1.296E8`.
3. In the **Max Time Step** list, select **User Defined**.
4. In the **Max Time Step** box, type `8.64E5`.
5. Click **OK**.

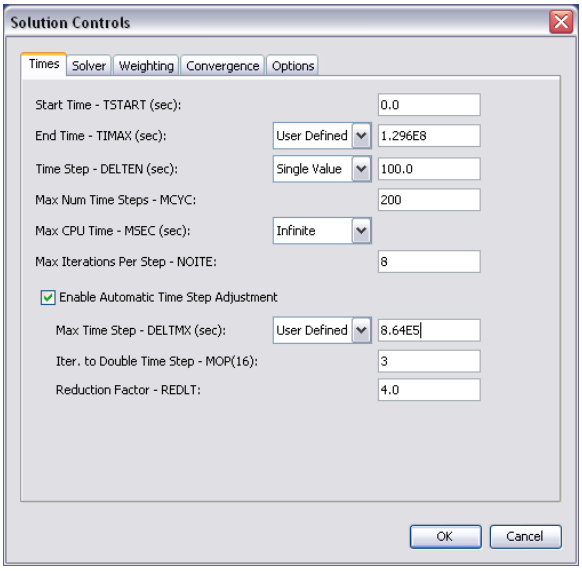

Figure 1.11. Solution Controls

Output Controls

1. On the **Analysis** menu, click **Output Controls**.
2. In the **Print and Plot Every # Steps** box, type `20`.
3. Click the **Fluxes and Velocities** check box to deselect the option.
4. Click the **Add TMVOC Variables** check box.
5. Click **OK**.

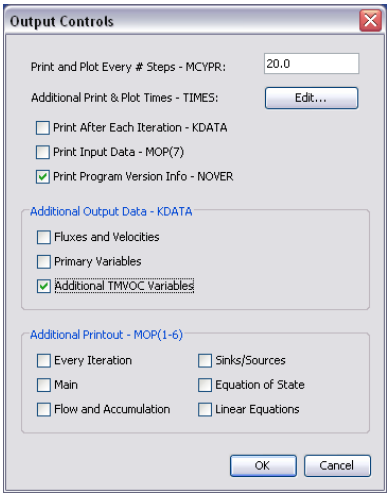

Figure 1.12. Output Controls

Saving

1. On the **File** menu, click **Save**.
2. Create a new folder named `Buck-lev-flow` and in the **File name** box, type `buck-lev-flow`.
3. Click **Save**.

TMVOC Analysis

1. On the **Analysis** menu, click **Run TOUGH2**.
2. Upon completion, the **Simulation Complete** dialog will appear. Click **OK**.
3. Click **Close** on the **Running TOUGH2** dialog.

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**.

1. In the **Time** list, select **1.296E8**.
2. In the **Scalar** list, select **SO**.

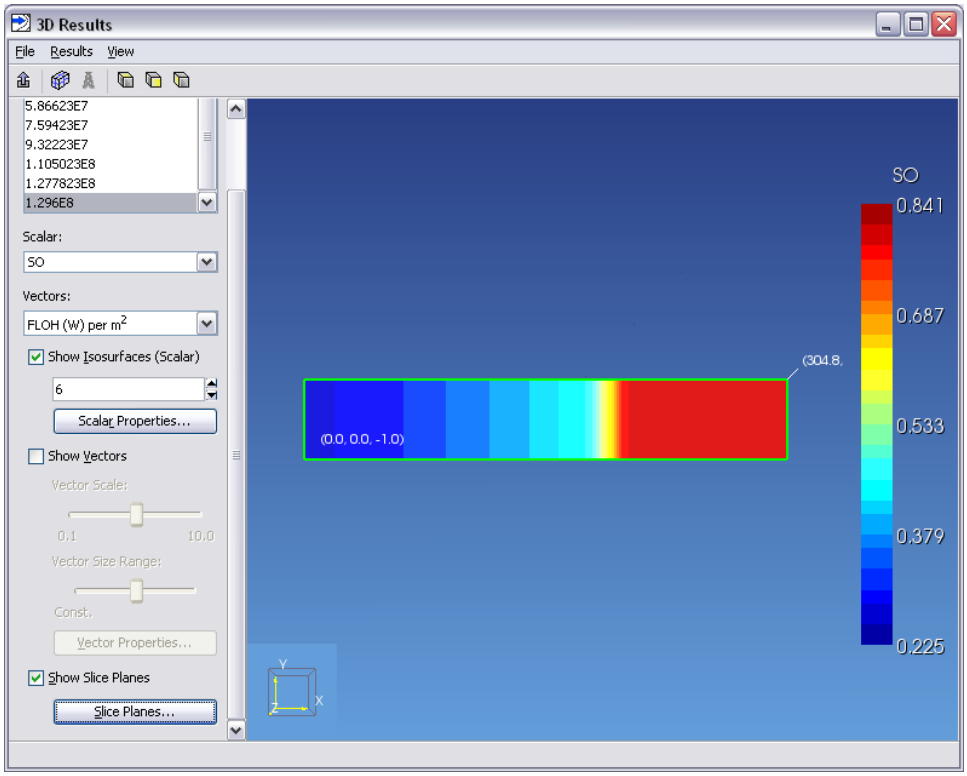

Figure 1.13. 3D Results

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)**.

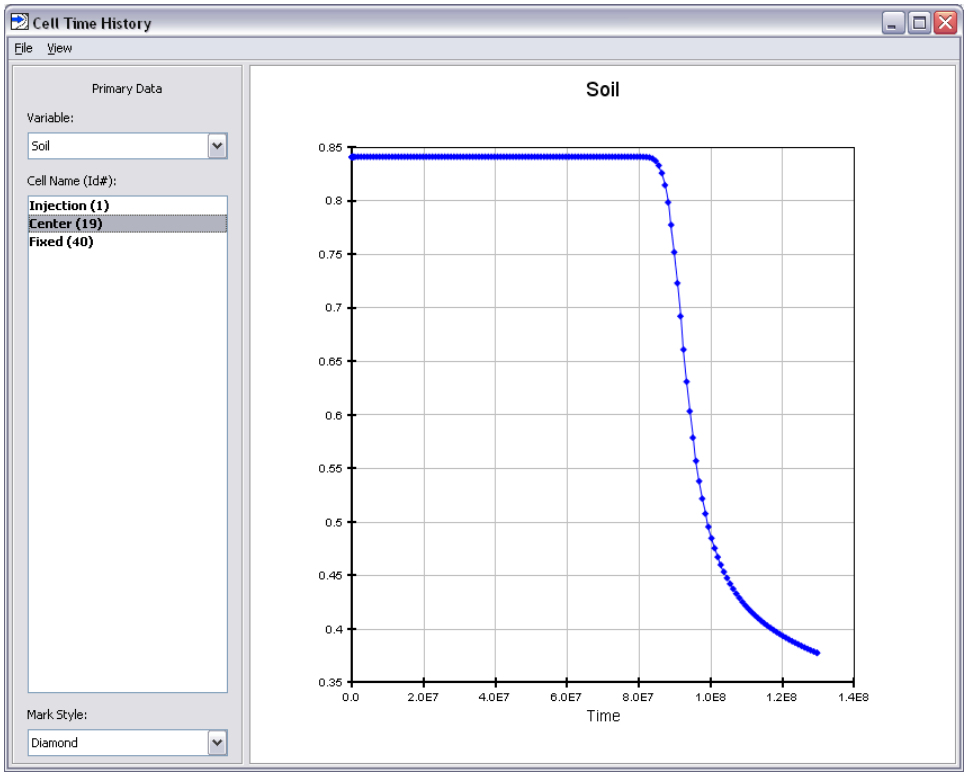

Figure 1.14. Time history plot of oil saturation in center cell.