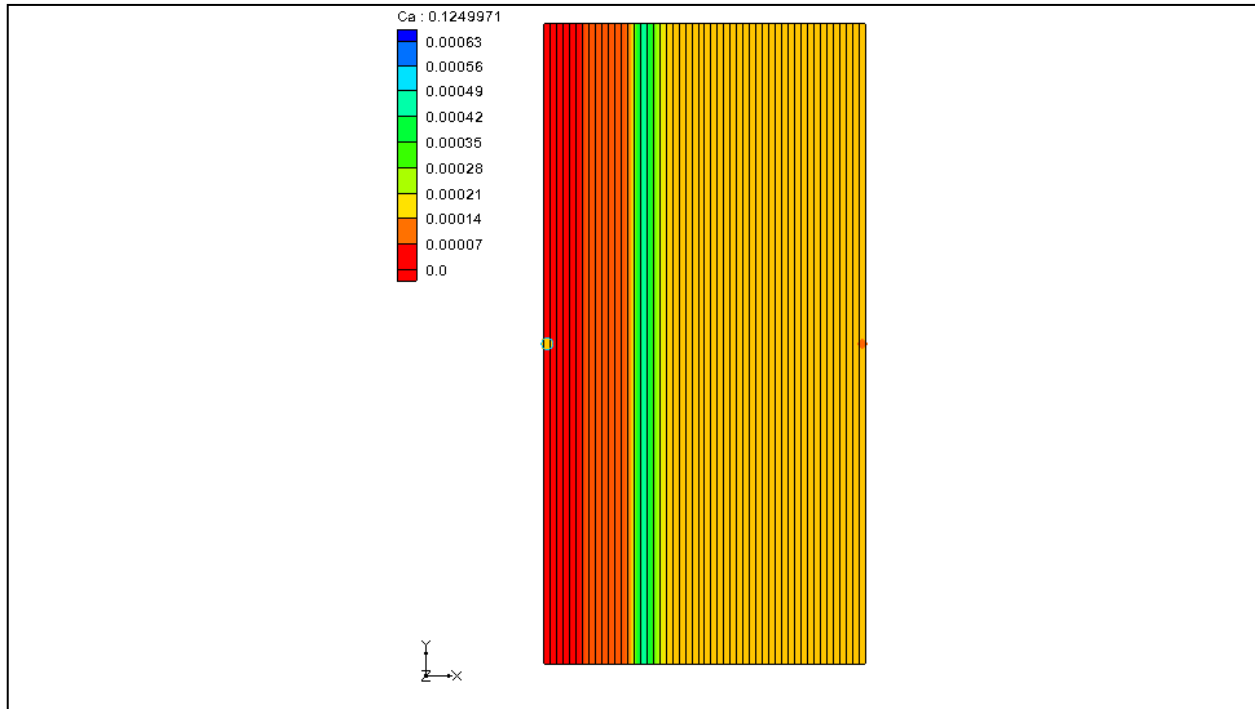*GMS 10.3 Tutorial*

PHT3D – Transport and Mineral Reactions

PHT3D Geochemical Reactions

Objectives

Learn about transport and mineral reactions in PHT3D.

Prerequisite Tutorials

- MT3DMS – Grid Approach

Required Components

- Grid Module
- MODFLOW
- MT3D
- PHT3D

Time

- 20–30 minutes

1   Introduction

PHT3D is a multi-component transport model for three-dimensional reactive transport in saturated porous media developed and maintained by Henning Prommer and Vicent Post (2010).[1] PHT3D is a combination of MT3DMS and PHREEQC-2. PHREEQC-2 allows for a variety of low temperature, aqueous-geochemical reactions.

The simulation of mineral dissolution and precipitation reactions is one of the key features of PHT3D, and one or more of them will be included in many typical model applications. The case described in this tutorial was originally presented by Engesgaard and Kipp (1992)[2] for a model verification of their MST1D code against the CHMTRNS model by Noorishad et al. (1987).[3] It involves a one-dimensional, model domain in which an aqueous water composition that is in equilibrium with two minerals, calcite and dolomite, is successively replaced, that is, flushed by water of a different chemical composition, leading to multiple precipitation-dissolution fronts. Dolomite is not present initially but is formed temporally.

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1 Prommer, H., and Post, V. (2010). A reactive multicomponent transport model for saturated porous media. User's Manual v2.10.

2 Engesgaard, P., and Kipp, K.L. (1992). A geochemical transport model for redox-controlled movement of mineral fronts in groundwater flow systems: A case of nitrate removal by oxidation of pyrite. *Water Resource Research* 28: 2829–2843.

3 Noorishad, J., Carnahan, C.L., and Benson, L.V. (1987). A report on the development of the non-equilibrium reactive chemical transport code CHMTRNS. (Berkeley, CA: Lawrence Berkeley Laboratory).

2   Description of Problem

In order to follow the discretisation chosen by Engesgaard and Kipp (1992), the project will create a model domain of 0.5 m length divided into 50 grid cells of 0.01 m length, 1 m width and 1 m height (50 columns, 1 row and 1 layer). A steady-state flow rate Q_{well} of 0.259 m3/d is required to achieve a pore-velocity of 0.083 m/d for the given porosity of 0.32. The total simulation time is 0.2430 days. It is divided into 210 time steps.

3   Getting Started

Do the following to get started:

1. If GMS is not running, launch GMS.

2. If GMS is already running, select the *File* / **New** command to ensure the program settings are restored to the default state.

4   The Flow Model

Before setting up the PHT3D simulation, a MODFLOW solution must exist to be used as the flow field for the transport simulation. In the interest of time, import a previously created MODFLOW simulation.

1. Select the **Open** 📂 button to bring up the *Open* dialog.

2. Locate and open the directory entitled *Tutorials\PHT3D\MineralReactions* then select the file entitled "start.gpr".

3. Click the **Open** button to import the file.

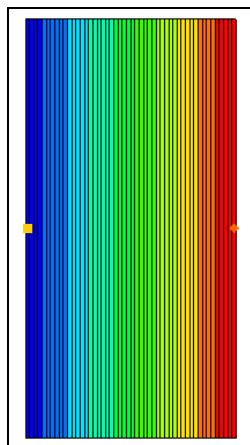The flow model has already been created in this example.

Figure 1   Flow model

5   Save the Project with a New Name

Before continuing, save the project with a new name.

1. Select the *File |* **Save As** command to bring up the *Save As* dialog.

2. Change the *File name* to **"**mineral_dis_pre.gpr" and click **Save**.

It's a good idea to save the work periodically.

6   Building the Transport Model

With a flow solution, it is possible to set up the PHT3D transport simulation.

6.1   Initializing the Simulation

First, initialize the simulation.

1. Right-click the Project Explorer and select **Expand All**.

2. Right-click on the "🔳 grid" item and select the **New MT3DMS** command to
    open the *Basic Transport Package* dialog.

3. Under the *Model* section in the dialog, select *PHT3D.*

6.2   PHT3D Reaction Definition

In some cases, this next step would be to prepare a problem-specific reaction module.
However, for simple problems, such as those that only include equilibrium reactions, this
is not the case. All of the aqueous species, components, and minerals needed to simulate
this LEA-based reactive transport problem are already included in the original
PHREEQC-2 database. This means that a user-defined set of equilibrium reactions does
not need to be created. Instead, use the PHREEQC-2 database.

To specify the reaction definitions, proceed as follows:

1. Select the **Define Species** button to open the *PHT3D Options* dialog.

This dialog allows for the definition the species uses as well as PHT3D general options.
Notice that the first item available is *General Options*.

2. Select *Equilibrium Species* from the list box on the left of the dialog.

Notice that it is not possible to view any candidate equilibrium species because a
PHREEQC database has not yet been selected. Now it is necessary to select a PHREEQC
database.

3. Select the **Open** 📂 button next to *PHREEQC database* to bring up an *Open* dialog.

4. Locate and open the directory entitled *Tutorials\PHT3D\MineralReactions* then select the file entitled "pht3d_datab.dat".

5. Select the **Open** button to load the file.

GMS has read the PHREEQC database and made available the different components included in the file. Now select the components to model.

6. Turn on the *Active* check box in the spreadsheet window for*: Ca, Mg, Cl* and *C(4)*. Note that the *pH* and *pe* will not be explicitly selected as these species are automatically included in all simulations.

7. Select the *Equilibrium Minerals/Phases* option in the left window.

8. Turn on the *Active* check box in the right window for *Calcite* and *Dolomite*.

Now that the selection of the species to include in the simulation is completed, accept the other default options in the dialog.

9. Select the **OK** to close the *PHT3D Options* dialog.

6.3   Initial concentrations

The next step is to specify the initial concentrations that define the hydrogeochemistry of the aquifer at the start of the simulation (Time = 0).

1. In the spreadsheet, select *Ca* under *Species* to highlight it.

2. Enter a value of "0.000123" for the *Starting Conc. (moles/liter)*.

Use the same procedures described above to specify the initial concentrations for all the aqueous components and minerals in the following two tables.

Note, that the aqueous concentrations are always defined in units of mol/l. In contrast, the unit for the initial concentrations of minerals is not mass per volume of water, i.e., *mol/l,* **but is defined as mass per bulk volume,** mol/l_{volume}.

Table 1   Aqueous concentrations used in this tutorial

Aqueous component	C_{init} (mol/l$_w$)
Ca	0.000123
Mg	0.0
Cl	0.0
C(4)	0.000123
pH	9.91
pe	4.0

Table 2   Mineral concentrations used in this tutorial

Mineral	C_{init} (mol/l$_v$)
Calcite ($CaCO_3$)	0.00003906
Dolomite ($CaMg(CO_3)_2$)	0.0

6.4   Packages

Next, select which packages to use.

1. Select the **Packages** button to open the *MT3DMS/RT3D Packages* dialog.

2. Turn on the following packages:

   - *Advection Package*

   - *Dispersion Package*

   - *Source/Sink Mixing Package*

3. Select the **OK** to close the *MT3DMS/RT3D Packages* dialog.

6.5   Porosity Array

Finally, define the porosity for the cells. The problem has a constant porosity of 0.32.

1. Select the **Porosity** button to open the *Porosity* dialog.

2. Select **Constant → Grid** button to open the *Grid Value* dialog.

3. Enter "0.32" then select the **OK** to close the *Grid Value* dialog.

4. Select the **OK** button to exit the *Porosity* dialog.

This completes the definition of the Basic Transport package data. Leave the other options at the default values.

5. Select the **OK** button to exit the *Basic Transport Package* dialog.

6.6   Run Options

Next, tell MT3DMS to always use the same MODFLOW solution to define the flow field. This will allow the transport simulation to be saved under a different name without having to re-run MODFLOW.

1. Select the *PHT3D* / **Run Options** command to open the *Run Options* dialog.

2. Select the *Single run with selected MODFLOW solution* option.

3. Select the **OK** to close the *Run Options* dialog.

7   Advection Package

The Advection Package has been included in the simulation. Use the default settings in the package so nothing needs to be changed.

8   Dispersion Package

Now edit the inputs to the dispersion package. To enter the data for the Dispersion package, do the following:

1. Select the *PHT3D* / **Dispersion Package** command to open the *Dispersion Package* dialog.

2. Select the **Longitudinal Dispersivity** button to open the *Longitudinal Dispersivity* dialog.

3. Select the **Constant → Grid** button to open the *Grid Value* dialog.

4. Enter a value of "0.0067" and select the **OK** to close the *Grid Value* dialog.

5. Select the **OK** button to exit the *Longitudinal Dispersivity* dialog.

6. Select the **OK** button to exit the *Dispersion Package* dialog.

9   Adding Inflow Concentrations

The flow model has been set up with an injection well on the left of the model and a constant head boundary condition on the right. The flow should move from left to right through the model grid. By default, water entering the model from the well will have a concentration of 0.0 for each of the species in the model. It is necessary to change the concentrations in the water from the injection well.

9.1   Assigning Inflow Concentrations

1. Choose the **Select Cells** 📦 tool.

2. Right-click on the left-most cell and select the **Sources/Sinks** command to open the *MODFLOW/PHT3D Sources/Sinks* dialog.

3. In the left window, select *PH3TD: Point SS* item.

4. Select the **Add BC** button.

5. Change the *Type* to "well (WEL)".

6. Enter the inflow concentrations as listed in Table 3 below.

Table 3   Inflow Concentrations

Aqueous component	C_{inflow} (mol/l$_w$)
Ca	0.0
Mg	0.001
Cl	0.002
C(4)	0.0
pH	7.0
pe	4.0

7. Select the **OK** button to exit the *MODFLOW/PHT3D Sources/Sinks* dialog.

10   Saving the Simulation and Running PHT3D

Now to save the simulation and run PHT3D.

1. Select the **Save** 🖫 button.

2. Select the *MODFLOW* | **Run MODFLOW** command.

3. Select **Close** when the *MODFLOW* simulation finishes.

4. Select the *PHT3D* | **Run PHT3D** command.

5. When the *PHT3D* simulation is finished, click the **Close** button.

11   Viewing the Solution

After PHT3D finished running, GMS automatically reads in the computed concentrations, mass files, and output file produced by PHT3D. All of this data is under a new folder in the Project Explorer called "mineral_dis_pre (PHT3D)".

1. If necessary, expand the " mineral_dis_pre (PHT3D)" folder from the Project Explorer.

2. Select the " Ca" dataset.

3. Click on the first time step in the *Time Step Window* below the Project Explorer.

4. Use the up and down arrows to view the different time steps.

11.1   Time Series Data Plot

Next, generate the time series data plot related to the concentrations.

1. Select the " Dolomite" dataset.

2. Select the **Plot Wizard** button to open the *Plot Wizard* dialog.

3. Select the *Active Dataset Time Series* plot.

4. Select the **Finish** button to close the *Plot Wizard* and generate the plot.

5. Choose the **Select Cells** tool and select any cell on the model.

The concentration of dolomite over time should now be visible. Note that dolomite is not present initially but is formed temporally.

12   Conclusion

This concludes the "PHT3D – Transport and Mineral Reactions" tutorial. Here are key concepts in this tutorial:

- How to define species in PHT3D using the original PHREEQC-2 database.

- How to specify the concentrations for a particular species.