THUNDERHEAD ENGINEERING

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

TOUGHREACT Example: Aqueous Transport with Adsorption and Decay

PetraSim 2016.1

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Overview

Using TOUGHREACT

TOUGHREACT is an extension of the original TOUGH2 simulator that is available as a simulator mode in PetraSim. The TOUGHREACT simulator supports a subset of the TOUGH2 EOS modules. The supported EOS modules are EOS1, EOS2, EOS3, EOS4, EOS9, and ECO2N. You can perform a TOUGHREACT simulation by selecting the TOUGHREACT simulator mode and one of the available EOS modules when creating a new model.

In PetraSim, options relating to TOUGHREACT are presented under the **TOUGHREACT** menu item in the main window. These options allow you to configure the reactive transport solver, simulation output, chemical zones, and other TOUGHREACT-specific parameters.

It is also possible to disable reactive transport during a TOUGHREACT simulation. This will effectively revert the simulator to TOUGH2 mode. This option is available in the **Global Properties** dialog, on the **Analysis** tab.

Input Files

A TOUGHREACT simulation requires four input files. These files are listed below:

- flow.inp -- This is the standard TOUGH2 input file
- solute.inp -- The chemical "geography" of the analysis
- chemical.inp -- The chemical parameters
- thermodb.txt -- The thermodynamic database

PetraSim creates each of these files into your simulation directory. However, the filenames cannot be changed. The naming scheme for the simulation output files follows a similar pattern. To avoid overwriting previous simulation input and output data, you must run each analysis in a separate directory.

Thermodynamic Database

A thermodynamic database listing the composition of many different species and minerals has been included with PetraSim. PetraSim will automatically load this database. A valid database must be loaded prior to the inclusion of species or the definition of reactive zones. This is because the species used to build up the zones are loaded from the thermodynamic database. If you choose to use a custom database, you must ensure that it is loaded before configuring any species or zones. To load a custom thermodynamic database:

1. First create or open a TOUGHREACT model.
2. On the **TOUGHREACT** menu, click **Thermodynamic Database.**
3. Select your custom thermodynamic database.
4. Click **OK**.

Aqueous Transport with Adsorption and Decay (EOS9)

Description

This problem is the first example in the TOUGHREACT manual. It is a 1-D problem, 12 m in length, with a unit area, divided into 60 blocks of 0.2 m thickness, as shown in Figure 1.

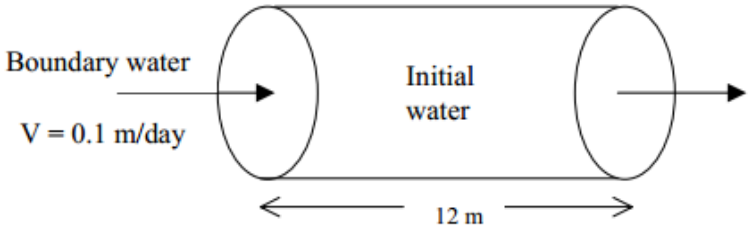

Figure 1: Aqueous Transport with Adsorption and Decay Model, after (1)

The completed PetraSim model file for this example problem may be found in a zip file on PetraSim's documentation web site. Download the *resources.zip* file and the **t2react_example1.sim** file is located in the **t2react_example1** folder.

Create the TOUGHREACT model

We first will create a new model using TOUGHREACT and EOS9 and specify a default model boundary:

1. On the **File** menu, click **New**.
2. For the **Simulator Mode**, select **TOUGHREACT v1.2**.
3. For the **Equation of State (EOS)**, select **EOS9.**
4. For the **Model Bounds (Default)**, enter the values from Table 1.
5. Click **OK**.

Table 1: Model Boundary Dimensions

Axis	Min (m)	Max (m)
X	0.0	12.0
Y	0.0	1.0
Z	0.0	1.0

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. You can select other units for the input parameters. If you do this, PetraSim will remember your selection the next time you open a model:

1. On the **View** menu, click **Unit System.**
2. Select the units you wish to use for each parameter.
3. To reset to the default TOUGH2 units, click **Reset**.

Note: You can always 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 TOUGHREACT 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 **T2REACT Example 1** and in the **File Name** box, type **t2react_example_1.sim**.
3. Click **Save.**

Specify the Solution Mesh

Specifying the mesh takes two steps. First we must enter the Z divisions per layer. By default, the model is created with a single layer in the Z direction and a single cell through the layer. This matches our desired input, so no changes need to be made to the layers.

To create the mesh:

1. On the **Model** menu, click **Create Mesh.**
2. In the **X Cells** box, type **60.**
3. In the **Y Cells** box, type **1.**
4. Click **OK** to create the mesh (Figure 2)**.**

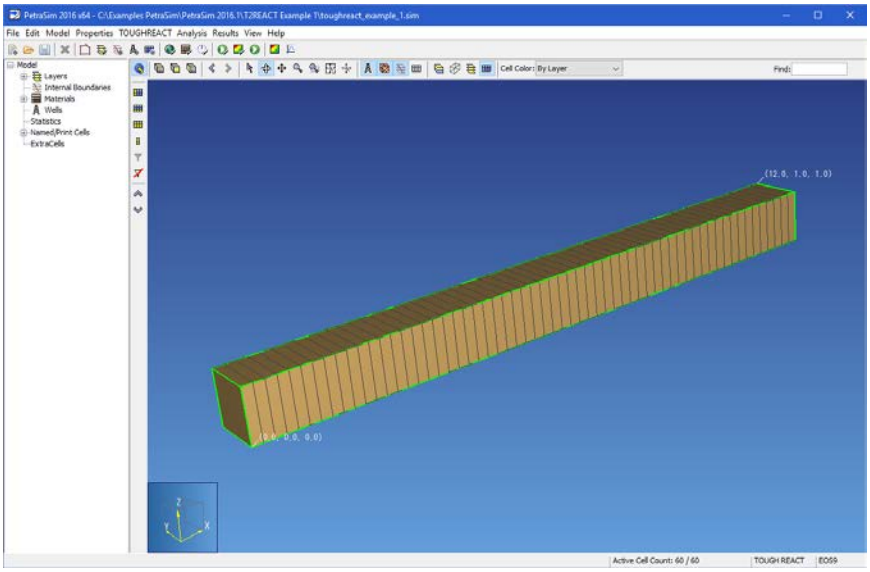

Figure 2: After creating the mesh

Global Properties

Global properties are properties that apply to the entire model.

Simulation Name

To set the simulation name:

1. On the **Properties** menu, click **Global Properties.**
2. In the **Name** box, type **TOUGHREACT Example 1.**
3. Click **OK.**

EOS Data

The EOS (Equation of State) tab displays options for EOS9.

1. In the **Global Properties** dialog, click the **EOS** tab.
2. In the **Reference Pressure (Pa)** box, type **1E5**.
3. In the **Reference Temperature (C)** box, type **4**.
4. Click **OK** to close the **Global Properties** dialog.

Material Properties

To specify the material properties, you use the **Material Data** dialog. This example requires one material.

Material Data

1. On the **Properties** menu, click **Edit Materials.**
2. In the materials list, select **ROCK1**.
3. In all three **Permeability** boxes (X, Y, and Z), type **6.51E-12**.
4. In the **Wet Heat Conductivity** box, type **0.0**.
5. In the **Specific Heat** box, type **952.9**.
6. Click **Apply** to save the changes.

In addition to the physical rock parameters, we also need to specify the relative permeability and capillary pressure functions for this material. These options can be found in the **Additional Material Data** dialog.

Relative Permeability

To specify the relative permeability function:

1. Click the **Additional Material Data** button.
2. Click the **Relative Perm** tab.
3. In the **Relative Permeability** list, select **Linear Functions**.
4. In the **Slmin** box, type **.333**.
5. In the **Slmax** box, type **1.0**.
6. In the **Sgmin** box, type **-0.1**.
7. In the **Sgmax** box, type **0.0**.

Capillary Pressure

To specify the capillary pressure function:

1. Click the **Capillary Press** tab.
2. In the **Capillary Pressure** list, select **Linear Function**.
3. In the **CPmax** box, type **9.7902E3**.
4. In the **A** box, type **0.333**.
5. In the **B** box, type **1**.
6. Click **OK** to exit the **Additional Material Data** dialog.
7. Click **OK** again to save your settings and exit the **Material Data** dialog.

Initial Conditions

The initial state of each cell in the model must be defined. The **Default Initial Conditions** dialog is used to define initial conditions that will be applied to the entire model. You can also specify initial conditions by cell, by region, by layer, or by importing the results of a previous analysis. For any analysis, the specific initial conditions will depend on several factors including EOS selection, simulator mode, and the initial state of the simulation.

Correct specification of initial conditions is essential for proper convergence and obtaining a correct result. In general, the initial conditions need to be physically meaningful. Often this requires an initial state analysis in which a model is run to obtain initial equilibrium conditions before the analysis of interest (geothermal production, VOC spill, etc.) is run.

To set the global initial conditions:

1. On the **Properties** menu, click **Initial Conditions.**
2. In the list, select **Pressure**.
3. In the **Pressure** box, type **1.001E5**.
4. Click **OK** to exit the **Default Initial Conditions** dialog.

Define Boundary Conditions

Boundary conditions can be defined for individual cells. We will define conditions for injection and production cells.

Water Source

We will inject into the cell on the left and produce from the cell on the right.

Injection

To define the injection cell:

1. Right-click the leftmost cell (ID=001) and click **Edit Cells.**
2. **I**n the **Cell Name** box, type **Injection**.
3. Click the **Sources/Sinks** tab.
4. Under **Injection**, select **Water**.

5. In the **Rate** box, type **1.16E-4**.
6. Because EOS9 is an isothermal analysis, the enthalpy value need not be set.
7. Click the **Print Options** tab.
8. Click **Print Time Dependent Flow and Generation Data.**
9. Click **OK** to save changes and close the dialog.

Similar steps are followed to define production in the model.

Production

To define the production cell:

1. Right-click the rightmost cell (ID=060) and click **Edit Cells.**
2. In the **Cell Name** box, type **Production.**
3. Click the **Sources/Sinks** tab.
4. Under **Production**, click **Mass Out.**
5. In the **Rate** box, type **1.16E-4.**
6. Click the **Print Options** tab.
7. Click **Print Time Dependent Flow and Generation Data.**
8. Click **OK** to save changes and close the dialog.

Print Center Cell Data

We will also choose a cell in the center of the model for which time history data will be printed.

1. Right-click on a cell near the center (for example, Cell ID 030) to edit the cell properties. In the popup menu click **Edit Cells.**
2. In the **Cell Name** box, type **Center.**
3. Click the **Print Options** tab.
4. Click **Print Time Dependent Flow and Generation Data.**
5. Click **OK** to save changes and close the dialog.

Solution Controls

We will now define the solution options. Options relating the time step and other solution controls 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 **100 days**.[1]
3. In the **Time Step** box, type **10 s**.
4. In the **Max Num Time Steps** list, type **2000**.
5. Click the **Enable Automatic Time Step Adjustment** checkbox.

[1] Most input boxes taking a time input will allow the user to enter the time in seconds (**s**), minutes (**min**), hours (**h**), months (**month**), and years (**yr**). If no unit is specified, seconds will be used.

6. In the **Max Time Step** list, select **User Defined** and in the **Max Time Step** box, type **0.1 days**.

Weighting

1. In the **Solution Controls** dialog, click the **Weighting** tab.
2. As the **Density at Interface** option, select **Average of Adjacent Elements**.

Convergence

1. In the **Solution Controls** dialog, click the **Convergence** tab.
2. In the **Relative Error Criterion** box, type **1.0E-6**.
3. Click **OK** to exit the **Solution Controls** dialog.

Output Controls

By default, the simulation will print output every 100 time steps. We can change the resolution of the output in the **Output Controls** dialog.

1. On the **Analysis** menu, click **Output Controls.**
2. In the **Print and Plot Every # Steps** box, type **500**.
3. In the **Additional Output Data** group, select **Fluxes and Velocities**, **Primary Variables**, and **Additional TOUGHREACT Variables**.

In addition to printing output every 500 steps, we can also specify times for which we want to view data in the **Additional Print Times** dialog.

To specify additional times for output:

1. On the **Output Controls** dialog, click the **Edit** button to open the **Additional Print Times** dialog.
2. In the **Times** table, type **4.32E6** and **8.64E6**.
3. Click **OK** to exit the **Additional Print Times** dialog.
4. Click **OK** to exit the **Output Controls** dialog.

TOUGHREACT Solution Parameters

We will now set the TOUGHREACT parameters. In this example, we are doing this last, since the entire model will lie in the same zone. However, if we wanted to define different zones in the model, we would specify the TOUGHREACT parameters first.

TOUGHREACT solution parameters can be entered on the **Solution Parameters** dialog.

To open the **Solution Parameters** dialog:

1. On the **TOUGHREACT** menu, click **Solution Parameters**.
2. Select **Advanced** from the list on the left to display the **Advanced Options** pane. Under the Advanced Options, click **Print Porosity, Permeability, Capillary Pressure Changes**.
3. Next, select **Times and Convergence** from the list on the left to open the **Time Stepping and Convergence Options** pane.
4. In the **Max Iterations to Solve Geochemical System** box, type **300**.

5. In the **Relative Sorption Concentration Tolerance** box, type **1.0E-6**.
6. Click **OK** to exit the **Solution Parameters** dialog.

TOUGHREACT Output Options

TOUGHREACT output options can be changed on the **Output Options** dialog.

1. On the **TOUGHREACT** menu, click **Output Options**.
2. In the **Grid Block Output Frequency(s)** box, type **40**.
3. For **Aqueous Concentration Output**, select **Write Total Aqueous Component Concentrations**.
4. For **Aqueous Concentration Units**, select **mol/L Liquid**.
5. For **Mineral Abundance Units**, select **Change in Volume Fraction**.
6. Click **OK** to exit the **Output Options** dialog.

TOUGHREACT Chemical Components

TOUGHREACT chemical components can be specified in the Chemical Components dialog. To open the Chemical Components dialog:

1. On the **TOUGHREACT** menu, select **Chemical Components**.

To define the primary species:

1. In the list on the left of the **Chemical Components** dialog, select **Primary Species**.
2. In the **Thermodynamic Database** list in the middle of the dialog, select **h+**, **h2o**, **na+**, **skdd1**, **skdd2**, and **skdd3**.
3. Click the --> button to move the selected species into the **Current Simulation** list on the right, as shown in Figure 3.

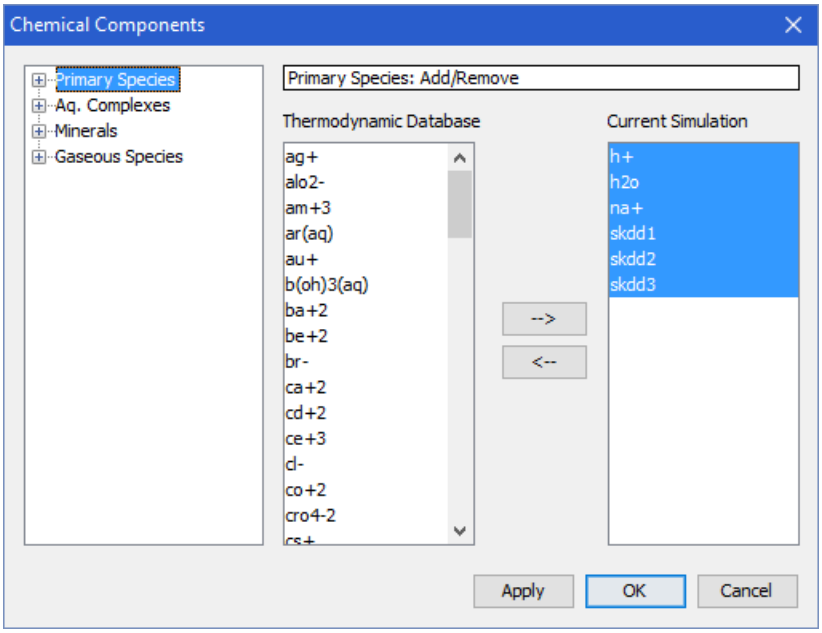

Figure 3: Primary Species

4. Click **Apply** to add the selected species to the analysis.

The parameters specific to each type can be viewed and changed by clicking on that type in the subtree under **Primary Species** in the list on the left.

To edit parameters for na+:

1. Click to expand the **Primary Species** list.
2. Click to select **na+**.
3. In the pane on the right, select **Output Concentration History at Selected Cells**. This will output additional data for cells that have previously been identified for printing time history data.

To edit parameters for skdd1:

1. Select **skdd1** in the list.
2. In the pane on the right, select **Output Concentration History at Selected Cells**.
3. Select **Enable Kd and Decay**.
4. In the **Decay Constant** box, type **0.0**.

To edit parameters for skdd2:

1. Select **skdd2** in the list.
2. In the pane on the right, select **Output Concentration History at Selected Cells**.
3. Select **Enable Kd and Decay**.
4. In the **Decay Constant** box, type **4.0113E-7**.

To edit parameters for skdd3:

1. Select **skdd3** in the list.
2. In the pane on the right, select **Output Concentration History at Selected Cells**.
3. Select **Enable Kd and Decay**.
4. In the **Decay Constant** box, type **4.0113E-7**.
5. Click **OK** to exit the **Chemical Components** dialog.

TOUGHREACT Zone Data

The next task is to create the zone data, which can be done in the **Geochemical Zones** dialog.

To open the **Geochemical Zones** dialog:

1. On the **TOUGHREACT** menu, click **Zone Data**. There will not be any zones in the model.

To create the initial water zone:

1. Select **Water (Initial)** in the list on the left.
2. Click **Add**.
3. In the **Create a New Zone** dialog, type **Water Zone** and click **OK**.
4. Click **Apply**.
5. In the list on the left, click + beside **Water (Initial)** to expand the subtree.
6. In the subtree under **Water (Initial)**, click **Water Zone** to display the zone parameters in to the right of the list.
7. Enter the data that is shown in Table 2.

Table 2: Water Zone Data

Species	Constraint	CGUESS	CTOT
h+	Amount (mol)	1.0e-7	1.0e-7
h20	Amount (mol)	1.0	1.0
na+	Amount (mol)	1.0e-10	1.0e-10
skdd1	Amount (mol)	1.0e-10	1.0e-10
skdd2	Amount (mol)	1.0e-10	1.0e-10
skdd3	Amount (mol)	1.0e-10	1.0e-10

To create the boundary water zone:

1. Select **Water (Boundary)** in the list on the left.
2. Click **Add**
3. In the **Create a New Zone** dialog, type **Water Boundary Zone** and click **OK**.
4. Click **Apply**.
5. In the list on the left, click + beside **Water (Boundary)** to expand the subtree.
6. In the subtree under **Water (Boundary)**, click **Water Boundary Zone** to display the zone parameters to the right of the list.
7. Enter the data that is shown in Table 3.

Table 3: Water Zone Data

Species	Constraint	CGUESS	CTOT
h+	Amount (mol)	1.0e-7	1.0e-7
h20	Amount (mol)	1.0	1.0
na+	Amount (mol)	1.0e-4	1.0e-4
skdd1	Amount (mol)	1.0e-4	1.0e-4
skdd2	Amount (mol)	1.0e-4	1.0e-4
skdd3	Amount (mol)	1.0e-4	1.0e-4

To create the permeability porosity zone:

1. Select **Permeability Porosity** in the list on the left.
2. Click **Add**.
3. In the **Create a New Zone** dialog, type **Perm/Por Zone** and click **OK**.
4. Click **Apply**.
5. In the list on the left, click + beside **Permeability Porosity** to expand the subtree.
6. In the subtree under **Permeability Porosity**, click **Perm/Por Zone** to display the zone parameters to the right of the list.
7. Select **Cubic Law**.

To create the linear Kd zone:

1. Select **Linear Kd** in the list on the left.
2. Click **Add**.
3. In the **Create a New Zone** dialog, type **Linear Kd Zone** and click **OK**.
4. Click **Apply**.
5. In the list on the left, click + beside **Linear Kd** to expand the subtree.
6. In the subtree under **Linear Kd**, click **Linear Kd Zone** to display the zone parameters to the right of the list.
7. For **skdd1** and **skdd3**, in the **Density** box, type **2.6** and in the **Kd** box, type **4.2735E-2** (Figure 4).
8. Click **OK** to exit the **Geochemical Zones** dialog.

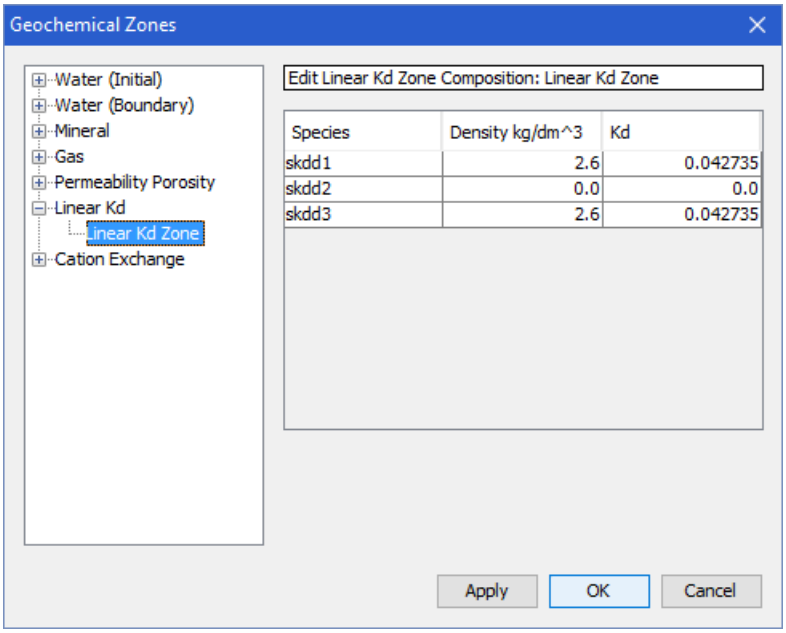

Figure 4: Linear Kd zone

Associate Zones with Mesh

The last task is to associate zones with the mesh. This can be done in two ways: by region or by cell. Initially the model is one layer with one region, but the default layer can be subdivided into more regions by using internal boundaries. This can be useful, since it is also possible to assign material data and initial conditions by region. In this case, the model will remain a single region.

We will associate the zones with the default region. The association will trickle down to the region's cells. To select the region and assign the Zones, in the **3D View**:

1. In the tree view, under the **Layers** subtree, select **Default**.
2. Under the **Edit** menu, click **Properties** to open the **Edit Layers** dialog.
3. Click the **Chemical Zones** tab.
4. Select **Set Zone Data**.
5. From the **Initial Water Zone**, **Boundary Water Zone**, **Permeability/Porosity Zone**, and **Linear Kd Zone** lists, select the respective zones that have previously been created.
6. Click **OK** to exit the **Edit Layers** dialog.

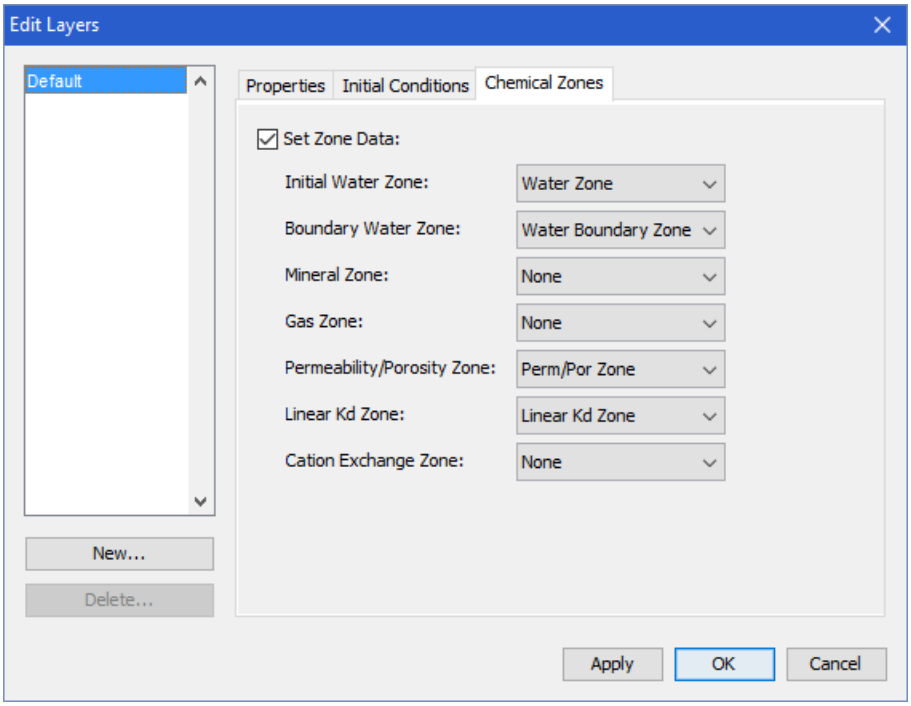

Figure 5: Associating the chemical zones with the mesh

Save and Run

The input is complete and you can run the simulation.

1. On the **File** menu, click **Save**.
2. To run the simulation: on the **Analysis** menu, click **Run T2react**.

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.
2. Because this is a 1-D model, the isosurfaces do not display the data well. To turn off the isosurfaces, clear the **Show Isosurfaces** checkbox.
1. To create a slice plane with contours, click **Slice Planes**.
2. In the **Axis** list, select **Y**.
3. In the **Coord** box, type **.5**.
4. Click **Close** to close the **Slice Planes** dialog.

To view 3D results, as shown in Figure 6:

1. In the **Time(s)** list, select **4.32E06**.
2. In the **Scalar** list, select **na+**.
3. Click the **Front View** for a good viewing perspective.

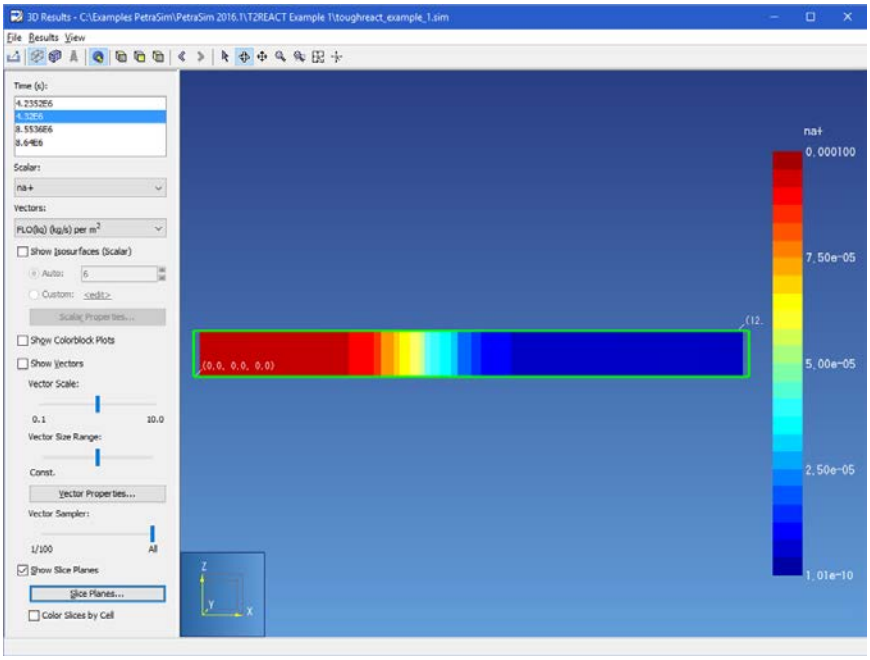

Figure 6: 3D Results

View Cell History Plots

You can view time history plots with the **Cell Time History** dialog:

1. On the **Results** menu, click **Cell History Plots**

The **Cell Time History** dialog will be displayed. In this window, you can display time history data using a plotting parameter and a list of cells. For example, to view the **na+** time history for the Center cell, as shown in Figure 7:

1. In the **Variable** list, select **na+**.
2. In the **Cell Name (Id#)** list, select **Center**.

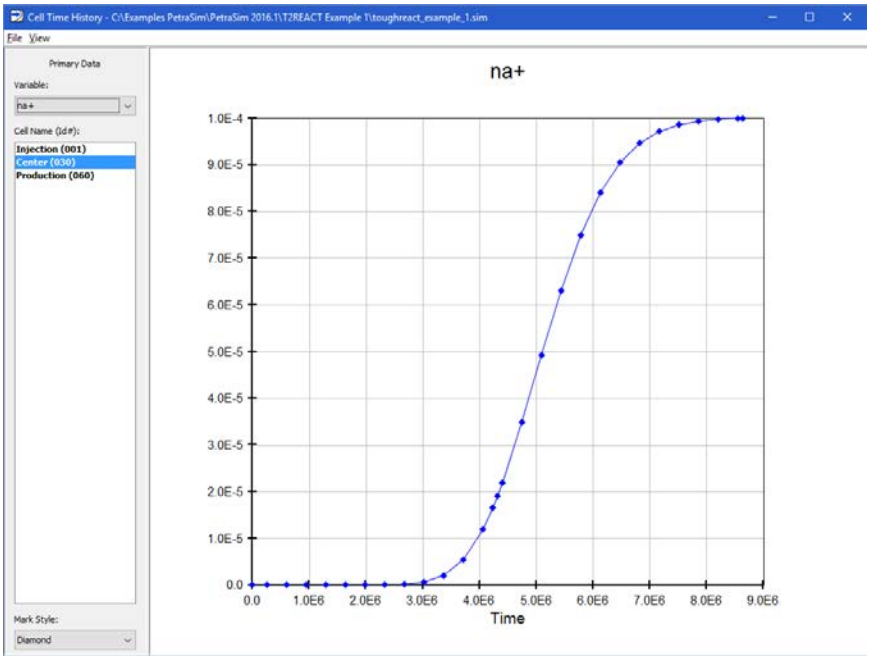

Figure 7: Cell History

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