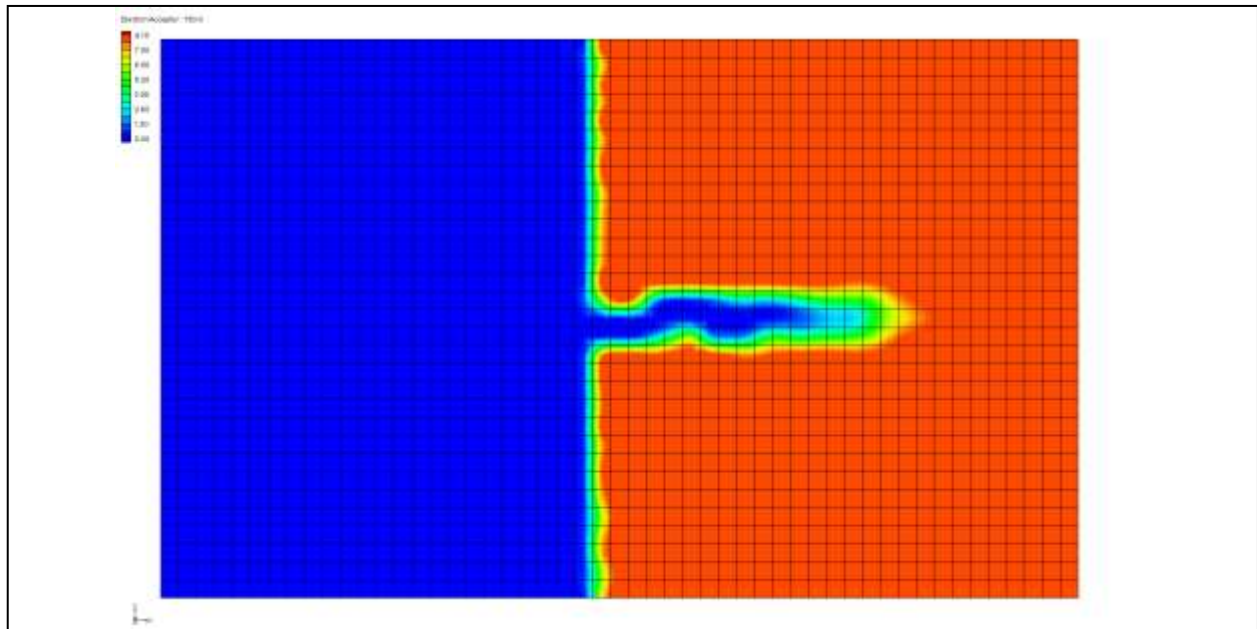


GMS 10.0 Tutorial

RT3D – Double-Monod Model



Objectives

Use GMS and RT3D to model the reaction between an electron donor and an electron acceptor, mediated by an actively growing microbial population that exists in both soil and aqueous phases.

Prerequisite Tutorials

- RT3D – Instantaneous Aerobic Degradation

Required Components

- Grid Module
- MODFLOW
- RT3D

Time

- 25-40 minutes



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1 Introduction

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 exists in both soil and aqueous phases. Since the flow model used in this simulation is the same as the flow model used in the “RT3D – Instantaneous Aerobic Degradation” tutorial, 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

Here are the steps of this tutorial:

1. Import a MODFLOW model
2. Define RT3D inputs and boundary conditions.
3. Run MODFLOW.
4. Run RT3D.
5. View the results.

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 follows:

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

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 this equation:

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

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 this equation:

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

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:

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

The conceptual model used here for representing attached bacteria cells is similar to the macroscopic model described by Baveye and Valocchi (1989).¹ The model also assumes first-order kinetic expressions for representing bacterial attachment and detachment processes (Taylor and Jaffé, 1990; and Hornberger et al., 1992).² 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

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1. Baveye, P. and Valocchi, A.J. (1989). An Evaluation of Mathematical Models of the Transport of Biologically Reacting Solutes in Saturated Soils and Aquifers. *Water Resources Research*, 25(6): 1413–1421.
 2. Taylor, S.W., and Jaffé, P.R. (1990). Substrate and Biomass Transport in a Porous Medium. *Water Resources Research*, 26(9): 2181–2194; and Hornberger, G.M., Mills, A.L., and Herman, J.S. (1992). Bacterial Transport in Porous Media: Evaluation of a Model Using Laboratory Observations. *Water Resources Research*, 28(3): 915-938.

Clement et al. (1996) may be integrated within this modeling approach.³ 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 the following:

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

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

$$\begin{aligned} \frac{d[X]}{dt} = & -Y_{X/D} \mu_m \left([X] + \frac{\rho \tilde{X}}{\phi} \right) \left(\frac{[D]}{K_D + [D]} \right) \left(\frac{[A]}{K_A + [A]} \right) + \\ & \frac{K_{det} \rho \tilde{X}}{\phi} - K_{att} [X] - K_e [X] \dots\dots\dots (7) \end{aligned}$$

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

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

3 Description of Problem

The problem in this tutorial is similar to the problem described in the “RT3D – BTEX Degradation with Multiple Electron Acceptors” tutorial. 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 m³/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

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3. Clement, T.P., Hooker, B.S., and Skeen, R.S. (1996). Macroscopic Models for Predicting Changes in Saturated Porous Media Properties Caused by Microbial Growth. *Ground Water*, 34(5): 934–942.

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, the user 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 assumed to be as follows: 0.0 mg/L, 9.0 mg/L, 2×10^{-17} (value for X in mg/L), and 3.0×10^{-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 $\rho = 1.6 \times 10^6$ mg/L and $\phi = 0.3$, the initial value of soil bacterial concentration can be expressed (when converted to a 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

Do the following to get started:

1. If GMS is not running, launch GMS.
2. If GMS is already running, select *File* / **New** 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. Click the **Open**  button.
2. Locate and open the file entitled *Tutorials\RT3D\flowmod*.
3. Select the file entitled “flowmod.gpr.”
4. Click **Open**.

At this point, the user should see a grid appear.

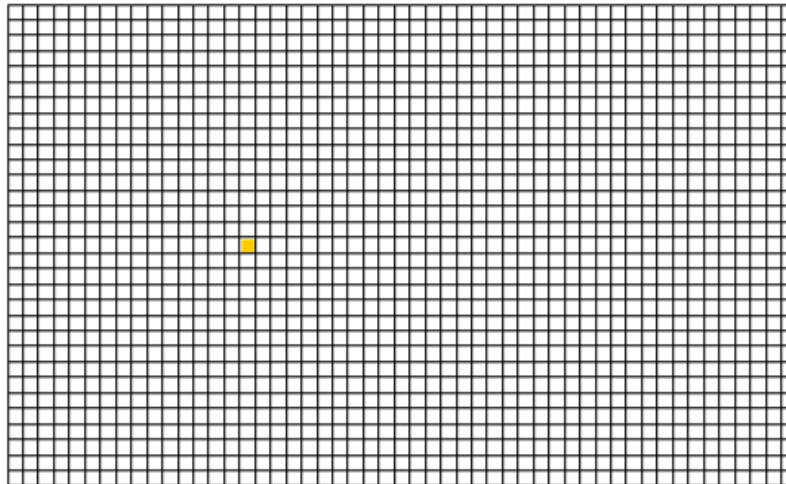



Figure 1 The grid imported with the flowmod.gpr file

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, the user 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. Expand the “3D Grid Data” folder in the Project Explorer.
2. In the Project Explorer, right-click on the “grid”  item.

3. Select the **New MT3D** command.

This initializes MT3D/RT3D and brings up the *Basic Transport Package* dialog.

8 The Basic Transport Package

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

1. Select the *RT3D* option in the *Model* section of the dialog.
2. Select the **Packages** button to open the *MT3D/RT3D Packages* dialog.
3. Turn on the following packages:
 - *Advection Package*
 - *Dispersion Package*
 - *Source/Sink Mixing Package*
 - *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 being modeled are listed by name. The next step is to define the starting concentration for each of these species. The default starting concentration is zero. The user will use the default value for the electron donor, but the user will use non-zero values for the electron acceptor (9.0 mg/L), the aqueous phase bacteria (2×10^{-17} mg/L), and the solid phase bacteria (3×10^{-9} mg bacteria/mg of soil).

1. In the *Basic Transport Package* dialog, select *Electron Acceptor* from the list of species.
2. Enter a value of “9.0” for the starting concentration.
3. Enter a starting value of “2e-17” for the *Aqueous-Phase Bacteria*.
4. Enter a starting value of “3e-9” for the *Soil-Phase Bacteria*.

8.2 Porosity

Next, it is necessary to consider the porosity, which should be set 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, the user will use a single stress period with a length of 730 days (two years).

1. Select the **Stress Periods** button to open the *Stress Periods* dialog.
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, the user 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 are needed for simple post-processing options, the user will specify that a solution be saved every 73 days (every time step).


1. Select the **Output Control** button to open the *Output Control* dialog.
2. Select the *Print or save at specified times* option.
3. Select the **Times** button to open the *Variable Time Steps* dialog.
4. Select the **Initialize Values** button to open the *Initialize Time Steps* dialog.
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, the user must define the concentrations of the 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.

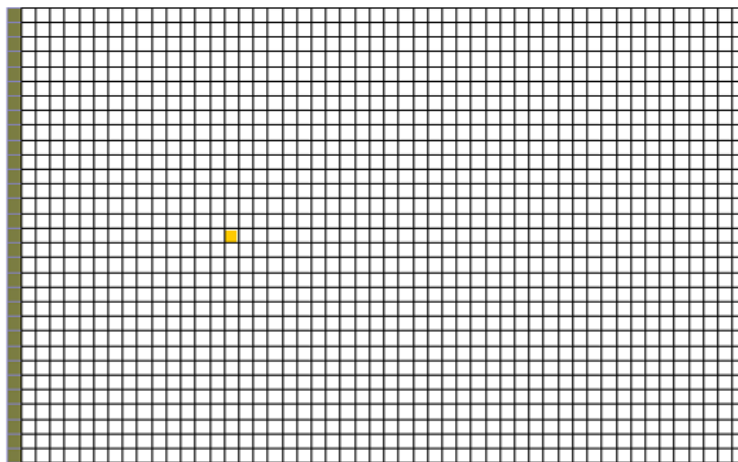


Figure 2 Selecting the cells on the left side of the grid

3. Select the *RT3D* / **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 *RT3D* | **Advection Package** command to open the *Advection Package* dialog.
2. Select the “Method of characteristics (MOC)” option in the drop-down menu for *Solution scheme*.
3. Select the **OK** button to exit the dialog.

11 The Dispersion Package

Next, the user 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 *RT3D* | **Dispersion Package** command to open the *Dispersion Package* dialog.
2. Enter a value of “0.3” for the *TRPT* value.
3. Select the **Longitudinal Dispersivity** button to open the *Longitudinal Dispersivity* dialog.
4. Select the **Constant** → **Grid** button to open the *Grid Value* dialog.
5. Enter a value of “10.0.”
6. Select **OK**.
7. Click **OK** to exit the *Longitudinal Dispersivity* dialog.
8. Select **OK** to exit the *Dispersion Package* dialog.

12 The Source/Sink Mixing Package

Next, the user will define the concentration at the spill location. The user 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 cell containing the injection well (spill location) by clicking anywhere in the interior of the cell.
2. Select the *RT3D* | **Point Sources/Sinks** command.
3. Click the **Add BC** button near the bottom of the dialog.
4. Change the *Type (ITYPE)* to “well (WEL).”
5. In the *Electron Donor* column, enter a concentration of “500” (mg/L).
6. Select the **OK** button to exit the dialog.

13 The Chemical Reaction Package

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

1. Select the *RT3D* | **Chemical Reaction Package** command to open the *RT3D Chemical Reaction Package* dialog.
2. In the *Reaction parameters* section, set *umax* 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, the user 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 *Tutorials\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, select the **Close** button.

15 Running RT3D

At this point, it is possible to save the model and run RT3D.


To run RT3D:

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


16 Viewing the Results

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

16.1 Electron Donor

1. Select the “Electron Donor”  dataset from the Project Explorer. (The user 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 *Contour Options*  button.
4. Change the *Contour 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 side to the right side, as expected.

16.2 Electron Acceptor


Next, the user will view the electron acceptor solution.

1. Select the “Electron Acceptor”  dataset 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, the user will view the solution for the aqueous-phase bacteria.

1. Select the “Aqueous-phase bacteria”  dataset 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, the user will view the solution for the solid-phase bacteria.

1. Select the “Solid-phase bacteria”  dataset from the Project Explorer.

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

17 Conclusion

This concludes the tutorial.