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T2VOC Example:

One Dimensional Gas Diffusion of an Organic Chemical

PetraSim 5

Table of Contents

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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.

One Dimensional Gas Diffusion of an Organic Chemical (T2VOC)

Description

This example demonstrates one dimensional gas diffusion of an organic chemical with phase partitioning - as described in the T2VOC User's Guide (1).

A horizontal column has an initial temperature of 10° C and an initial pressure of 101325 Pa. The left cell has a fixed thermodynamic state and acts as a source of chlorobenzene. The geometry of the problem is shown in Figure 1.

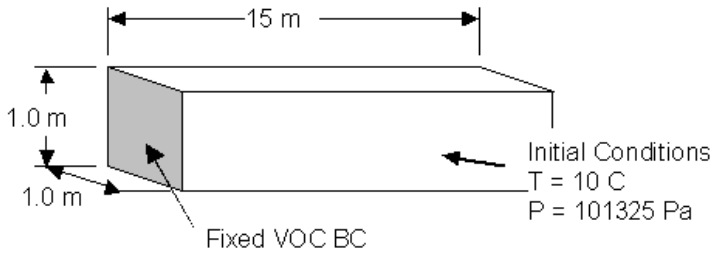

Figure 1: Example Problem Overview

We will use a mesh with 150 cells in the horizontal direction.

Create a T2VOC Model

We will first create a new model using the T2VOC EOS.

From the **File** menu, select **New…** to open the **New Model** dialog.

1. For the **Simulator Mode**, choose **TOUGH2**.
2. For the **Equation of State (EOS)**, choose **T2VOC**.
3. For the **Model Bounds**, enter the values from Table 1.

Table 1: Model boundary dimensions

Axis	Min (m)	Max (m)
X	0.0	15.0
Y	0.0	1.0
Z	0.0	1.0

Click **OK** to close the **New Model** dialog and create the model.

You can rotate, pan, and zoom the model using the mouse and **Shift** and **Alt** keys. The resulting boundary is shown in Figure 2. PetraSim will automatically add labels for the min point and max point of the boundary.

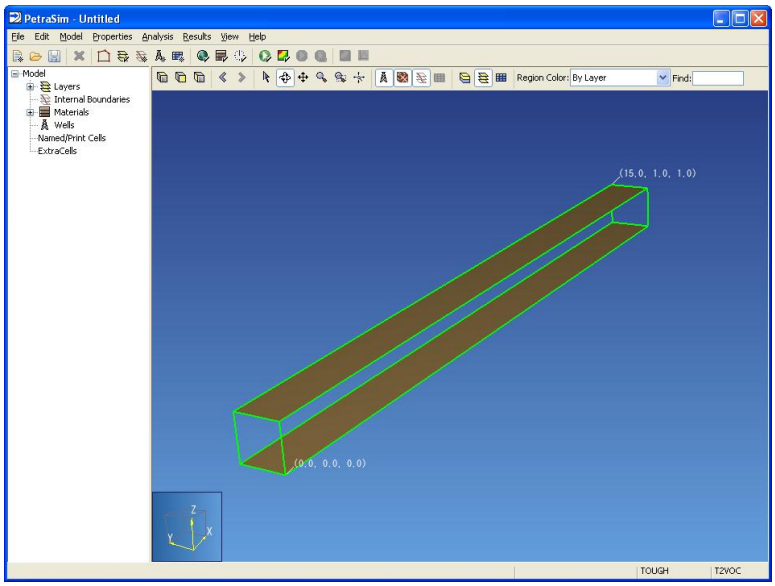

Figure 2: The Model Boundary

Specify the Solution Mesh

The solution mesh must be specified in two steps. First the Z divisions must be specified per layer. Then the mesh can be created using the **Create Mesh** dialog.

Specify Z Divisions

We must first specify one Z division for the default layer. To do so, we will open the **Edit Layers** dialog. On the **Model** menu, select **Edit Layers…**.

1. In the layers list in the left-hand pane, select the **Default** layer.
2. In the right-hand pane, select **Regular** for **Dz**.
3. In the **Cells** box, type *1*.
4. In the **Factor** box, type *1.0*.

Click **OK** to apply the changes and close the **Edit Layers** dialog.

Create the Mesh

We will now create the radial solution mesh using the **Create Mesh** dialog. To open the dialog, on the **Model** menu, select **Create Mesh…**.

1. For the **Mesh Type**, select **Regular**.
2. For the **Divisions**, select **Regular**.
3. In the **X Cells** box, type *150*.
4. In the **Y Cells** box, type *1*.

5. For both **X** and **Y Factor**s, type *1.0*.

Click **OK** to create the mesh.

Global Properties

Global properties are those properties that apply to the entire model. In this example we will set the simulation name and configure the simulation VOC. To edit global properties, you can use the **Global Properties** dialog.

On the **Properties** menu, select **Global Properties…**.

Simulation Name

1. In the **Global Properties** dialog, select the **Analysis** tab.
2. In the **Name** box, type *T2VOC Problem 1*.

EOS Data

The EOS (Equation of State) tab displays options for the T2VOC simulator. In this example, we will perform an isothermal (no heat flow) analysis. We will also specify a variant of chlorobenzene as the simulation VOC and specify the Air-Vapor diffusion constant.

In the **Global Properties** dialog, select the **EOS** tab.

By default, the simulator will run in isothermal mode. Nothing needs to be changed.

To specify the VOC, you will need to create a variant of chlorobenzene using the **Edit VOC Data** dialog.

1. Click **Edit VOC Data…**.
2. Click **New**.
3. In the **Name** box, type *Chlorobenzene Ex 1*.
4. In the **Based On** list, select **Chlorobenzene (STD)**.
5. Click **OK**. This creates a new VOC.
6. Update the values for **CHEMP.4**, **CHEMP.6**, and **CHEMP.7** according to the values shown in Table 2, Table 0.3, and Table 4.
7. Click **OK** and ensure that the selected **Simulation VOC** is **Chlorobenzene Ex 1**.
8. This simulation will use gas diffusion. You can enable gas diffusion by setting the **Air-Vapor Diffusion** to a non-zero value. In the **Air-Vapor Diffusion** box, type *2.13e-5*.
9. Click **OK** to close the **Global Properties** dialog.

Table 2: Chlorobenzene Ex 1 (CHEMP.4)

Field	Value
Reference Density for NAPL	1106.0
Reference Temperature for NAPL	293
Reference Binary Diffusivity of VOC in Air	8.0e-6
Reference Temperature for Gas Diffusivity	283.15
Chemical Diffusivity Exponent	1.0

Table 0.3: Chlorobenzene Ex 1 (CHEMP.6)

Field	Value
SOLA	7.99e-5
SOLB	0.0
SOLC	0.0
SOLD	0.0

Table 4: Chlorobenzene Ex 1 (CHEMP.7)

Field	Value
Chemical Organic Carbon Partition Coef	0.15
Default Fraction of Organic Carbon in Soil	0.005
VOC Biodegradation Decay Constant	0.0

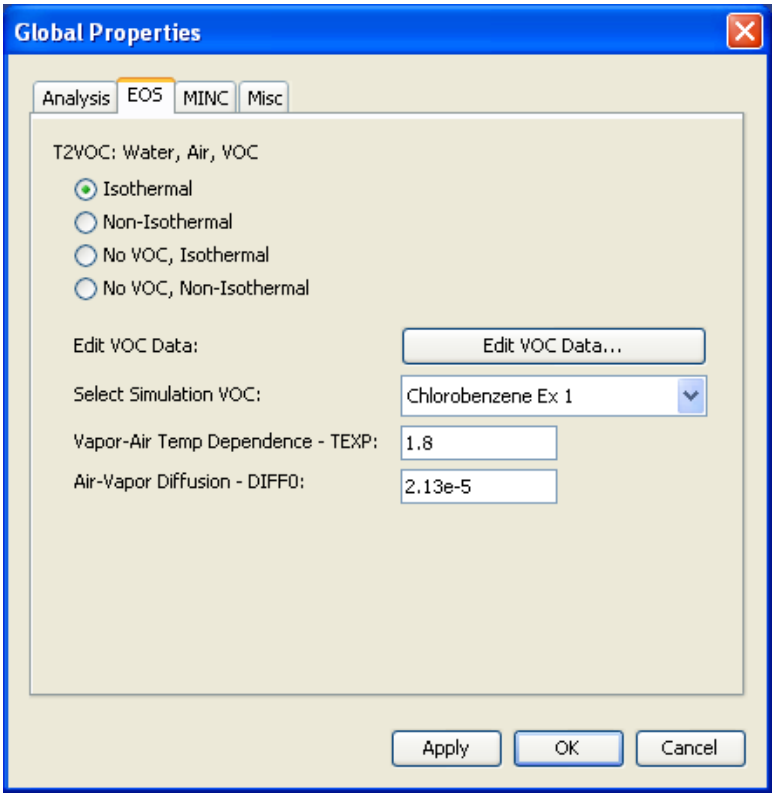

Figure 3: T2VOC Simulation Parameters

Material Properties

To specify the material properties, you can use the **Material Data** dialog.

1. On the **Properties** menu, click **Edit Materials…**.
2. In the **Name** box, type *DIRT1*.

3. In the **Density** box, type *2650.0*.
4. In the **Porosity** box, type *0.4*.
5. In all three **Permeability** boxes, type *1e-14*.
6. In the **Wet Heat Conductivity** box, type *3.1*.
7. In the **Specific Heat** box, type *1000.0*.
8. Click **Apply** to save the changes.

We still need to specify the relative permeability function and fraction of organic carbon for this material. These options can be found in the **Advanced Material Data** dialog. To open this dialog, click the **Additional Material Data…** button.

To specify the relative permeability function:

1. Select the **Relative Perm** tab.
2. In the **Relative Permeability** list, select **Stone's 3-Phase**.
3. In the $\mathbf{S_{wr}}$ box, type *0.4*.
4. In the $\mathbf{S_{nr}}$ box, type *0.1*.
5. In the $\mathbf{S_{gr}}$ box, type *1.0e-3*.
6. In the **n** box, type *1.0*.

The default capillary pressure (none) is correct for this example.

To specify the fraction of organic carbon:

1. Select the **Misc** tab.
2. In the **Fraction of Organic Carbon** box, type *0.005*.

Click **OK** to exit the **Additional Material Data** dialog.

Click **OK** again to save your settings and exit the **Material Data** dialog.

Initial Conditions

You can control the initial state of the primary variables using initial conditions. Primary variable selection will depend on several factors including EOS selection, simulator mode, and the initial state of the simulation. You can edit initial conditions globally and on a cell-by-cell basis.

To edit global initial conditions: on the **Properties** menu, select **Initial Conditions…**.

For this example, we will initialize all cells to a two-phase water and air state. There is no initial chlorobenzene saturation. To set the initial conditions:

1. Select the **Two-Phase Water/Air** state option.
2. In the **Pressure** box, type *101325.0*.
3. In the **Temperature** box, type *10.0*.
4. In the **Water Saturation** box, type *0.25*.
5. In the **VOC Mole Fraction in Air** box, type *0.0*.

6. Click **OK**.

Boundary Conditions

We will inject chlorobenzene into the model using a cell-specific initial condition. Then we will force the state of that cell to remain constant. To edit individual cells, you can use the **3D View**.

Every cell in the model has a unique ID number. You can find and select cells based on their ID number using the **Find** field in the upper-right corner of the **3D View**. In this example, cell 1 will be the chlorobenzene source. To find and select cell 1:

1. In the **Find** box, type *1*.
2. Press *ENTER*. The cell should be selected and shown in the center of the **3D View**.

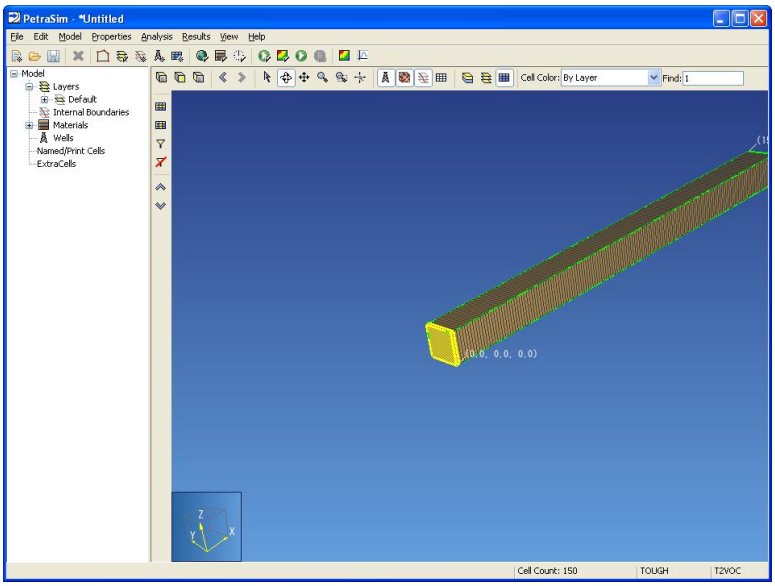

Figure 4: Finding a Cell in the 3D View

You can now edit the properties of cell 1. Ensure cell 1 is selected. On the **Edit** menu, select **Properties…**.

To force the state of this cell to remain constant throughout the simulation, you can adjust its type. Select the **Properties** tab. Then, in the **Type** list, select **Fixed State**.

Now you can give the cell a custom initial condition that will remain constant throughout the simulation. Select the **Initial Conditions** tab. To enter the custom initial conditions:

1. Select **Specify Initial Conditions by Cell**.
2. Select the **Three-Phase Water/Air/NAPL** state.
3. In the **Gas Saturation** box, type *0.75*.
4. In the **Water Saturation** box, type *0.2*.

Notice that we did not explicitly specify a NAPL saturation. With the gas saturation at *0.75* and the water saturation at *0.2* the NAPL saturation will be *0.05*. T2VOC will perform this calculation during the simulation.

Click **OK** to close the **Edit Cell Data** dialog.

Solution Controls

We will now adjust the time step T2VOC will use while executing the simulation. Options relating the time step and other simulation options can be found in the **Solution Controls** dialog.

To open the **Solution Controls** dialog: on the **Analysis** menu, click **Solution Controls…**.

For this example, we will adjust the end time, increase the maximum number of time steps, and limit the size of the maximum time step.

1. In the **End Time** box, type *1 yr*.
2. In the **Max Num Time Steps** box, type *350*.
3. In the **Max Time Step** list, select **User Defined**.
4. In the **Max Time Step** box, type *5 days*.

Click **OK** to exit the **Solution Controls** dialog.

Output Controls

By default, T2VOC will print output every 100 time steps. We can increase the resolution of the output with the **Output Controls** dialog.

1. On the **Analysis** menu, click **Output Controls…**.
2. In the **Print and Plot Every # Steps** box, type *5*.
3. Click **OK** to exit the **Output Controls** dialog.

Save and Run

The input is complete and you can now run the simulation. Bear in mind that T2VOC generates many output files and they will overwrite the output from any previous simulations in a directory. If you haven't already, you may want to save your model in a directory specifically intended for the simulation results. For example:

1. On the **File** menu, click **Save**.
2. Create a new folder named *t2voc_problem_1* and in the **File Name** box, type *t2voc_prob1.sim*.
3. Click **Save**.

To run the simulation, on the **Analysis** menu, click **Run TOUGH2**.

During the solution, a graph will display the time step size. In this case, the time steps increase until they remain constant at the specified maximum.

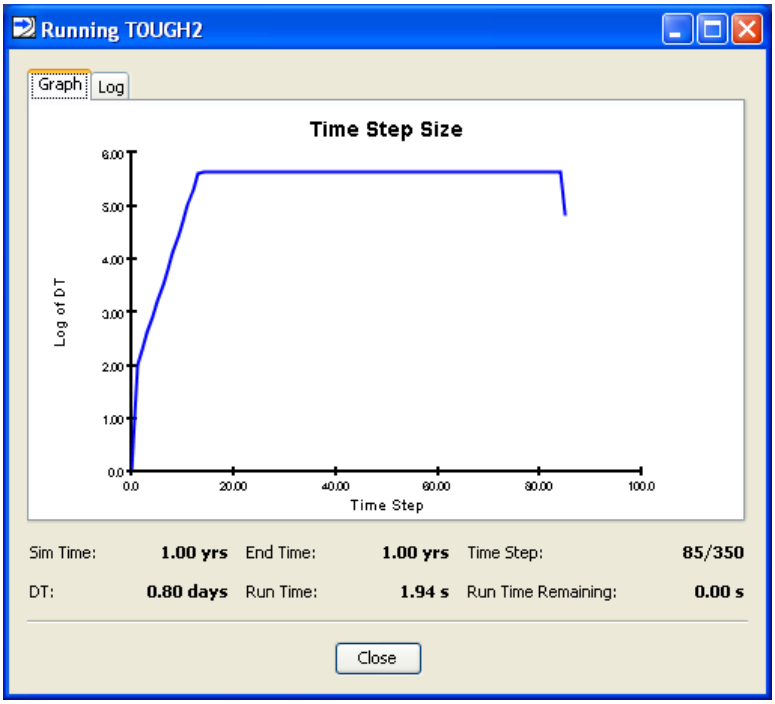

Figure 5: Running T2VOC

View 3D Results

To view the 3D results for a simulation

1. On the **Results** menu, click **3D Results**. The data for the current simulation will be automatically loaded and displayed.

To view the VOC concentration for the last time step.

1. In the **Time(s)** list, select the last entry (**3.156E07**).
2. In the **Scalar** list, select **CVOCGAS**.
3. Click to clear the **Show Isosurfaces** checkbox.

To add a slice plane on which contours will be displayed, click **Slice Planes…**. For this example we will show one slice plane. To configure the slice plane

1. In the **Axis** list, select **Z**.
2. In the **Coord** box, type *0.5*.
3. Ensure that the **Scalar** check box is checked.
4. Click **Close**.

Your results should now look similar to the screenshot in Figure 6. You can now see the gas-phase VOC concentration emanating from the left side of the model.

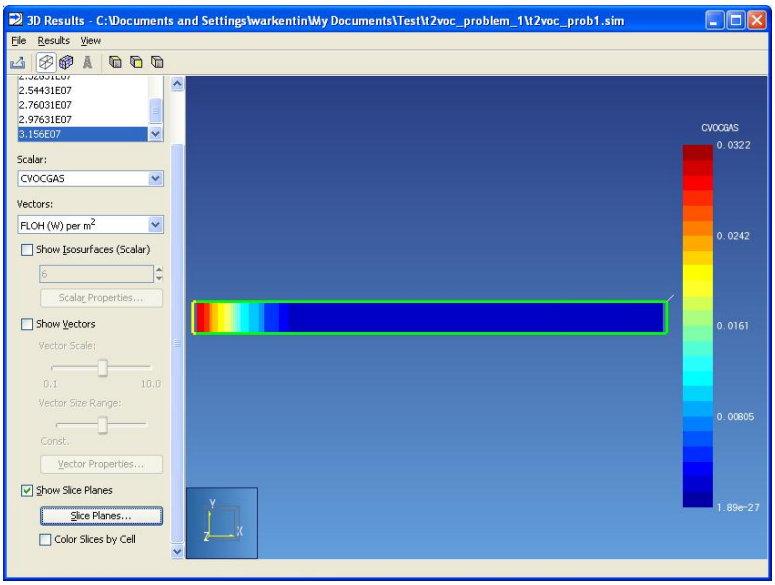

Figure 6: T2VOC 3D Results

Close the **3D Results** window.

References

1. **Falta, Ronald, et al., et al.** *T2VOC User's Guide.* Berkeley, CA, USA : Earth Sciences Division, Lawrence Berkeley National Laboratory, March 1995. LBNL-36400.

2. **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.