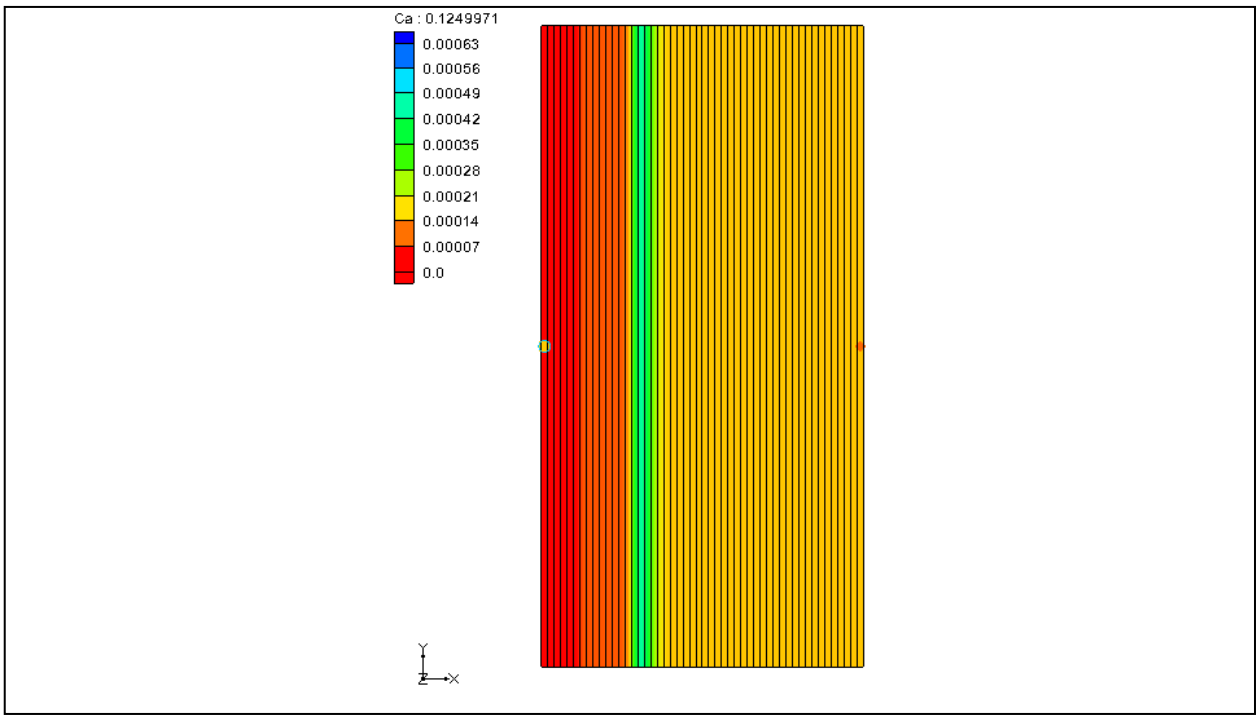
GMS v. 9.2

GMS 9.2 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
- MODFLOW
- MT3D
- PHT3D

Time

- 30-60 minutes

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1 Contents

2 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. 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) for a model verification of their MST1D code against the CHEMTRNS model by Noorishad et al. (1987). 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, i.e., flushed by water of a different chemical composition, leading to multiple precipitation-dissolution fronts. Dolomite is not present initially but is formed temporally.

3 Description of Problem

In order to follow the discretisation chosen by Engesgaard and Kipp (1992), we 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.

4 Getting Started

If you have not yet done so, launch GMS. If you have already been using GMS, you may wish to select the *File* | *New* command to ensure the program settings are restored to the default state.

5 The Flow Model

Before setting up the PHT3D simulation, we must first have a MODFLOW solution that will be used as the flow field for the transport simulation. In the interest of time, we will read in a previously created MODFLOW simulation.

1. Select the *Open* button  .
2. Locate and open the directory entitled **Tutorials\PHT3D\MineralReactions**.
3. Select the file entitled **start.gpr**.
4. Select the *Open* button.

The flow model has already been created in this example.

6 Save the Project With a New Name

Before we continue, let's save the project with a new name.

1. Select the *File* | *Save As* command.
2. Save the project with the name **mineral_dis_pre.gpr**.

It's a good idea to save your work periodically as you proceed.

7 Building the Transport Model

Now that we have a flow solution, we are ready to set up the PHT3D transport simulation.

7.1 Initializing the Simulation

First, we will initialize the simulation.

1. Expand the items in the *Project Explorer*.
2. Right-click on the **grid** and select the *New MT3D* command.
3. Under the *Model* section in the dialog, select *PHT3D.*

7.2 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 PHREEEQC-2 database. This means that we don't have to define our own set of equilibrium reactions but we can simply use the PHREEQC-2 database. To specify the reaction definitions, proceed as follows:

1. Select the *Define Species* button.

This dialog allows us to define the species that we will use 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.

We can see that we are unable to view any candidate equilibrium species because we have not yet selected a PHREEQC database. Let's select a PHREEQC database now.

3. Select the *Open* button next to *PHREEQC database*.
4. Locate and open the directory entitled **Tutorials\PHT3D\MineralReactions**.
5. Select the file entitled **pht3d_datab.dat**.
6. Select the *OK* button.

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

7. Turn on the *Active* check box in the spreadsheet window for: **Ca, Mg, Cl and C(4)**. Note that we will not explicitly select **pH** and **pe** as these species are automatically included in all simulations.
8. Select the *Equilibrium Minerals/Phases* option in the left window.
9. Turn on the *Active* check box in the right window for: **Calcite** and **Dolomite**.

We are now done selecting the species to include in our simulation; we will accept the other default options in the dialog.

10. Select the *OK* button.

7.3 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 spread sheet select the **Ca** *Species*.
2. Enter a value of **0.000123** for the starting concentration.

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

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, i.e.,** mol/l_{volume}.

Table 7-1. Aqueous concentrations used in this tutorial.

Aqueous component	C_{init} (mol/l_w)
Ca	**1.23×10^{-4}**
Mg	**0.0**
Cl	**0.0**
C(4)	**1.23×10^{-4}**
pH	**9.91**
pe	**4.0**

Table 7-2. Mineral concentrations used in this tutorial.

Mineral	C_{init} (mol/l_v)
Calcite ($CaCO_3$)	**3.906×10^{-5}**
Dolomite ($CaMg(CO_3)_2$)	**0.0**

7.4 Packages

Next, we will select which packages we wish to use.

1. Select the *Packages* button.
2. Turn on the following packages:
   - *Advection Package*
   - *Dispersion Package*
   - *Source/Sink Mixing Package*
3. Select the *OK* button.

7.5 Porosity Array

Finally, we will define the porosity for the cells. Our problem has a constant porosity of 0.32.

1. Select the *Porosity* button in the *Basic Transport Package* dialog.
2. In the *Porosity* dialog, select *Constant -> Grid* button.
3. Enter **0.32**.
4. Select the *OK* button twice to exit both dialogs.

This completes the definition of the Basic Transport package data. We can leave the other options at the default values.

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

7.6 Run Options

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

1. Select the *PHT3D* | *Run Options* command.
2. Select the *Single run with selected MODFLOW solution* option.
3. Select the *OK* button.

8 Advection Package

The Advection Package has been included in our simulation and we will use the default settings in the package so we do not need to edit anything in the Advection package.

9 Dispersion Package

Now we will edit the inputs to the dispersion package. To enter the data for the Dispersion package:

1. Select the *PHT3D* | *Dispersion Package* command.
2. Select the *Longitudinal Dispersivity* button.
3. Select the *Constant* → *Grid* button.
4. Enter a value of **0.0067** and select the *OK* button.

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

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

10 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. We expect flow to 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 our model. We want to change the concentrations in the water from the injection well.

10.1 Assigning Inflow Concentrations

1. Choose the *Select Cells* tool  .

2. Right click on the left-most cell and select *Sources/Sinks* command.

3. In the left window, select **MT3D: Point SS** item.

4. Select the *Add BC* button.

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

6. Enter the inflow concentrations listed in the table below.

Table 10-1. Inflow Concentrations

Aqueous component	C_{inflow} (mol/l_w)
Ca	**0.0**
Mg	**1.0×10^{-3}**
Cl	**2.0×10^{-3}**
C(4)	**0.0**
pH	**7.0**
pe	**4.0**

7. Select the *OK* button to exit the dialog.

11 Saving the Simulation and Running PHT3D

We are now ready to save the simulation and run PHT3D.

8. Select the *Save*  button.

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

10. Select *Close* when the simulation finishes.
11. Select the *PHT3D* | *Run PHT3D* command.
12. When the simulation is finished, click the *Close* button.

12 Viewing the Solution

After PHT3D finished running, GMS automatically read 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* data set.
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.

12.1 Time Series Data Plot

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

1. Select the *Dolomite* data set.
2. Select the *Plot Wizard* button.
3. Select the *Active Data Set Time Series* plot.
4. Select the *Finish* button.
5. Choose the *Select Cells* tool.
6. Select any cell on the model.

You should be able to see the concentration of *Dolomite* over time. Note that *Dolomite* is not present initially but is formed temporally.

13 Conclusion

This concludes the *PHT3D – Transport and Mineral Reactions* tutorial. Here are the things that you should have learned in this tutorial:

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

- How to specify the concentrations for a particular species.

