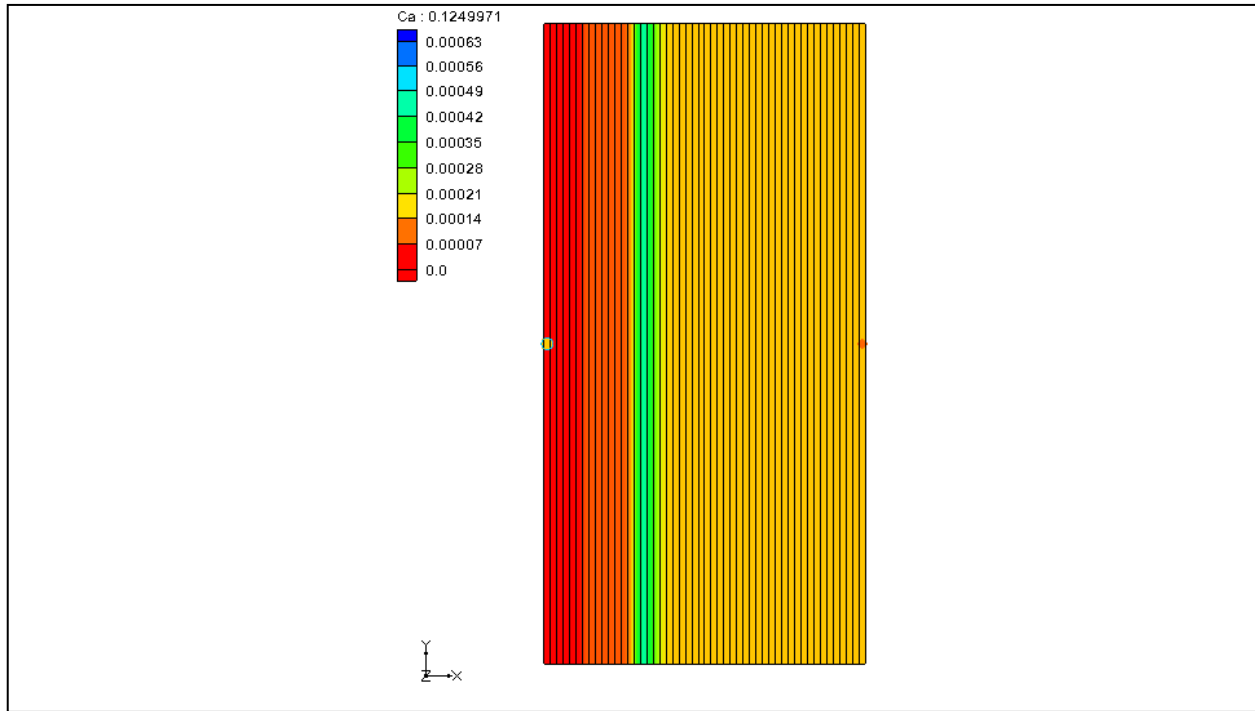


*GMS 10.0 Tutorial*

***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



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## 1 Introduction

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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).<sup>1</sup> 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)<sup>2</sup> for a model verification of their MST1D code against the CHMTRNS model by Noorishad et al. (1987).<sup>3</sup> 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).

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## 2 Description of Problem

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In order to follow the discretisation chosen by Engesgaard and Kipp (1992), the user 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  $Q_{\text{well}}$  of 0.259 m<sup>3</sup>/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.

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## 3 Getting Started

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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.

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## 4 The Flow Model

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

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## 5 Save the Project with a New Name

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Before continuing, save the project with a new name.

1. Select the *File* | **Save As** command.
2. Change the project name to “mineral\_dis\_pre.gpr.”
3. Click **Save**.

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

## 6 Building the Transport Model


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Now that the user has a flow solution, it is possible to set up the PHT3D transport simulation.

### 6.1 Initializing the Simulation

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First, the user will initialize the simulation.

1. Expand the items in the Project Explorer.
2. Right-click on the “grid”  item.
3. Select the **New MT3D** command to open the *Basic Transport Package* dialog.
4. Under the *Model* section in the dialog, select *PHT3D*.

### 6.2 PHT3D Reaction Definition

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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 the user doesn't have to define his or her own set of equilibrium reactions but can simply use the PHREEQC-2 database. To specify the reaction definitions, proceed as follows:

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

This dialog allows for the definition the species that the user 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.

The user can see that it is not possible to view any candidate equilibrium species because the user has not yet selected a PHREEQC database. Now it is necessary to 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, the user can select the components the user wants to model.

7. Turn on the *Active* check box in the spreadsheet window for: *Ca*, *Mg*, *Cl* and *C(4)*. Note that the user 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*.

The user is now done selecting the species to include in the simulation; the user will accept the other default options in the dialog.

10. Select the **OK** button.

### 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 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 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<sub>volume</sub>.**

Table 1 Aqueous concentrations used in this tutorial

Aqueous component	C <sub>init</sub> (mol/l <sub>w</sub> )
Ca	1.23 x 10 <sup>-4</sup>
Mg	0.0
Cl	0.0
C(4)	1.23 x 10 <sup>-4</sup>
pH	9.91
pe	4.0

Table 2 Mineral concentrations used in this tutorial

Mineral	C <sub>init</sub> (mol/l <sub>v</sub> )
Calcite (CaCO <sub>3</sub> )	3.906 x 10 <sup>-5</sup>
Dolomite (CaMg(CO <sub>3</sub> ) <sub>2</sub> )	0.0

### 6.4 Packages

Next, the user will select which packages to use.

1. Select the **Packages** button to open the *MT3D/RT3D Packages* dialog.
2. Turn on the following packages:
  - *Advection Package*
  - *Dispersion Package*
  - *Source/Sink Mixing Package*
3. Select the **OK** button.

## 6.5 Porosity Array

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Finally, the user will define the porosity for the cells. The 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 to open the *Grid Value* dialog.
3. Enter “0.32.”
4. Select the **OK** button.
5. Select the **OK** button to exit the *Porosity* dialog.

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

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

## 6.6 Run Options

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Next, the user will tell MT3DMS to always use the same MODFLOW solution to define the flow field. This will allow the user 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.

## 7 Advection Package

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The Advection Package has been included in the simulation. The user will use the default settings in the package, so nothing needs to be changed.

## 8 Dispersion Package

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Now the user will 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.”
5. Select the **OK** button.
6. Select the **OK** button to exit the *Longitudinal Dispersivity* dialog.
7. Select the **OK** button to exit the *Dispersion Package* dialog.


## 9 Adding Inflow Concentrations

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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

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1. Choose the **Select Cells**  tool.
2. Right-click on the left-most cell.
3. Sselect **Sources/Sinks** command to open the *MODFLOW/PHT3D Sources/Sinks* dialog.
4. In the left window, select *PH3TD: Point SS* item.
5. Select the **Add BC** button.

6. Change the *Type* to “well (WEL).”
7. Enter the inflow concentrations as listed in the table below.


Table 3 Inflow Concentrations

Aqueous component	$C_{inflow}$ (mol/l <sub>w</sub> )
Ca	0.0
Mg	$1.0 \times 10^{-3}$
Cl	$2.0 \times 10^{-3}$
C(4)	0.0
pH	7.0
pe	4.0

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



## 10 Saving the Simulation and Running PHT3D

Now save the simulation and run PHT3D.

1. Select the **Save**  button.
2. Select the *MODFLOW* / **Run MODFLOW** command.
3. Select **Close** when the simulation finishes.
4. Select the *PHT3D* / **Run PHT3D** command.
5. When the simulation is finished, click the **Close** button.

## 11 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”  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

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

1. Select the “Dolomite”  dataset.
2. Select the **Plot Wizard**  button.
3. Select the *Active Dataset Time Series* plot.
4. Select the **Finish** button.
5. Choose the **Select Cells**  tool.
6. Select any cell on the model.

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

## 12 Conclusion

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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.