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TOUGHREACT Example:
CO2 Disposal in Deep Saline Aquifers

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**.

CO2 Disposal in Deep Saline Aquifers (ECO2N)

Description

This problem is example five in the TOUGHREACT manual. It is a 1-D radial problem in which CO2 is injected into a well field 100 m in depth and extending with a 100,000 m radius. CO2 is injected at a rate of 90 kg/s, which is approximately equivalent to that generated by a 300 MW coal-fired power plant. The CO2 injection continues for 100 years. This problem demonstrates the restart feature to run for an additional 900 years with no additional CO2 injection.

Entering all the parameters for the geochemical system in this example problem can be time-intensive. A partially completed PetraSim file (**geochem_basic.sim**) containing only the parameters for chemical components can be found in the resources archive on the PetraSim support website. If this file is opened, the example problem can be continued from the section **Create the Model Boundary**. The web site also contains completed PetraSim files for both parts of this problem (**co2_disposal_p1** and **co2_disposal_p2**).

Create the TOUGHREACT model

We first will create a new model using TOUGHREACT and ECO2N 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 **ECO2N.**
4. Click **OK** to create the new model.

We will edit the geometry of the model later. For now we will focus on the geochemical problem description.

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 2** and then a subfolder **Part 1**. In the **File Name** box, type **co2_disposal_p1.sim**.
3. Click **Save.**

Global Properties

We will first define all material and chemical properties, beginning by defining analysis options related to the equation of state (ECO2N).

To edit global properties:

1. On the **Properties** menu, click **Global Properties.**
2. Click the **Analysis** tab.
3. In the **Name** box, type **CO2 Injection**.
4. Click the **EOS** tab.
5. Select **Isothermal**.
6. In the **Brine Density in CO2** box, select **Independent**.
7. Click **OK** to exit the **Global Properties** dialog.

Material Properties

We next define the material properties. Since this problem uses only one material, we will simply modify the default material.

Material Data

1. On the **Properties** menu, click **Edit Materials.**
2. In the **Name** box, type **SAND**.
3. In the **Porosity** box, type **0.3**.
4. In the three (x, y, and z) permeability boxes, type **1.0E-13**.
5. In the **Wet Heat Conductivity** box, type **2.51**.
6. In the **Specific Heat** box, type **920**.

Relative Permeability

1. Click **Additional Material Data** to open the **Additional Material Data** dialog.
2. Click the **Relative Perm** tab.
3. In the **Relative Permeability** list, select **van Genuchten-Mualem Model**.
4. In the **RP(1)** box, type 0.457.
5. In the **Slr** box, type **0.3**.
6. In the **Sls** box, type **1.0**.
7. In the **Sgr** box, type **0.05**.

Capillary Pressure

1. Click the **Capillary Press** tab.

2. In the **Capillary Pressure** list, select **van Genuchten Function**.
3. In the **CP1(1)** box, type **0.457**.
4. In the **Slr** box, type **0.0**.
5. In the **1/P0** box, type **5.1E-5**.
6. In the **Pmax** box, type **1.0E7**.
7. In the **Sls** box, type **0.999**.

Miscellaneous

1. Click the **Misc** tab.
2. In the **Pore Compressibility** box, type **4.5E-10**.
3. Click **OK** to exit the **Additional Material Data** dialog.
4. Click **OK** again to exit the **Material Data** dialog.

Initial Conditions

To open the **Default Initial Conditions** dialog:

1. On the **Properties** menu, click **Initial Conditions.**
2. In the dropdown box, select **Two Fluid Phases (P, Xsm, Sg, T)**.
3. In the **Pressure** box, type **2.0E7**.
4. In the **Temperature** box, type **75.0**.
5. In the **Gas Saturation** box, type **0.0**.
6. In the **Salt Mass Fraction** box, type **0.06**.
7. Click **OK** to exit the **Default Initial Conditions** dialog.

TOUGHREACT Solution Parameters

TOUGHREACT solution parameters can be set in the **Solution Parameters** dialog. To open the **Solution Parameters** dialog:

1. On the **TOUGHREACT** menu, click **Solution Parameters**.

Click **Standard**.

1. Click to select **Enable Gaseous Species Transport**.

Click **Advanced**.

1. Click to clear **Ignore Mineral Dissolution/Precipitation Effects on Flow**.
2. Under **Effect of CO2 and H2O Reactions on Flow**, click to select **CO2 and H2O**.

Click **Validation**.

1. In the **Max Stochiometric Ionic Strength** box, type **6.0**.

Click **Times and Convergence**.

1. In the **Relative Transport Concentration Tolerance**, type **1.0E-6**.
2. In the **Relative Sorption Concentration Tolerance**, type **1.0E-6**.

Click **Diffusion Coefficients**.

1. In the **Aqueous Species Diffusion Coefficient** box, type **1.0E-9**.
2. In the **Gaseous Species Diffusion Coefficient** box, select **User Defined** and type 1.1E-5.
3. Click **OK** to exit the **Solver Parameters** dialog.

TOUGHREACT Output Parameters

TOUGHREACT output parameters can be set in the **Output Options** dialog. To open the **Output Options** dialog:

1. On the **TOUGHREACT** menu, click **Output Options.**
2. Under **Aqueous Concentration Output**, select **Write Total Aqueous Component Concentrations**.
3. Under **Mineral Abundance Units**, select **Change in Volume Fraction**.
4. 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**.

The thermodynamic database contains the master list of chemical components. To use a species (of any type), we first add the species to the simulation, then configure the simulation-specific properties for that species.

Primary Species

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 **alo2-**, **ca+2**, **cl-**, **fe+2**, **h+**, **h2o**, **hco3-**, **k+**, **mg+2**, **na+**, **o2(aq)**, **sio2(aq)**, and **so4-2**.
3. Click the --> button to move the selected species into the **Current Simulation** list on the right.
4. Click **Apply** to add the selected species to the analysis.

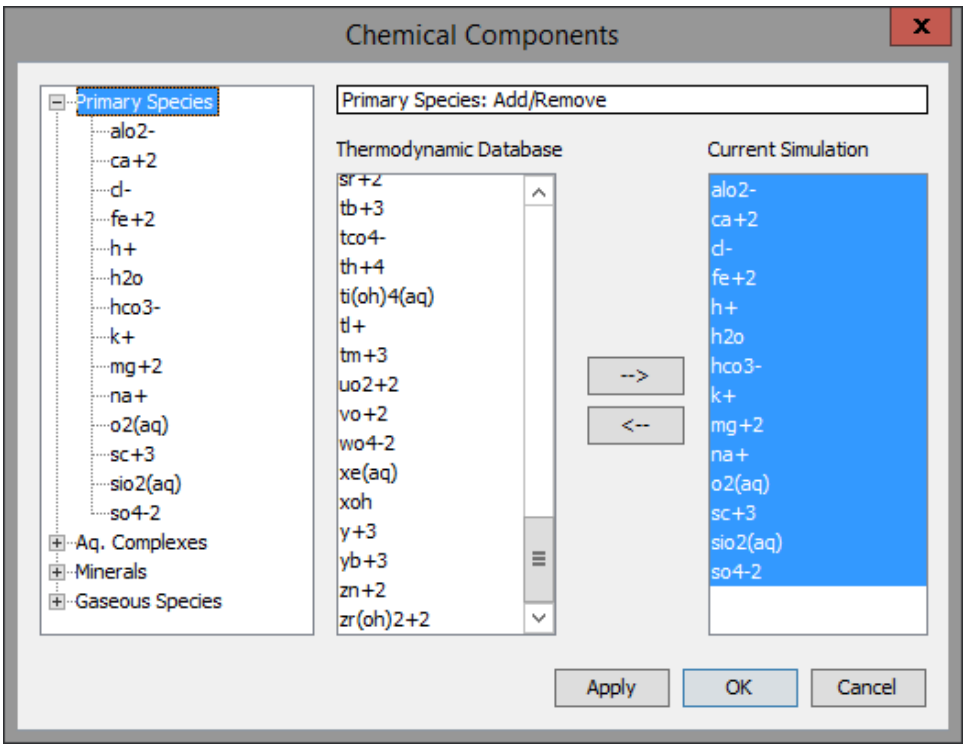

Figure 1: Primary Species

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. For this simulation, there is no need to edit any additional parameters.

Aqueous Complexes

A similar process is used to define the aqueous complexes:

1. In the list on the left of the **Chemical Components** dialog, select **Aq. Complexes**.
2. Click **Select Species Individually**.
3. In the **Thermodynamic Database** list in the middle of the dialog, select **acetic~acid(aq)**, **al(oh)2+**, **al(oh)3(aq)**, **al+3**, **aloh+2**, **cacl+**, **cacl2(aq)**, **caco3(aq)**, **cahco3+**, **caoh+**, **caso4(aq)**, **ch4(aq)**, **co2(aq)**, **co3-2**, **fe+3**, **fecl+**, **fecl4-2**, **feco3(aq)**, **fehco3+**, **h2(aq)**, **h2s(aq)**, **h3sio4-**, **halo2(aq)**, **hs-**, **hso3-**, **kcl(aq)**, **kso4-**, **mgcl+**, **mghco3+**, **mgso4(aq)**, **naalo2(aq)**, **nacl(aq)**, **naco3-**, **nahco3(aq)**, **nahsio3(aq)**, **naoh(aq)**, **naso4-**, **oh-**, and **so2(aq)**.
4. Click the --> button to move the selected species into the **Current Simulation** list on the right.
5. Click **Apply** to add the selected species to the analysis.

Minerals

A similar process is used to define the minerals:

1. In the List on the left of the **Chemical Components** dialog, select **Minerals**.

2. In the **Thermodynamic Database** in the middle of the dialog, select **albite~low**, **ankerite-2**, **calcite**, **chlorite**, **dawsonite**, **dolomite-2**, **hematite**, **illite**, **k-feldspar**, **kaolinite**, **magnesite**, **oligoclase**, **pyrite-2**, **quartz**, **siderite-2**, **smectite-ca**, and **smectite-na**.
3. Click the --> button to move the selected species into the **Current Simulation** list on the right.
4. Click **Apply** to add the selected minerals to the analysis.

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

Each mineral has unique dissolution, precipitation, and additional mechanisms properties. The values for each of these properties for each mineral are shown in Table 1 and Table 2. Pyrite is a bit different than the other minerals and its properties are shown in Table 3 and Table 4. This section will demonstrate how to specify the properties for **albite~low**, then you should be able to enter the remaining mineral properties by following the same pattern and referring to the tables.

Please note, if table entries are blank, then those parameters should not be set. The mineral **calcite** is considered to be at equilibrium and no parameters for dissolution, precipitation, or additional mechanisms should be specified. The mineral **quartz** has no additional mechanisms. Several minerals have only 1 additional mechanism. There is no table column for **Initial Volume Fraction**, as all minerals should be given the same value for that parameter, *1.0e-6*.

Select **albite~low** in the list under **Minerals**.

To edit dissolution rate parameters for **albite~low**:

1. Under **Specify Kinetic Constraints**, click to select **Dissolution**.
2. Click **Edit.** This will open the **Edit dissolution Rate Parameters** dialog.
3. In the **Activation Energy – EA** box, type **69.8** (from Table 1).
4. In the **Rate Constant k25** box, type **2.7542e-13** (from Table 1).
5. Click **OK** to save changes and exit the **Edit Dissolution Rate Parameters** dialog.

To edit precipitation rate parameters for **albite~low**:

1. Under **Specify Kinetic Constraints**, click to select **Precipitation**.
2. Click **Edit**. This will open the **Edit Precipitation Rate Parameters** dialog.
3. On the **Options** tab, in the **Initial Volume Fraction** box, type **1.0e-6**.
4. Click the **Energy** tab.
5. In the **Activation Energy – EA** box, type **69.8** (from Table 1).
6. In the **Rate Constant k25** box, type **2.7542e-13** (from Table 1).
7. Click **OK** to save changes and exit the **Edit Dissolution Rate Parameters** dialog.

To add additional mechanisms for **albite~low**:

1. Under **Rate Constant Dependence on pH**, click to select **Specify Additional Mechanisms**.
2. Click **Edit**. This will open the **Edit Additional Mechanisms** dialog.

3. Click **New**. This will create **Mechanism (1)**.
4. In the **Rate Constant** box, type **6.9183e-11** (from Table 2).
5. In the **Activation Energy** box, type **65.0** (from Table 2).
6. In the table, in the **Species** list, select **h+** (from Table 2).
7. In the table, in the **Exponent** box, type **0.457** (from Table 2).
8. Click **Apply** to save the changes to **Mechanism (1)**.
9. Click **New**. This will create **Mechanism (2)**.
10. In the **Rate Constant** box, type **2.5119e-16** (from Table 2).
11. In the **Activation Energy** box, type **71.0** (from Table 2).
12. In the table, in the **Species** list, select **h+** (from Table 2).
13. In the table, in the **Exponent** box, type **-0.572** (from Table 2).
14. Click **OK** to save changes and exit the **Edit Dissolution Rate Parameters** dialog.

All other selected minerals should be edited in this fashion, using the values shown in Table 1 and Table 2. Data for **pyrite-2** can be found in Table 3 and Table 4. Empty table cells indicate that the existing data is already correct and that new data need not be entered (i.e. if there is no entry for a particular option, do not enable that option).

Table 1: Dissolution and Precipitation Data for Minerals

Mineral	Initial Vol Frac	Activation Energy	Rate Constant k25
albite~low	1e-6	69.8	2.7542E-13
ankerite-2	1e-6	62.76	1.2598E-09
calcite	1e-6		
chlorite	1e-6	88	3.0200E-13
dawsonite	1e-6	62.76	1.2598E-09
dolomite-2	1e-6	52.2	2.9512E-08
hematite	1e-6	66.2	2.5119E-15
illite	1e-6	35	1.6596E-13
k-feldspar	1e-6	38	3.8905E-13
kaolinite	1e-6	22.2	6.9183E-14
magnesite	1e-6	23.5	4.5709E-10
oligoclase	1e-6	69.8	1.4454E-13
quartz	1e-6	87.7	1.0233E-14
siderite-2	1e-6	62.76	1.2598E-09
smectite-ca	1e-6	35	1.6596E-13
smectite-na	1e-6	35	1.6596E-13

Table 2: Additional Mechanism Data for Minerals

	Mechanism(1)			Mechanism(2)		
Mineral	**Rate Constant**	**Activation Energy**	**n(H+) Exponent**	**Rate Constant**	**Activation Energy**	**n(H+) Exponent**
albite~low	6.9183E-11	65.0	0.457	2.5119E-16	71.0	-0.572
ankerite-2	6.4565E-04	36.1	0.500			
calcite						
chlorite	7.7624E-12	88.0	0.500			
dawsonite	6.4565E-04	36.1	0.500			
dolomite-2	6.4565E-04	36.1	0.500			
hematite	4.0738E-10	66.2	1.000			
illite	1.0471E-11	23.6	0.340	3.0200E-17	58.9	-0.400
k-feldspar	8.7096E-11	51.7	0.500	6.3096E-22	94.1	-0.823
kaolinite	4.8978E-12	65.9	0.777	8.9125E-18	17.9	-0.472
magnesite	4.1687E-07	14.4	1.000			
oligoclase	2.1380E-11	65.0	0.457			
quartz						
siderite-2	6.4565E-04	36.1	0.500			
smectite-ca	1.0471E-11	23.6	0.340	3.0200E-17	58.9	-0.400
smectite-na	1.0471E-11	23.6	0.340	3.0200E-17	58.9	-0.400

Table 3: Dissolution and Precipitation Data for pyrite-2

	Dissolution		Precipitation		
Mineral	**Activation Energy**	**Rate Constant k25**	**Initial Vol Frac**	**Activation Energy**	**Rate Constant k25**
pyrite-2	0.0	0.0	1e-6	56.9	4.0000e-11

Table 4: Additional Mechanism Data for pyrite-2

	Mechanism(1)			Mechanism(2)		
Mineral	**Rate Constant**	**Activation Energy**	**Exponent**	**Rate Constant**	**Activation Energy**	**Exponent**
pyrite-2	3.0200e-8	56.9	[h+, -0.5] [fe+3, 0.5]	2.8184e-5	56.9	[o2(aq), 0.5]

To save these changes: click **Apply**.

Gaseous Species

1. In the list on the left of the **Chemical Components** dialog, select **Gaseous Species**.
2. In the **Thermodynamic Database** list in the middle of the dialog, select **co2(g)**.
3. Click the --> button to move co2(g) into the **Current Simulation** list on the right.
4. Click **Apply** to add the selected species to the analysis.
5. Click **OK** to exit the **Chemical Components** dialog.

TOUGHREACT Zone Data

Geochemical zones describe the initial chemical composition of the model. You can define geochemical zones using the **Geochemical Zones** dialog. To open the **Geochemical Zones** dialog:

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

To create the 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 to the right of the list.
7. Edit each cell in the table, setting the **Constraint**, **CGUESS**, and **CTOT** values for each species as shown in Table 5.

Table 5: Water (Initial) Zone

Species	Constraint	CGUESS	CTOT
alo2-	Amount (mol)	1.078E-08	1.361E-08
ca+2	Amount (mol)	4.479E-03	4.737E-03
cl-	Amount (mol)	0.9109	1.001
fe+2	Amount (mol)	2.615E-07	3.022E-07
h+	Amount (mol)	8.48E-08	0.0432
h2o	Amount (mol)	1	1
hco3-	Amount (mol)	1.841E-03	4.562E-02
k+	Amount (mol)	5.805E-03	5.980E-03
mg+2	Amount (mol)	2.348E-05	2.669E-05
na+	Amount (mol)	0.9006	0.9905
o2(aq)	Amount (mol)	2.763E-66	-8.646E-02
sio2(aq)	Amount (mol)	9.203E-04	1.034E-03
so4-2	Amount (mol)	1.443E-16	1.324E-09

8. Click **Apply**.

To create the mineral zone:

1. Select **Mineral** in the list on the left.
2. Click **Add**.
3. In the **Create a New Zone** dialog, type **Mineral Zone** and click **OK**.
4. Click **Apply**.
5. In the list on the left, click + beside **Mineral** to expand the subtree.

6. In the subtree under **Mineral**, click **Mineral Zone** to display the zone parameters to the right of the list.
7. Edit each cell in the table, setting the **Vol. Fraction**, **Grain Radius**, **Surface Area**, and **Units** values for each mineral as shown in Table 6.

Table 6: Mineral Zone

Mineral	Vol. Fraction	Grain Radius	Surface Area	Units
albite~low	0	0.001	9.8	cm^2/g mineral
ankerite-2	0	0.001	9.8	cm^2/g mineral
calcite	0.01929			
chlorite	0.04556	0.001	9.8	cm^2/g mineral
dawsonite	0	0.001	9.8	cm^2/g mineral
dolomite-2	0	0.001	9.8	cm^2/g mineral
hematite	0.00497	0.001	12.87	cm^2/g mineral
illite	0.00954	0.001	151.63	cm^2/g mineral
k-feldspar	0.08179	0.001	9.8	cm^2/g mineral
kaolinite	0.02015	0.001	151.63	cm^2/g mineral
magnesite	0	0.001	9.8	cm^2/g mineral
oligoclase	0.19795	0.001	9.8	cm^2/g mineral
pyrite-2	0	0.001	12.87	cm^2/g mineral
quartz	0.57888	0.001	9.8	cm^2/g mineral
siderite-2	0	0.001	9.8	cm^2/g mineral
smectite-ca	0	0.001	151.63	cm^2/g mineral
smectite-na	0.03897	0.001	151.63	cm^2/g mineral

8. Click **Apply**.

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-Poro 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-Pore Zone** to display the zone parameters to the right of the list.
7. For **Permeability Law**, select **Cubic Law**.
8. Click **Apply**.
9. Click **OK** to exit the **Geochemical Zones** dialog.

Saving the Geochemical Data File as a Starting Point for a New Analysis

All of the problem data that is not specific to a particular geometry and loading condition has now been defined. At this point, save the data by clicking **Save As** on the **File** menu, and typing **geochem_basic.sim** as the file name. We can now open geochemical data and click **Save As** on the **File** menu, giving the new name as **co2_disposal_p1.sim**. Anytime you want to create a model that uses the same (or similar)

geochemical data, you can open the **geochem_basic.sim** file and save it as a different file as a starting point for a different analysis. In this manner you can avoid repeating all the data input.

In continuing this example, model specific data will now be entered and simulated.

Create the Model Boundary

To create the boundary for this model, use the **Edit Boundary** dialog. To create the model boundary:

1. On the **Model** menu, click **Edit Boundary.**
2. Click the **Quick Set Min/Max** button ( ) from the toolbar to open the **Set Boundary** dialog.
3. Enter the values from Table 7.
4. Click **OK** to close the **Set Boundary** dialog and preview the new model boundary.
5. Click **OK** to close the **Edit Boundary** dialog and commit the changes.

Table 7: Model Boundary Dimensions

Axis	Min (m)	Max (m)
X	0.0	1E5
Y	0.0	1.0

Edit the Default Layer

We will now set the Z bounds of the default layer. Under the **Model** menu, select **Edit Layers** to open the **Edit Layers** dialog:

1. Select the default layer from the list on the left.
2. For the **Top**, enter **0**.
3. For the **Base**, enter **-100**.
4. Click **OK** to commit the changes and close the **Edit Layers** dialog.

To make this model easier to visualize, we will change the view scale.

1. On the **View** menu, click **Scale Axes**.
2. For the **X Factor**, enter **.005**.
3. For the **Y Factor**, enter **100.0**.
4. Click **OK** to set the view scale. The model should now appear as shown in Figure 2.

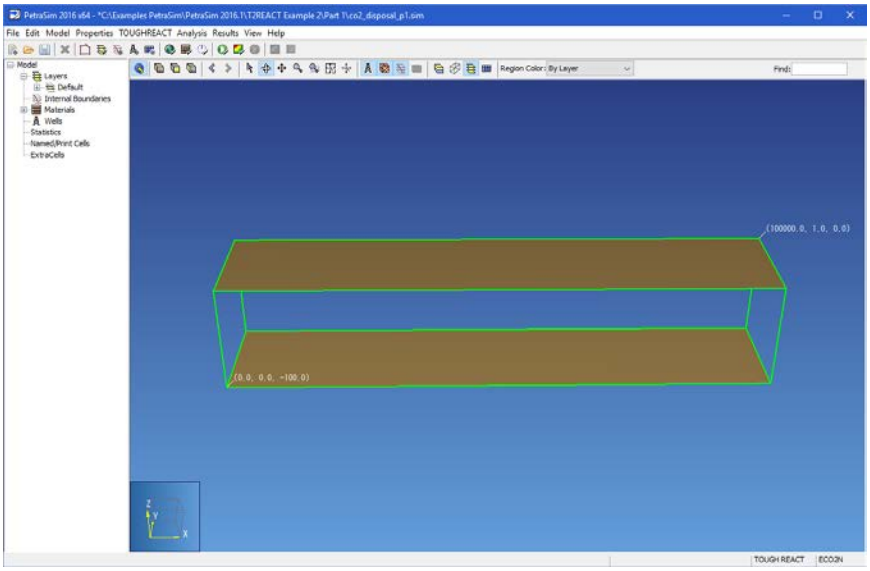

Figure 2: Model after applying view scale.

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. For the **Mesh Type**, select **Radial**.
3. For the **Divisions**, select **Regular.**
4. In the **Radial Cells** box, type **100**.
5. In the **Factor** box, type **1.1096251**.
6. Click **OK** to create the mesh.

This 100 mesh grid used here is different than the 130 cell meshmaker mesh used in the example problem write-up from the TOUGHREACT user's manual. The style of the mesh used in TOUGHREACT user's manual would require a logarithmic capability in PetraSim's meshmaker mesh creator that is currently not supported. The 100 cell logarithmic mesh used in this example problem appears to be sufficient based on a sensitivity analysis (Figure 3) of the Sg parameter after 100 years of simulation with different mesh sizes.

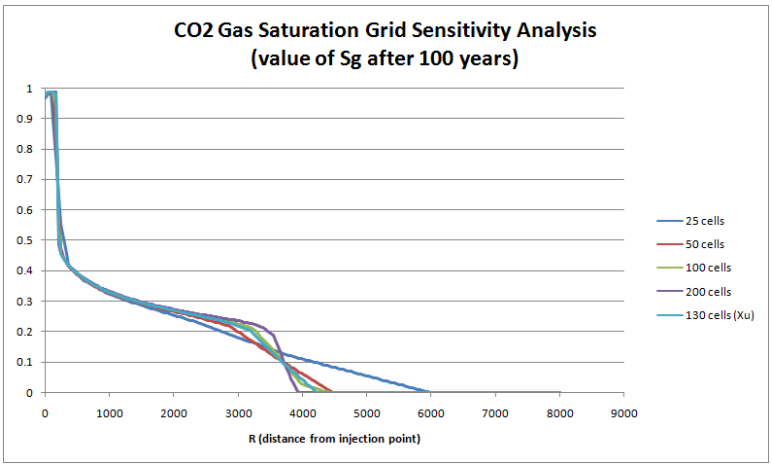

Figure 3: CO2 Injection

To use a 200 cell mesh, change the value of the **Radial Cells** parameter to 200 and the value of the **Factor** parameter to **1.04950055**. The running time of this simulation is linear in the number of cells. It takes approximately 10 minutes to run the first 100 years of the simulation with 100 cells. This time would be doubled for 200 years.

Define Boundary Conditions

To edit cells, you can use the **3D View**. In this case, we will use the **3D View** to define boundary conditions in the model.

In this model, CO2 is injected into the center at 90 kg/s. Since this is an RZ grid, the center cell is the min X cell (far left). Since this is an isothermal simulation, it will not be necessary to specify an enthalpy for the injected CO2 - we will leave this value at 0.0.

To select and edit the injection cell:

1. In the **Find** box, type **1**, then press **Enter**. Cell 1 will be selected and centered in the **3D View**.
2. On the **Edit** menu, click **Properties**. This will open the **Edit Cell Data** dialog.

To specify the properties for the injection cell:

1. In the **Cell Name** box, type **Injection**.
2. Click the **Sources/Sinks** tab.
3. Under **Injection**, click to select **CO2**.
4. In the **Rate** box, type **90**.
5. Click the **Print Options** tab.
6. Click **Print Time Dependent Flow and Generation (BC) Data**.
7. Click **OK** to close the **Edit Cell Data** 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.

1. On the **Analysis** menu, click **Solution Controls**.

Times

1. In the **Solution Controls** dialog, click the **Times** tab.
2. In the **End Time** box, type **100 years**.
3. In the **Time Step** box, type **1**.
4. In the **Max Num Time Steps** list, click **Infinite**.
5. In the **Max Time Step** list, select **User Defined**.
6. In the **Max Time Step** box, type **30 days**.

Solver

1. Click the **Solver** tab.
2. For the **Conjugate Gradient Solvers**, select **Stabilized Bi-Conjugate Gradient**.
3. In the **Max CG Iterations (Frac. Of Eqns.)** box, type **0.8**.
4. In the **CG Convergence Criterion** box, type **1e-7**.
5. Click **OK** to exit the **Solution Parameters** 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 **9999** (we will specify specific output times).

To specify specific 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 **3.15576E7**, **3.15576E8**, **1.57788E9**, **3.15576E9**, **1.57788E10**, **3.15576E10**, **6.31152E10**, and **1.57788E11**.
3. Click **OK** to exit the **Additional Print Times** dialog.
4. Click **OK** to exit the **Output Controls** dialog.

Associate Zones with Mesh

The last task is to associate zones with the mesh. This can be done in two ways, either by region or for individual cells. Initially the model is one region, but it 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 and we will specify zones for the entire domain.

To specify zone data:

1. In the **Tree View** at the left, under **Layers**, under the **Default** layer, click to select the **Default** region as shown in Figure 4.
2. Under the **Edit** menu, click **Properties** to open the **Edit Region Data** dialog.
3. Click the **Chemical Zones** tab.
4. Select **Set Zone Data**.
5. From the **Initial Water Zone**, **Mineral Zone**, and **Permeability/Porosity Zone** lists, select the respective zones that have previously been created.
6. Click **OK** to exit the **Edit Region Data** dialog.

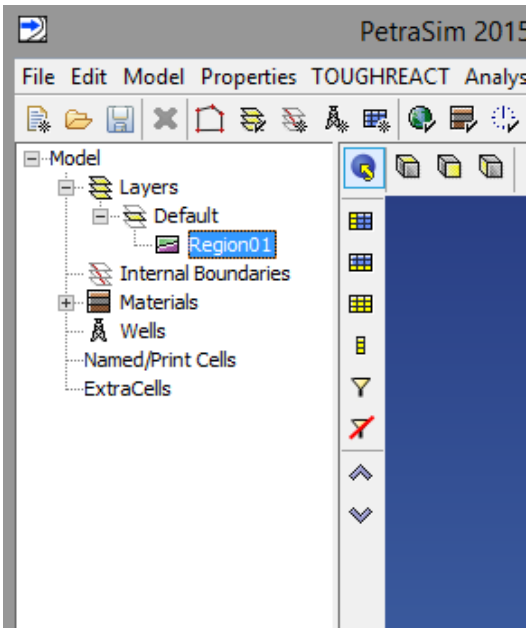

Figure 4: Selecting a region in the Tree View

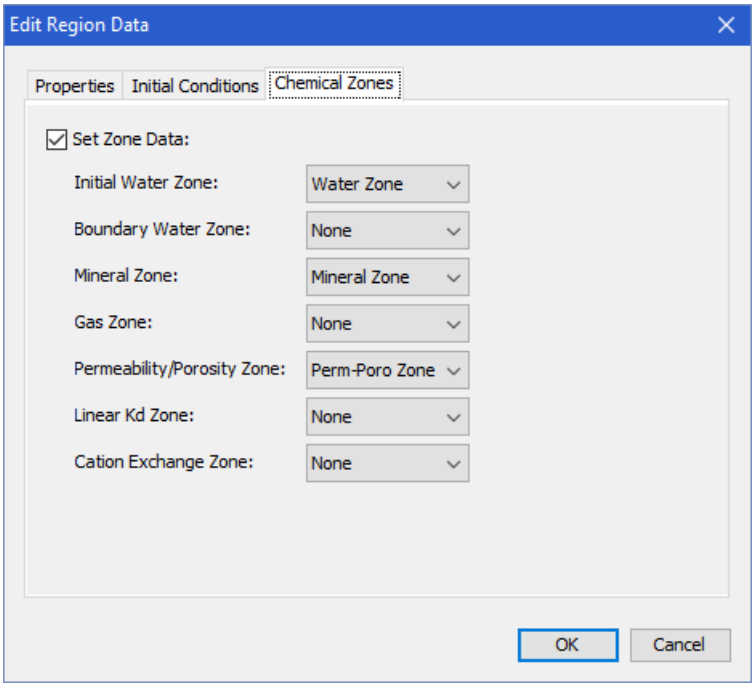

Figure 5: Zones Associated with Mesh

Save and Run

The input is complete and you can run the simulation. To retain the geochemical data as a reusable starting point, save this model as a different file in a separate directory. For example:

1. To run the simulation: on the **Analysis** menu, click **Run T2REACT**.

View Results

The best way to view results for this problem is to use the **Line Plot** feature in PetraSim. Line plots allow us to view the data in 2D as a function of distance from a point. In this case, we will view the data as it radiates from the center of the model (as a function of R). Line plots are available in the **3D Results** view.

To create a line plot:

1. On the **Results** menu, click **3D Results**.
2. In the **3D Results** view, on the **File** menu, click **Line Plot**.
3. In the **Line Plot** dialog, enter the following two points: Point1=**(0.0, 0.5, -50)**, Point2=**(8000, 0.5, -50)**, then click **OK**.

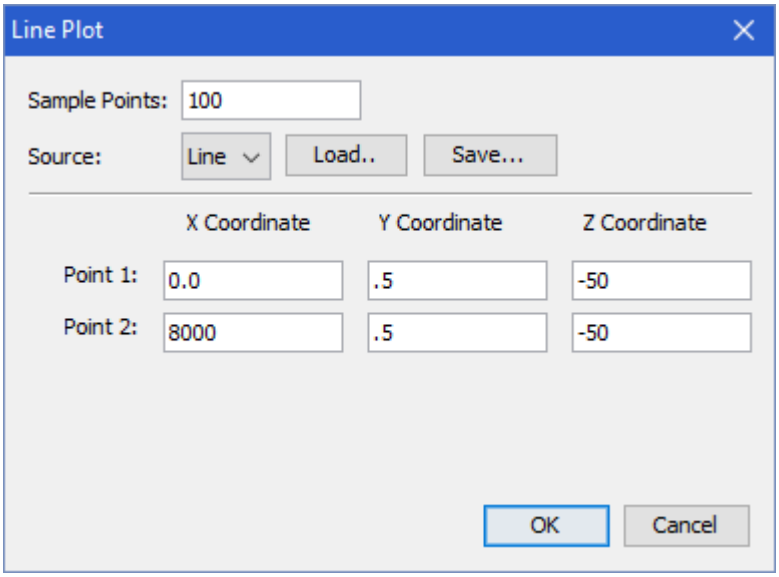

Figure 6: Preparing a Line Plot

In the **Line Plot** dialog, to show CO2 saturation (Sg):

1. In the **Variable** list, select **SG**.
2. In the **Time** list, select **3.1557E9**.

This result is shown in Figure 7.

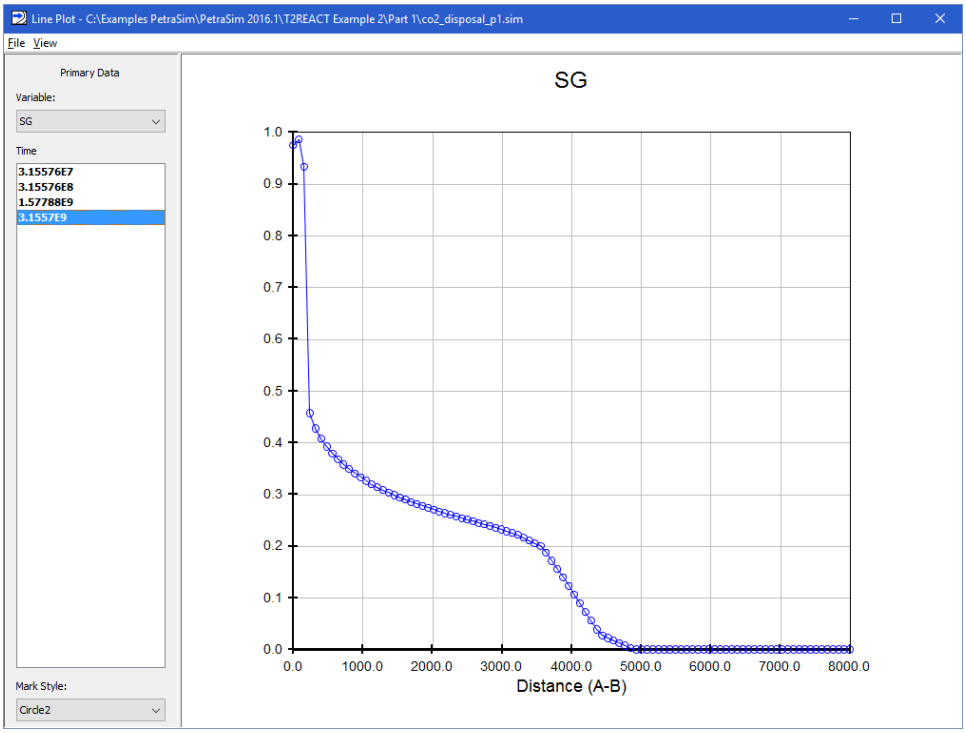

Figure 7: Line Plot of CO2 Saturation (SG)

The Continuation Run (Restart)

During the first part of this simulation, we injected 90 kg/s of CO2 into the aquifer for 100 years. During the second part, we will stop injecting CO2 and monitor the aquifer out to 1,000 years. Before proceeding, create a second folder on your computer for the restart run - otherwise the continuation run will overwrite the results from the first run.

1. On the **File** menu, click **Save As**.
2. Create a new folder named **Part 2**. Move to that folder.
3. In the **File Name** box, type **co2_disposal_p2.sim**.
4. Click **Save**.

Next, turn off the CO2 injection.

1. In the **Find** box, type **1**, then press **Enter**. Cell 1 will be selected and centered in the **3D View**.
2. On the **Edit** menu, click **Properties**. This will open the **Edit Cell Data** dialog.
3. Click the **Sources/Sinks** tab.
4. Under **Injection**, click to clear **CO2**.
5. Click **OK** to exit the **Edit Cell Data** dialog.

Add Restart Data

We will use the initial conditions and geochemical data from the end of the previous simulation, to start the continuation run. To enable the simulation restart feature:

1. On the **TOUGHREACT** menu, click **Restart Options.**
2. In the **Restart Options** dialog, click to enable **Activate Simulation Restart**.
3. For **Initial Conditions (SAVE)**, click **Browse** and select the SAVE file from the previous run.
4. For **Geochem Data (savechem)**, click **Browse** and select the savechem file from the previous run.
5. Click **OK**, to save changes and close the **Restart Options** dialog.

Set a New End Time

To specify the new 1,000 year end time for the simulation:

1. On the **Analysis** menu, click **Solution Controls**.
2. In the **Solution Controls** dialog, in the **End Time** box, type **1000 yrs**.
3. Click **OK**, to save changes and close the **Solution Controls** dialog.

Start the Continuation Run

On the **Analysis** menu, click **Run T2React**.

View Results

To look at the total amount of sequestered CO2 after 1,000 years, we can create another line plot.

To create a line plot:

1. On the **Results** menu, click **3D Results**.
2. In the **3D Results** view, on the **File** menu, click **Line Plot…**.
3. In the **Line Plot** dialog, enter the following two points: Point1=**(0.0, .5, -50)**, Point2=(**8000, 0.5, -50)**, then click **OK**.

In the **Line Plot** dialog, to show total CO2 sequestered in minerals (SMco2):

1. In the **Variable** list, select **SMco2**.
2. In the **Time** list, select **3.1557E10**.

This result is shown in Figure 8.

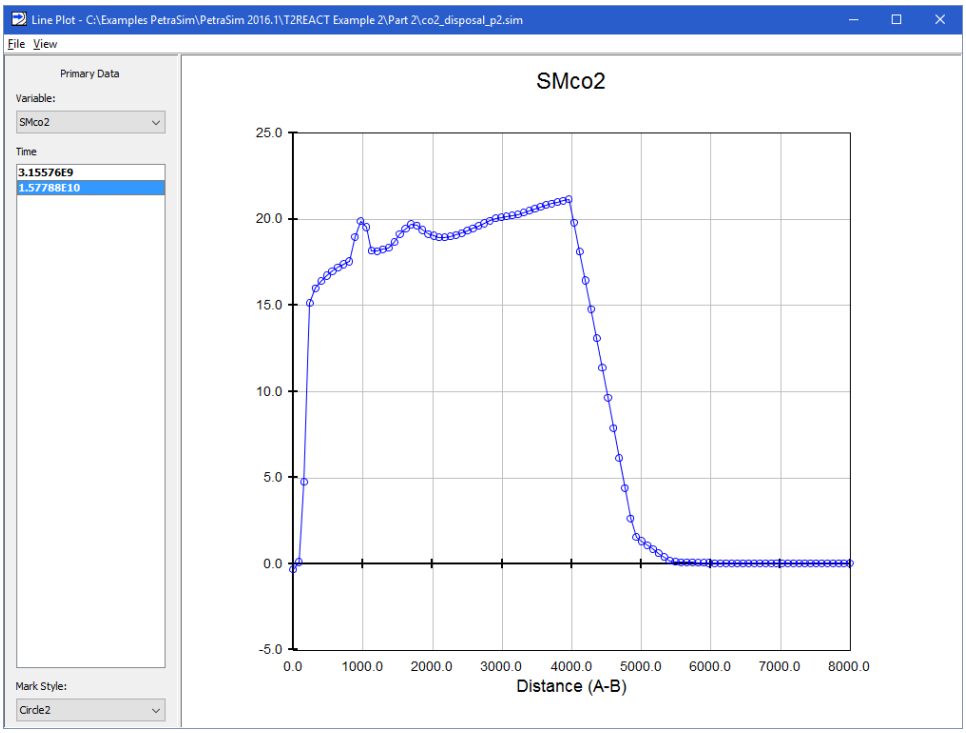

Figure 8: Line Plot of Total CO2 Sequestered in Minerals (SMco2)

You can also look at the mineral abundance as a function of x (R), using the **Line Plot** dialog.

References

1. **Xu, Tianfu, et al.** *TOUGHREACT User's Guide: A Simulation Program for Non-isothermal Multiphase Reactive Geochemical Transport in Variably Saturated Geologic Media.* Berkeley, CA, USA : Earth Sciences Division, Lawrence Berkeley National Laboratory, September 2004. LBNL-55460.

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.

3. **Pruess, Karsten and Garcia, J.** *Solutions of Test Problems for Disposal of CO2 in Saline Aquifers.* Berkeley, CA, USA : Earth Sciences Division, Lawrence Berkeley National Laboratory, December 2002. LBNL-51812.

4. **Pruess, Karsten, et al.** *Intercomparison of Numerical Simulation Codes for Geologic Disposal of CO2.* Berkeley, CA, USA : Earth Sciences Division, Lawrence Berkeley National Laboratory, December 2002. LBNL-51813.

5. **Pruess, Karsten.** *A TOUGH2 Fluid Property Module for Mixtures of Water, NaCl, and CO2.* Berkeley, CA, USA : Earth Sciences Division, Lawrence Berkeley National Laboratory, August 2005. LBNL-57952.