GMS TUTORIALS

RT3D – Double Monod Model

This tutorial illustrates the steps involved in using GMS and RT3D to model the reaction between an electron donor and an electron acceptor, mediated by an actively growing microbial population that exist in both soil and aqueous phases. Since the flow model used in this simulation is the same as the flow model used in *RT3D – Instantaneous Aerobic Degradation*, the steps involved in building the flow model will not be described in this tutorial. A pre-defined version of the flow model will be used.

1.1 Outline

This is what you will do:

1. Import a MODFLOW model
2. Define conditions.
3. Run MODFLOW.
4. Run RT3D.
5. Use the data calculator to convert units and view the results

1.2 Required Modules/Interfaces

You will need the following components enabled to complete this tutorial:

- Grid
- MODFLOW
- RT3D and ART3D

You can see if these components are enabled by selecting the *File* | *Register* command.

2 Description of the Reaction Model

Methods for enhancing in situ bioremediation of subsurface soil and groundwater involve injection or infiltration of a carbon source (or electron donor), nutrients, and other electron acceptors to stimulate the growth of native microbes. In addition, bioengineered suspension cultures of contaminant degrading organisms may be also added to increase the amount of attached and suspended biomass in the subsurface. These two types of active remediation techniques can be used to bioremediate contaminated source zones or to establish a biobarrier to prevent plume migration and/or to enhance plume attenuation. The successful use of subsurface microbes for bioremediation requires an understanding of coupled flow, transport, and reaction processes that control bacterial growth and migration patterns. The Dual-Monod model, available in the RT3D code, can be used to develop such understanding by simulating the coupled reactive transport and microbial growth. The model is developed in a general format; therefore, the interaction between any electron donor and acceptor mediated by any type of microbial population can be simulated by varying appropriate kinetic constants. Advanced users can modify this basic formulation and couple it with other packages, such as the sorption package, to simulate more realistic bioremediation scenarios (any such modified reaction models can be easily implemented via the user-defined reaction option).

Assuming the linear-equilibrium model for modeling sorption, and the Dual-Monod model for modeling bacterial growth, the fate and transport equation for an electron donor (hydrocarbon, for example) in a multi-dimensional saturated porous media can be written as:

$$R_D \frac{\partial [D]}{\partial t} = \frac{\partial}{\partial x_i}\left(D_{ij} \frac{\partial [D]}{\partial x_j} \right) - \frac{\partial}{\partial x_i}\left(v_i [D] \right) + \frac{q_s}{\phi}[D_s] - \mu_m \left([X] + \frac{\rho \tilde{X}}{\phi} \right) \left(\frac{[D]}{K_D + [D]} \right) \left(\frac{[A]}{K_A + [A]} \right) \quad \text{..... (1)}$$

where [D] is the electron donor concentration in the aqueous phase [ML^{-3}], [D_s] is the donor concentration in the sources/sinks [ML^{-3}], D_{ij} is the dispersion coefficient; [X] is the aqueous phase bacterial cell concentration [ML^{-3}], $\tilde{X}$ is the solid-phase cell concentration (mass of bacterial cells per unit mass of porous media [MM^{-1}]), [A] is the electron acceptor concentration in the aqueous phase [ML^{-3}], R_H is the retardation coefficient of the hydrocarbon, K_D is the half saturation coefficient for the electron donor [ML^{-3}], K_A is the half saturation coefficient for the electron acceptor [ML^{-3}], and μ_m is the contaminant utilization rate [T^{-1}]. The model assumes that the degradation reactions occur only in the aqueous phase, which is usually a conservative assumption.

The fate and transport of the electron donor (oxygen, for example) can be modeled using the equation:

$$R_A \frac{\partial [A]}{\partial t} = \frac{\partial}{\partial x_i}\left(D_{ij} \frac{\partial [A]}{\partial x_j} \right) - \frac{\partial}{\partial x_i}\left(v_i [A] \right) + \frac{q_s}{\phi}[A_s] - Y_{A/D}\,\mu_m \left([X] + \frac{\rho \tilde{X}}{\phi} \right) \left(\frac{[D]}{K_D + [D]} \right) \left(\frac{[A]}{K_A + [A]} \right) \quad \text{..... (2)}$$

where $Y_{A/D}$ is the stoichiometric yield coefficient, and R_A is the retardation coefficient of the electron acceptor.

The fate and transport of bacteria in the aqueous phase can be described using the equation:

$$\frac{\partial [X]}{\partial t} = \frac{\partial}{\partial x_i}\left(D_{ij} \frac{\partial [X]}{\partial t} \right) - \frac{\partial}{\partial x_i}\left(v_i [X] \right) + \frac{q_s}{\phi}[X_s] - K_{att}[X] + \frac{K_{det}\rho \tilde{X}}{\phi} + Y_{X/D}\,\mu_m [X] \left(\frac{[D]}{K_D + [D]} \right) \left(\frac{[A]}{K_A + [A]} \right) - K_e [X] \quad \text{..... (3)}$$

where K_{att} is the bacterial attachment coefficient [T^{-1}], K_{det} is the bacterial detachment coefficient [T^{-1}], and K_e is the endogenous cell death or decay coefficient [T^{-1}].

The growth of attached-phase bacteria can be described using an ordinary differential equation of the form:

$$\frac{d\tilde{X}}{dt} = \frac{K_{att}\phi [X]}{\rho} - K_{det}\tilde{X} + Y_{X/D}\,\mu_m \tilde{X} \left(\frac{[D]}{K_D + [D]} \right) \left(\frac{[A]}{K_A + [A]} \right) - K_e \tilde{X} \quad \text{..... (4)}$$

The conceptual model used here for representing attached bacteria cells is similar to the macroscopic model described by Baveye and Valocchi (*Wat. Resour. Res.,* 25, 1413-1421,1989). The model also assumes first-order kinetic expressions for representing bacterial attachment and detachment processes (Taylor and Jaffe, *Wat. Resour. Res.,* 26, 2181-2194,1990, and Hornberger et al., *Wat. Resour. Res.,* 28, 915-938, 1992). Permeability and porosity changes caused by bacterial growth are ignored in this formulation. However, if required, macroscopic models for biomass-affected porous-media properties described by Clement et al. (*Ground Water*, 34, 934-942, 1996) may be integrated within this modeling approach. It should be noted that a lot of active research is currently underway to gain an increased understanding of bacteria transport in porous media because currently available bacterial transport models (including the model used here) are arguably approximate. Therefore, application of this model to real situations should be always supported by field- or laboratory-scale data.

The reactive-transport model discussed above was set-up as a RT3D reaction package with three mobile species (to represent electron donor, electron acceptor, and aqueous bacteria) and one immobile species (to represent attached soil bacteria). After

employing the reaction-operator splitting strategy, the reaction package for the problem reduces to:

$$\frac{d[D]}{dt} = -\frac{\mu_m}{R_D}\left([X] + \frac{\rho\tilde{X}}{\phi}\right)\left(\frac{[D]}{K_D + [D]}\right)\left(\frac{[A]}{K_{[A]} + [A]}\right) \quad \text{..... (5)}$$

$$\frac{d[A]}{dt} = -\frac{Y_{A/D}\,\mu_m}{R_A}\left([X] + \frac{\rho\tilde{X}}{\phi}\right)\left(\frac{[D]}{K_D + [D]}\right)\left(\frac{[A]}{K_A + [A]}\right) \quad \text{..... (6)}$$

$$\frac{d[X]}{dt} = -Y_{X/D}\,\mu_m\left([X] + \frac{\rho\tilde{X}}{\phi}\right)\left(\frac{[D]}{K_D + [D]}\right)\left(\frac{[A]}{K_A + [A]}\right) + \frac{K_{det}\rho\tilde{X}}{\phi} - K_{att}[X] - K_e[X] \quad \text{..... (7)}$$

$$\frac{d\tilde{X}}{dt} = \frac{K_{att}\phi[X]}{\rho} - K_{det}\tilde{X} + Y_{X/D}\,\mu_m\tilde{X}\left(\frac{[D]}{K_D + [D]}\right)\left(\frac{[A]}{K_A + [A]}\right) - K_e\tilde{X} \quad \text{..... (8)}$$

These four equations are coded into the double-monod reaction module.

3 Description of Problem

The problem we will be solving in this tutorial is similar to the problem described in the first tutorial (*RT3D – BTEX Degradation with Multiple Electron Acceptors*). The site is a 510 m X 310 m section of a confined aquifer with a flow gradient from left to right. An underground storage tank is leaking fuel hydrocarbon contaminants at 2 m^3/day at the location shown. Source concentration of BTEX is 500 mg/L. It will be assumed that the aquifer is initially clean and has very low levels of aerobic bacterial activity. The fuel hydrocarbon compounds are expected to serve as the carbon source, resuscitating the bacterial cells and activating them into a growth mode. This is a common subsurface phenomenon that occurs in most fuel-contaminated sites. Several field studies have observed the presence of enhanced levels of microbial activity near a source region, and low background levels outside the plume. In this example, we will simulate the transient changes in hydrocarbon, oxygen, and bacterial concentrations levels within the contaminated area.

Initial levels of hydrocarbon, oxygen, aqueous bacteria, and attached bacteria are assume to be: 0.0 mg/L, 9.0 mg/L, 2 x 10^{-17} (value for X in mg/L), and 3.0 x 10^{-9} (value for $\tilde{X}$ in mg of bacteria/mg of soil), respectively. Note the mass fraction unit used for representing soil bacterial cells will always yield small numbers. Using the value of soil porosity and bulk density, these numbers can be converted into standard mg/L units (liquid-volume basis) to get a better feel for bacterial concentration levels. For example, assuming ρ = 1.6 x 10^6 mg/L and ϕ = 0.3, the initial value of soil bacterial concentration can be expressed (converted to liquid volume basis using the formula: $\tilde{X}\,\rho/\phi$) as: 0.016 mg/L. While post processing output concentration in GMS, the data calculator will be

used to perform this unit conversion. This is recommended because extremely small numbers may not be displayed correctly in GMS.

Assumed values for other kinetic reaction constants are given below:

Constant	GMS Display	Value
μ_m	umax	0.125 day^{-1}
K_D	K_{ed}	0.12 mg/L
K_A	K_{ea}	0.1 mg/L
$Y_{x/D}$	$Y_{x/ed}$	0.05
$Y_{A/D}$	$Y_{ea/ed}$	3.0
K_{decay}	K_{decay}	0.001 day^{-1}
K_{att}	K_{att}	70.0 day^{-1}
K_{det}	K_{det}	1.0 day^{-1}

Sorption is assumed to be negligible for this site, hence the values of all retardation coefficients are assumed to be unity.

The first part of the problem will be to import a previously computed MODFLOW flow model of the site. Using this flow field, a reactive transport model will be then be defined using RT3D.

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 New command from the File menu to ensure the program settings are restored to the default state.

5 Importing the MODFLOW Model

The first part of the simulation is to import the MODFLOW flow model. A steady state flow model has been previously computed and is supplied with the tutorial files.

1. Switch to the *3D Grid Module* 
2. In the Open dialog, locate and open the file entitled **tutfiles\RT3D\flowmod\flowmod_MODFLOW\flowmod.mfs**.

At this point, you should see a grid appear.

6 Building the Transport Model

Now that the flow model is imported, the next step is to perform the RT3D simulation. For this part of the simulation, we will select the reaction, define the reaction data, define the supplemental layer data needed by RT3D, define the boundary conditions, and assign concentrations to the well.

7 Initializing the Model

To initialize the RT3D data:

1. Select the *MT3D* | *New Simulation* command.

8 The BTN Package

The next step is to initialize the data in the Basic Transport Package. First, we will initialize the data, select RT3D as the transport model, and select the appropriate packages.

1. Select the *RT3D* option.
2. Select the *Packages* button.
3. Select the *Advection Package*, the *Dispersion Package*, the *Source/Sink Mixing Package*, and the *Chemical Reaction Package*.
4. For the reaction type, select the *Double Monod Model* option.
5. Select the *OK* button to exit the *Packages* dialog.

8.1 Starting Concentration

Note that in the *Starting Concentration* section of the dialog, the species associated with the reaction we are modeling are listed by name. The next step is to define the starting concentration for each of these species. The default starting concentration is zero. We will use the default value for the electron donor, but we will use non-zero values for the electron acceptor (9.0 mg/L), the aqueous phase bacteria ($2x10^{-17}$ mg/L), and the solid phase bacteria ($3x10^{-9}$ mg bacteria/mg of soil).

1. Select *Electron Acceptor* from the list of species.
2. Select the Starting Concentration button.
3. Select the *Constant* → *Grid* button.
4. Enter a value of **9.0**.
5. Select the *OK* button.
6. Select the *OK* button to exit the *Starting Concentration* dialog.
7. Repeat these steps to enter a starting value of **2e-17** for the *Aqueous-Phase Bacteria* and **3e-9** for the *Soil-Phase Bacteria*.

8.2 Porosity

Next, we will define the porosity as 0.3. Since this is the default supplied by GMS, no changes need to be made.

8.3 Stress Periods

Next, we will define the stress periods. Since the injection rate and the boundary conditions do not change, we will use a single stress period with a length of 730 days (two years).

1. Select the *Stress Periods* button.
2. Enter a value of **730** for the *Length*.
3. Enter a value of **10** for the *Num time steps*.
4. Select the OK button to exit the Stress Periods dialog.

8.4 Output Options

Finally, we will define the output options. One binary solution file is created by RT3D for each of the species. By default, RT3D saves a solution at each transport step for each species. Since this results in large files containing more solutions than we need for the simple post-processing we intend to do, we will specify that a solution be saved every 73 days (every time step).

1. Select the *Output Control* button.
2. Select the *Print or save at specified times* option.
3. Select the *Times* button.
4. Select the *Initialize Values* button.
5. Enter **73.0** for the Initial time step size.
6. Enter **73.0** for the Maximum time step size.
7. Enter **730.0** for the Maximum simulation time.
8. Select the *OK* button to exit the *Initialize Time Steps* dialog.
9. Select the *OK* button to exit the *Variable Time Steps* dialog.
10. Select the *OK* button to exit the *Output Control* dialog.

This completes the input for the Basic Transport package.

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

9 Assigning Concentrations to the Left Boundary

The left boundary of the model is a constant head boundary. Since the head at the left boundary is greater than the head at the right boundary, the left boundary acts as a source and water enters the model from the left. Thus, we must define the concentrations of our species at the left boundary. The simplest way to do this is to mark the cells as specified concentration cells.

1. Select the *Select Cell* tool  .
2. Select the cells on the left boundary by dragging a box that just surrounds the cells.
3. Select the *MT3D* | *Cell Properties* command.
4. Change the *ICBUND* value to **–1**.
5. Select the *OK* button.

10 The Advection Package

The next step is to initialize the data for the Advection package.

1. Select the *MT3D* | *Advection Package* command.
2. Select the *Method of characteristics (MOC)* option.
3. Select the *OK* button to exit the dialog.

11 The Dispersion Package

Next, we will enter the data for the Dispersion package. The aquifer has a longitudinal dispersivity of 10.0 m and a transverse (horizontal) dispersivity of 3.0 m.

1. Select the *MT3D* | *Dispersion Package* command.
2. Select the *Longitudinal Dispersivity* button.
3. Select the *Constant* → *Grid* button.
4. Enter a value of **10.0** and select *OK*.
5. Enter a value of **0.3** for the *TRPT* value.
6. Select the *OK* button to exit the *Dispersion Package* dialog.

12 The Source/Sink Mixing Package

Next, we will initialize the Source/Sink Mixing package and define the concentration at the spill location. We will assign a concentration of 500 mg/L for the electron donor and leave the other concentrations at the default value of 0.0.

1. Select the MT3D | Source/Sink Mixing Package command.
2. In the Initialize Point Source/Sinks from MODFLOW section in the lower left corner of the dialog, select the Well button.
3. Using the horizontal scroll bar below the spreadsheet section, scroll over until the Electron Donor column is visible.
4. Change the Electron Donor value to **500.0**.
5. Select the OK button to exit the Source/Sink Mixing Package dialog.

13 The Chemical Reaction Package

Next, we will initialize the Chemical Reaction package and define appropriate reaction rate constants.

1. Select the MT3D | Chemical Reaction Package command.
2. In the Reaction Parameters section, click on the umax item and set its value to **0.125**.
3. Likewise, set the value of Yea / ed to **3.0**.

The rest of the constants will all be left at the default values.

4. Select the *OK* button.

14 Run MODFLOW

Before running RT3D, we will regenerate the MODFLOW solution.

1. Select the *File* | *Save As* command.
2. In the *Save As* dialog, change the path to the directory entitled *tutfiles\rt3d\monod*.
3. Enter "**bacteria**" for the file name.
4. Select the *Save* button to save the files.

To run MODFLOW:

5. Select the *MODFLOW* | *Run MODFLOW* command.
6. When the simulation is finished, close the window.

15 Running RT3D

At this point, we are ready to save the model and run RT3D.

To run RT3D:

1. Select the *MT3D* | *Run RT3D* command.
2. Select *Yes* at the prompt.
3. When the simulation is finished, select the *Close* button.

16 Viewing the Results

First, we will view the Electron Donor solution at 730 days.

16.1 Electron Donor

1. Select the *Electron Donor* data set from the *Project Explorer* (You may need to expand the *bacteria (RT3D)* solution folder.
2. Select the time step at t = **730** days from the *Time Step Window*.

To display color-filled contours:

3. Select the *Data* menu | *Contour Options* command.
4. Change the method to *Color fill*.
5. Select the *OK* button.

Recall that the electron donor solution represents the contaminant. The plume is moving from the left to the right side, as expected.

16.2 Electron Acceptor

Next, we will view the electron acceptor solution.

1. Select the *Electron Acceptor* data set from the *Project Explorer*.

Note that the electron acceptor solution is the inverse of the electron donor solution. The minimum value (the blue region) corresponds to the location of the plume.

16.3 Aqueous-Phase Bacteria

Next, we will view the solution for the aqueous-phase bacteria.

1. Select the Aqueous-phase bacteria data set from the Project Explorer.

Note that the bacteria are flourishing at the left end and around the edges of the plume where there is a combination of electron donors and electron acceptors.

16.4 Solid-Phase Bacteria

Finally, we will view the solid-phase bacteria. However, before viewing the data set, we need to adjust the data set. The mass fraction unit used for representing soil bacterial cells (mg of bacteria/mg of soil) always yields small numbers. The resulting concentrations are so small that they sometimes produce numerical round-off errors in the GMS contouring routines. Thus, we will first utilize the *Data Calculator* to convert to units of mg/L. For example, assuming $\rho = 1.6 \times 10^6$ mg/L and $\phi = 0.3$, the initial value of soil bacterial concentration can be converted to liquid volume basis using the formula: $\tilde{X}\,\rho/\phi$.

1. Select the *Data* | *Data Calculator* command.
2. Enter "**f*(1.6*10^6)/0.3**" in the *Expression* field (the *Soil-Phase Bacteria* data set should be listed as item *f*).
3. Enter "**Soil Bacteria**" in the *Result* field.
4. Select the *Compute* button.
5. Select the *Done* button.

Note that the distribution of the soil bacteria is similar to the distribution of the aqueous-phase bacteria.

16.5 Other Post-Processing Options

At this point, you may wish to experiment with the other post-processing options, including film loop animation and time series plots.

17 Conclusion

This concludes the tutorial.