



# **CHEMFLUX<sup>TM</sup>**

**2D / 3D Contaminant Transport Modeling Software**

## **Tutorial Manual**

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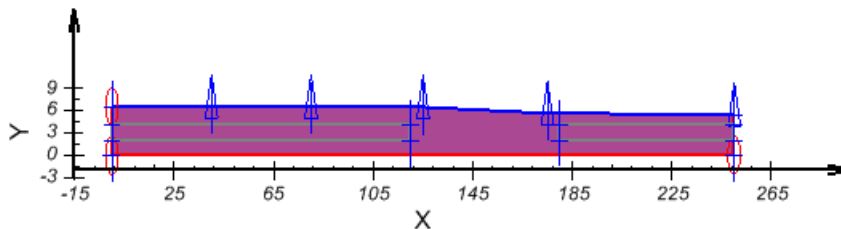
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# 1 A Two Dimensional Example Model

Sudicky (1989) developed the following example. The model considers flow and solute transport in a heterogeneous cross section with a highly irregular flow field, dispersion parameters that are small compared with the spatial discretization, and a large contrast between longitudinal and transverse dispersivities (Zheng and Wang 1999). Below is a description of the seepage model, including model dimensions, boundary conditions, soil properties, and the final flow regime. This is followed by step by step instructions on how to enter and solve the contaminant transport model.

Project Name: Tutorial  
 Model Name: Example2D  
 Minimum authorization required: FULL



It is important to note that you will be analyzing the SVFlux model before the ChemFlux model is completed.

## 1.1 Steady-State SVFLUX Solution

Project Name: Examples Model Name: ChemFlux2D

### • Model Dimensions

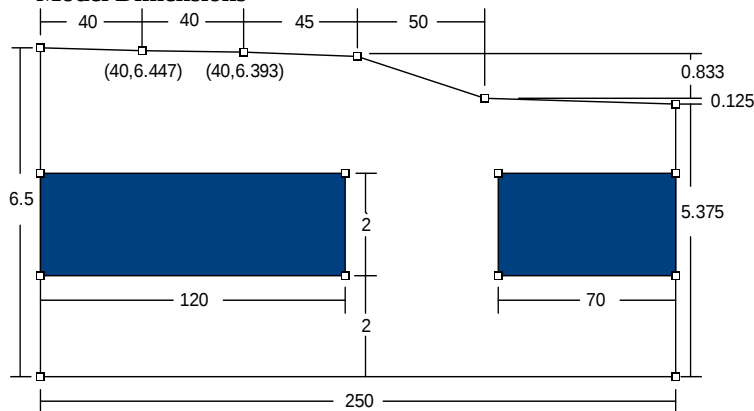


Figure 1: 2D example, model dimensions

- SVFLUX Boundary Conditions

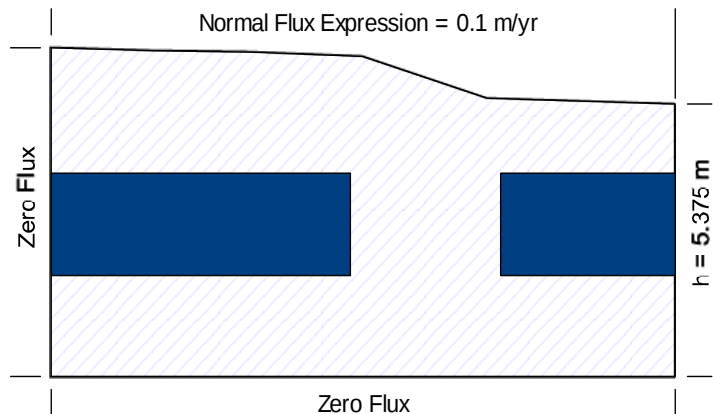


Figure 2: 2D example, seepage boundary conditions

- SVFLUX Soil Properties



Ksat = 5.0e-06 m/s  
ky-ratio = 1.0  
Volumetric water content = 0.35



Ksat = 1.0e-04 m/s  
ky-ratio = 1.0  
Volumetric water content = 0.35

A uniform volumetric water content was set by entering a soil water characteristic curve with three points, (0.0001,0.351), (100,0.35), and (1000,0.349). This soil water characteristic curve was used for both the soils in the model.



**T i p !**

Steady state seepage solutions do not require that the soil water characteristic curves have an initial positive slope. An initial positive slope is only required in transient models where the soil storage will change with time.

- SVFLUX Flow Regime

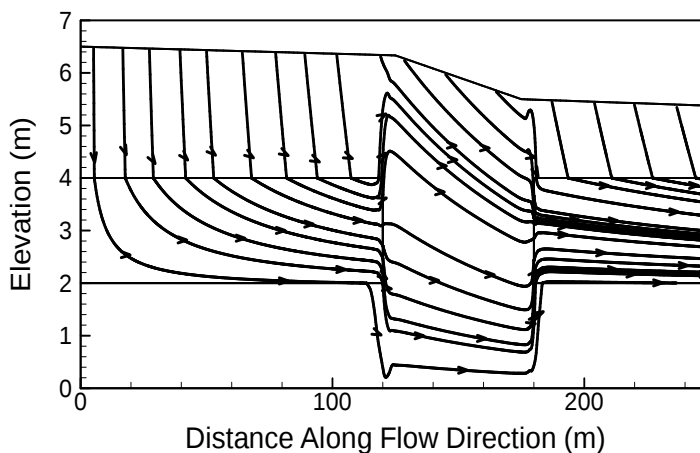


Figure 3: 2D example, flow regime



Tip!

Note that the model is completely saturated.

## 1.2 CHEMFLUX Solution Data

### • CHEMFLUX Boundary Conditions

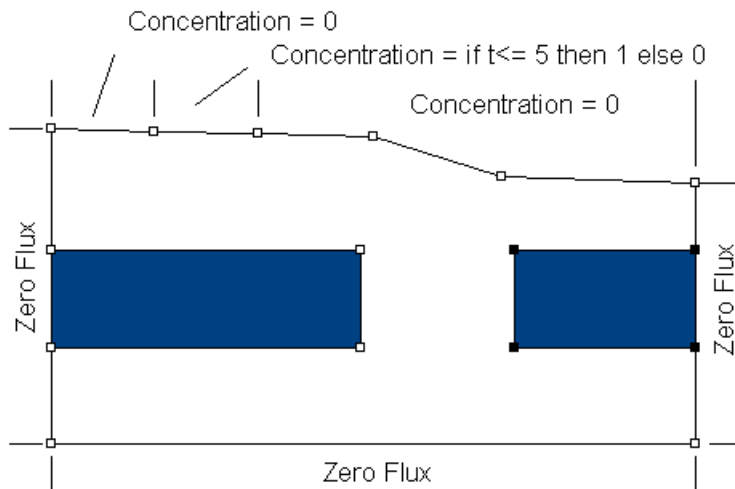


Figure 4: 2D example, CHEMFLUX boundary conditions

### • CHEMFLUX Soil Properties

Only one soil is used for the model with these properties:

Longitudinal Dispersivity,  $\alpha_L = 0.5\text{m}$

Transverse Dispersivity,  $\alpha_T = 0.005\text{m}$

Diffusion Coefficient,  $D^* = 0.0423\text{m}^2/\text{yr}$

## 1.3 SVFLUX Gradients File

A gradient file generated by SVFLUX is required for this example. The seepage model described above has been included in the model files distributed with the SVFLUX software. To generate the necessary seepage gradient file, follow these instructions.

1. Open the SVOOffice 2006 software.
2. From SVOOffice 2006 Manager select Examples as the Project.
3. Ensure that "SVFlux" is in the Application drop-down.
4. Select the model name ChemFlux2D.
4. Click OK.
5. Select Model > Reporting > Output Manager from the menu.
6. Add a transfer file to the Output Manager by pressing the Add Transfer output file button in the

- lower left in the New box.
7. Enter gradient2D as the file name. Select gradx and grady, then press the Add Selection button.
  8. Click OK to close the dialog.
  9. Select Solve > Analyze from the menu to run the model. A window will pop up asking if you would like to save the model file. If you would like to, save the model file.

When the model is finished, the necessary gradient file will be created in the solution folder automatically by SVFLUX. The file is called gradient2D.trn.

## 1.4 Adding a CHEMFLUX Project

The first step in defining a model is to decide the project under which the model is going to be organized. If the project is not yet included you must add the project before proceeding with the model. In this case, the model is placed under a project called Tutorial.

Follow these steps in order to add this project:

1. Access the SVOOffice 2006 Manager dialog.
2. Click New in the upper right of the Projects section.
3. The Create New Project dialog is opened along with a prompt asking for a new Project Name.
4. Type "Tutorial" as the new Project Name and press OK.

The Project Properties dialog is where information specific to each project is stored. This will include the Project Name, Project Folder, and Project Notes information.



The Project Name is the only required information needed to define a project. The rest of the fields are optional.

The dialog is opened ready to accept information.

It should be noted that once the project is defined it will be identified by the Project Name throughout the rest of the program. Also, CHEMFLUX does not allow you to specify two projects with the same Project Name.

5. Fill out the Project Properties dialog with the desired information.
6. To exit this dialog and return to SVOOffice 2006 Manager, click OK. The project information is automatically saved upon entry.

## 1.5 Adding a CHEMFLUX Model

The first step in defining a model is to decide the project under which the model is going to be organized. If the project is not yet included you must add the project before proceeding with the model. Once a project has been created any number of models may be stored in it.

When the SVOOffice 2006 Manager dialog is opened there will be a list of the projects that have been defined. In this case there is only the Tutorial project. To add a model:

1. Press the "New..." button under the 'Models' heading.
2. Select ChemFlux for the Application.
3. Enter Example2D in the Model Name box.
4. Select 2D for System, Transient for Type, Metric for Units, and Years for Time Units.
5. Click the OK button to save the model and close the New Model dialog.
6. The new model will automatically added be added to the Models list.



You will notice that there is no distinction between steady state and transient state in CHEMFLUX. This is because all models are considered to be transient state.

**T i p !**

## 1.6 Opening the CHEMFLUX Model

If the model was just added it will already be open in the workspace. When returning to the model, follow these steps to open it in the workspace:

1. Select the Tutorial Project.
2. Ensure that ChemFlux is selected from the Application drop-down.
3. Select the Example2D model.
4. The model may be opened by clicking the Open button or by double clicking on the model name.

## 1.7 Defining the CHEMFLUX Model

The following section provides instructions on how to begin defining the model in the workspace.

### 1.7.1 Import SVFLUX Geometry

Geometry must be imported from SVFLUX before any other modeling can be done in CHEMFLUX.

1. Select the Model > Geometry > Import Geometry > From Existing Model... menu.
2. The Import Geometries dialog will pop up. Select the appropriate project name, Examples.
3. Select the ChemFlux2D model.
4. Press the Import button.

The import includes any regions, region shapes, surfaces, surface grids and elevations. These parts of the model definition are fixed in CHEMFLUX. World coordinate system settings and features are also imported if present, but may be edited in CHEMFLUX.

### 1.7.2 Specify Settings

The first step in defining the model is to specify the settings that will be used for the model. To open the Settings dialog select Model > Settings in the workspace menu.

The Settings dialog will contain information about the current model System, Units, Time, and contaminant transport processes.

1. To open the Settings dialog select Model > Settings in the workspace menu.
2. Check Advection and Dispersion in the Processes box under the General tab.
3. Enter a Start Time of 0, a Time Increment of 1 yr, and an End Time of 20 yr.
4. Select the Advection tab.
5. Choose Import from SVFlux from the Advection Control option.
6. Click Browse.
7. Specify the file Examples\_ChemFlux2D\_2.trn that was generated by SVFLUX.
8. Press OK to close the Settings dialog.



It is very important that the .TRN file and the geometry are obtained from the same SVFLUX model.

**T i p !**

### 1.7.3 Define Material Properties

The next step in defining the model is to enter the material properties for the single soil that will be used in the model.

1. Open the Soils dialog by selecting Model > Soils > Manager from the menu.
2. Click the New... button to create a soil.
3. Enter "Soil#1" for the soil name.
4. Double-click on the new soil to open the Soil Properties dialog.
5. Move to the Dispersion tab.
6. Refer to the data provided under the "ChemFlux Solution Data" section at the beginning of this tutorial. Enter the Longitudinal Dispersivity,  $\alpha_L = 0.5m$ .
7. Enter the Transverse Dispersivity,  $\alpha_T = 0.005m$ .
8. Select Constant as the Diffusion option.
9. Enter the Diffusion Coefficient,  $D^* = 0.0423m^2/yr$ .
10. Close the Soil Properties and Soil Manager dialogs.

### 1.7.4 Assign Soils to Regions

A region in CHEMFLUX is the basic building block for a model. A region represents both a physical portion of soil being modeled and a visualization area in the CHEMFLUX CAD workspace. A region will have a set of geometric shapes that define its soil boundaries. Also, other modeling objects including features, flux sections, water tables, text, and line art are defined on any given region.

This model is divided into three regions, but the same soil will be assigned to each region. To specify the soil for the regions follow these steps:

1. Open the regions dialog selecting Model > Geometry > Regions from the menu.
2. Select Soil#1 from the drop-down as the soil for Region 1.
3. Repeat for Region 2 and Region 3.
4. Click OK to close the dialog.

### 1.7.5 Specify Boundary Conditions

Boundary conditions must be applied to region points. Once a boundary condition is applied to a boundary point this defines the starting point for that particular boundary condition. The boundary condition will then extend over subsequent line segments around the edge of the region in the direction in which the region shape was originally entered. Boundary conditions remain in effect around a shape until re-defined. The user may not define two different boundary conditions over the same line segment.

More information on boundary conditions can be found in Menu System > Model Menu > Boundary Conditions > 2D Boundary Conditions in your User's Manual.

The next step is to specify the boundary conditions. Refer to Figure 2 at the beginning of this tutorial. A zero flux condition will be defined on sides and base of the model with various concentration conditions being applied to the top boundary. The boundary conditions are applied to the outer Region 1; none are applied to the other 2 regions.

1. Select "Region 1" by going to Model > Geometry > Regions in the menu and clicking on Region 1.
2. Press OK to close the dialog.
3. From the menu select Model > Boundaries > Boundary Conditions. The Boundary Conditions dialog will open.

**Boundaries**

Region Name: Region 1      Select Shape Index: 585089471

| X   | Y     | Boundary Condition       | Expression or Data      | Units            |
|-----|-------|--------------------------|-------------------------|------------------|
| 0   | 0     | Flux Expression          | 0                       | g/yr/m...        |
| 250 | 0     | Continue                 |                         |                  |
| 250 | 5.375 | Concentration Expression | 0                       | g/m <sup>3</sup> |
| 175 | 5.5   | Continue                 |                         |                  |
| 125 | 6.333 | Continue                 |                         |                  |
| 80  | 6.393 | Concentration Expression | if t <= 5 then 1 else 0 | g/m <sup>3</sup> |
| 40  | 6.447 | Concentration Expression | 0                       | g/m <sup>3</sup> |
| 0   | 6.5   | Flux Expression          | 0                       | g/yr/m...        |

Update Selected Segment

Boundary Condition: Flux Expression      Length: 250 m

Expression: 0      Build Equation...

NOTE: boundary conditions defined at a point remain in effect until re-defined at a subsequent point

OK Cancel

4. Select the point (0,0) from the list.
5. From the Boundary Condition drop down select a Zero Flux boundary condition.
6. Repeat these steps to define the boundary conditions for the remaining Region 1 segment as shown in the diagram and in the screen-shot above. (Be sure to define a Zero Flux condition for the last point in the list).
7. Press OK to exit the dialog and save the defined boundary conditions.



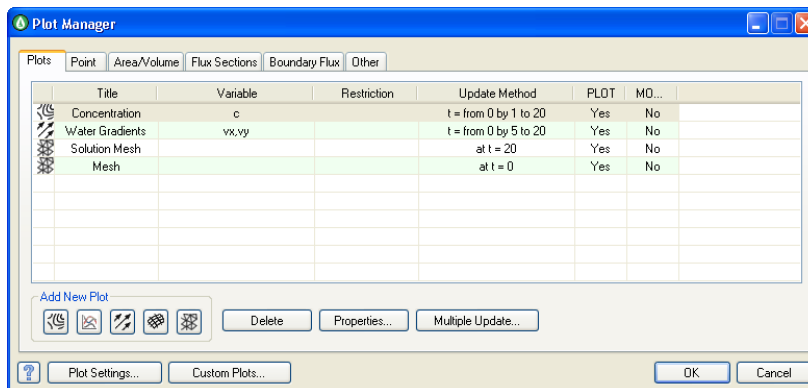
**Tip!**

Any boundary condition becomes the boundary condition for the following line segments that have a Continue boundary condition until a new boundary condition is specified.

## 1.8 Specify Plots

There are many plot types that can be specified to visualize the results of the model. A few will be generated for this tutorial example model including a plot of the solution mesh, concentration contours, and water gradient vectors.

1. Open the Plot Manager dialog by selecting Model > Reporting > Plot Manager from the menu.
2. The toolbar at the bottom left of the dialog contains a button for each plot type. Click on the Contour button to begin adding the first contour plot. The Plot Properties dialog will open.
3. Enter the title Concentration.
4. Select c as the variable to plot from the drop-down.
5. Select the PLOT from the Output Option tab.
6. Move to the Update Method tab and enter a Start Time = 0, a Time Increment = 1, and an End Time = 20.
7. Move to the Zoom tab and enter X = 100, Y = 0.1, Width = 100, and Height = 6.6.
8. Click OK to close the dialog and add the plot to the list.
9. Repeat steps 2 – 8 to create the remaining plots. Note that the Mesh plot does not require entry of a variable.
10. Click OK to close the Plot Manager and return to the workspace.



## 1.9 Specify Output Files

There are four output file types that can be specified to export the results of the model. One will be generated for this tutorial example model: a file to output variables for advanced visualization in the AcuMesh software.

1. Open the Output Manager dialog by selecting Model > Reporting > Output Manager from the menu.
2. The toolbar at the bottom left of the dialog contains a button for each output file type. Click on the AcuMesh button to begin adding the output file. The Output File Properties dialog will open.
3. Enter the title AcuMesh.
4. Press the Select All button.
5. Press the Add Selection button.
6. Check the Write File box found under the Output Options tab.
7. Click OK to close the dialog and add the output file to the list.

### 1.9.1 Setting Time Steps

The Output File Properties dialog also allows the user to define timesteps for the current model. This can be accessed by using the Update Method tab on the Output File Properties dialog.

1. Enter a Start Time of 0, a Time Increment of 1 yr, and an End Time of 20 yr.
2. Click OK to close the Output File Properties dialog and return to the workspace.
3. Click OK to close the Output Manager and return to the workspace.

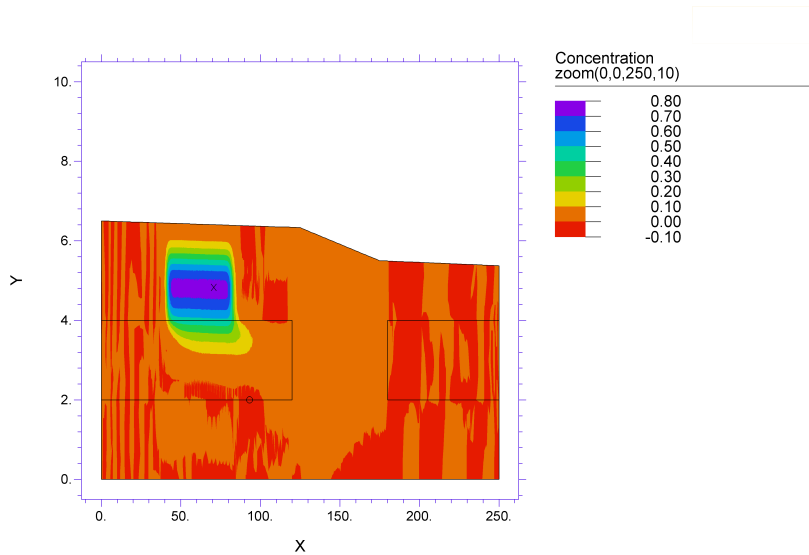
## 1.10 Analyze

The next step is to analyze the model. Select Solve > Analyze from the menu. This action will write the descriptor file and open the CHEMFLUX solver. The solver will automatically begin solving the model.

## 1.11 Results

After the model has finished solving, the results will be displayed in the dialog of thumbnail plots within the CHEMFLUX solver. Right-click the mouse and select Maximize to enlarge any of the thumbnail plots. The following is a short summary of plots illustrating the movement of the plume through the model for times of 8 years, 12 years, and 20 years.

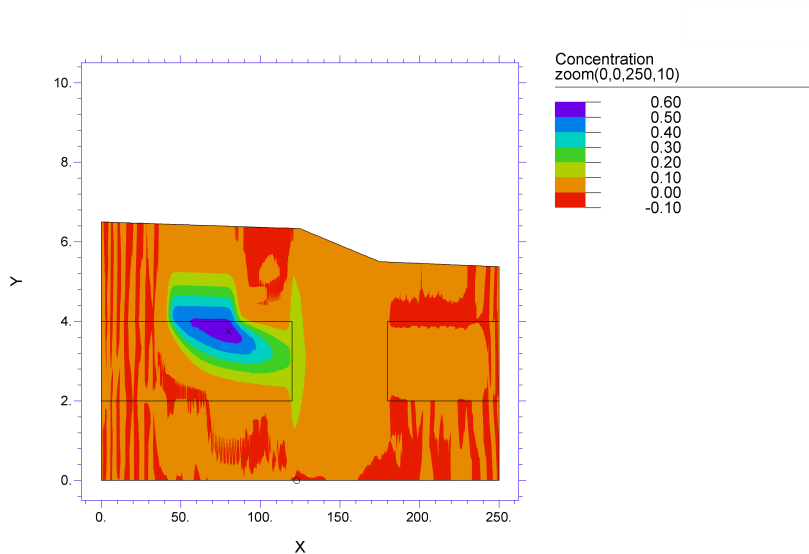
- Time = 8 years



Examples\_2DExample: Cycle=96 Time= 8.0000 dt= 0.1961 p2 Nodes=6375 Cells=3068 RMS Err= 2.9e-4  
Integral= 56.74936

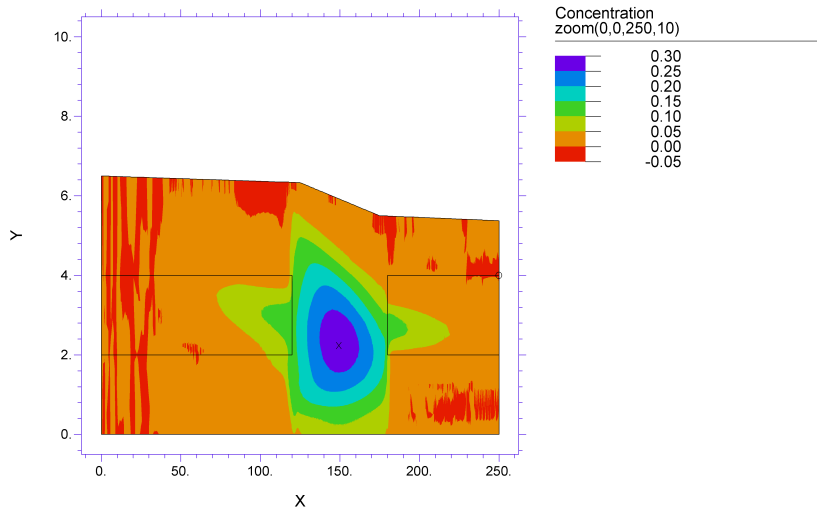
The source has been shut off for 3 years

- Time = 12 years



Examples\_2DExample: Cycle=129 Time= 12.000 dt= 0.1492 p2 Nodes=7314 Cells=3559 RMS Err= 3.6e-4  
Integral= 57.30137

- Time = 20 years

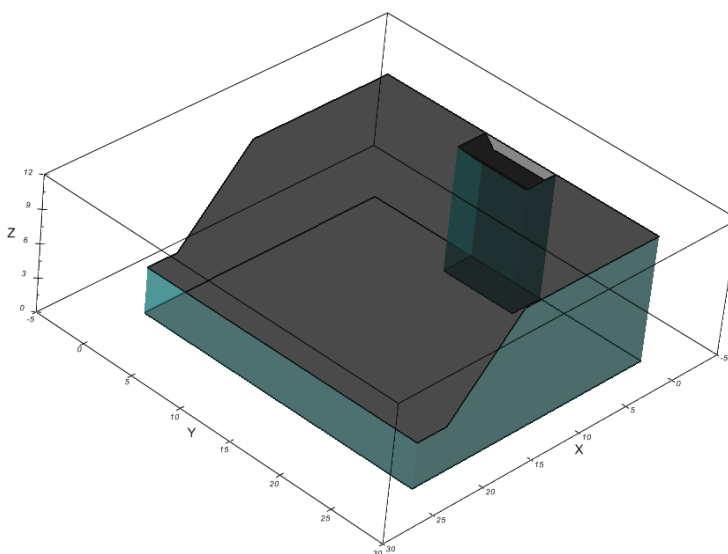


Examples\_2DExample: Cycle=178 Time= 20.000 dt= 0.3099 p2 Nodes=12577 Cells=6140 RMS Err= 3.7e-4  
Integral= 61.18735

## 2 A Three Dimensional Example Model

The following example will introduce you to the three dimensional model in CHEMFLUX. The model will be used to investigate if contaminant from a reservoir will travel to a river channel due to advection and dispersion processes within a 400 day time period. The 400 day time period was chosen as the time necessary to install a pumping well between the river channel and the reservoir. The well will be used to pump contaminant from the ground to ensure the plume will not reach the river channel. The example model begins with a brief description of the steady state seepage analysis completed to provide CHEMFLUX with computed seepage gradients. Next a detailed set of instructions guides the user through the creation of the 3D contaminant transport model.

Project Name: Tutorial  
Model Name: Example3D  
Minimum authorization required: STUDENT



It is important to note that you will be analyzing the SVFlux model before the ChemFlux model is completed.

### 2.1 Steady State SVFLUX Solution

Advection is known as the process by which solutes are transported by the bulk motion of the flowing groundwater Freeze & Cherry (1979). The bulk motion of the flowing groundwater or seepage gradients are solved using SVFLUX. SVFLUX calculates the seepage gradients and writes them to a text file. The CHEMFLUX solver then reads this text file when calculating the contaminant transport solution. Below is a description of the seepage model solved by SVFLUX.

Project Name: Examples      Model Name: ChemFlux3D

- **Model Dimensions**

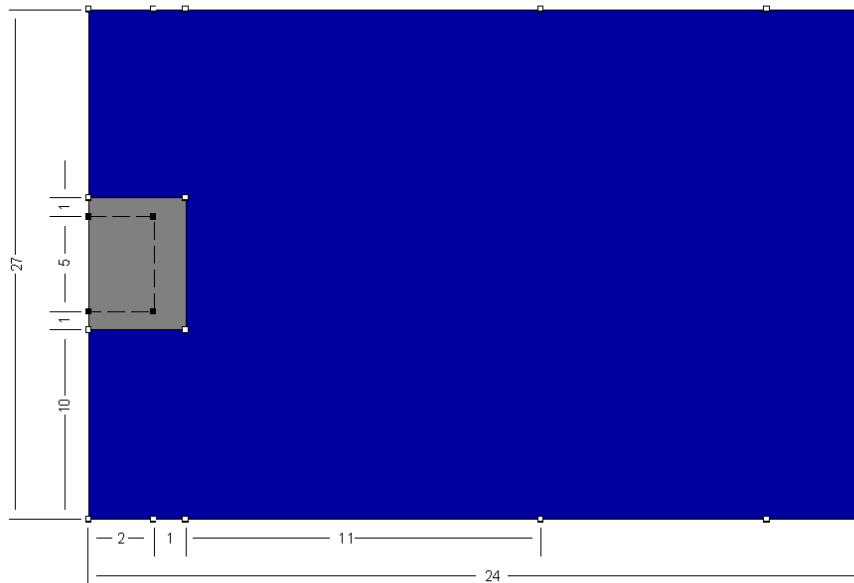


Figure 5: 3D Example; Model Dimensions

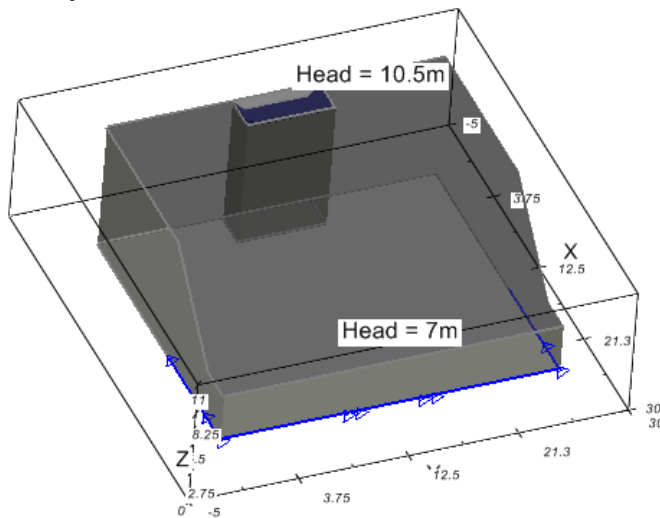
- **Surface 1 Grid**

| X | Y  | Z |  | X  | Y  | Z |
|---|----|---|--|----|----|---|
| 0 | 0  | 0 |  | 14 | 0  | 0 |
| 0 | 10 | 0 |  | 14 | 10 | 0 |
| 0 | 11 | 0 |  | 14 | 11 | 0 |
| 0 | 16 | 0 |  | 14 | 16 | 0 |
| 0 | 17 | 0 |  | 14 | 17 | 0 |
| 0 | 27 | 0 |  | 14 | 27 | 0 |
| 2 | 0  | 0 |  | 21 | 0  | 0 |
| 2 | 10 | 0 |  | 21 | 10 | 0 |
| 2 | 11 | 0 |  | 21 | 11 | 0 |
| 2 | 16 | 0 |  | 21 | 16 | 0 |
| 2 | 17 | 0 |  | 21 | 17 | 0 |
| 2 | 27 | 0 |  | 21 | 27 | 0 |
| 3 | 0  | 0 |  | 24 | 0  | 0 |
| 3 | 10 | 0 |  | 24 | 10 | 0 |
| 3 | 11 | 0 |  | 24 | 11 | 0 |
| 3 | 16 | 0 |  | 24 | 16 | 0 |
| 3 | 17 | 0 |  | 24 | 17 | 0 |
| 3 | 27 | 0 |  | 24 | 27 | 0 |

- **Surface 2 Grid**

| X | Y  | Z  |  | X  | Y  | Z  |
|---|----|----|--|----|----|----|
| 0 | 0  | 11 |  | 14 | 0  | 11 |
| 0 | 10 | 11 |  | 14 | 10 | 11 |
| 0 | 11 | 10 |  | 14 | 11 | 11 |
| 0 | 16 | 10 |  | 14 | 16 | 11 |
| 0 | 17 | 11 |  | 14 | 17 | 11 |
| 0 | 27 | 11 |  | 14 | 27 | 11 |
| 2 | 0  | 11 |  | 21 | 0  | 4  |
| 2 | 10 | 11 |  | 21 | 10 | 4  |
| 2 | 11 | 10 |  | 21 | 11 | 4  |
| 2 | 16 | 10 |  | 21 | 16 | 4  |
| 2 | 17 | 11 |  | 21 | 17 | 4  |
| 2 | 27 | 11 |  | 21 | 27 | 4  |
| 3 | 0  | 11 |  | 24 | 0  | 4  |
| 3 | 10 | 11 |  | 24 | 10 | 4  |
| 3 | 11 | 11 |  | 24 | 11 | 4  |
| 3 | 16 | 11 |  | 24 | 16 | 4  |
| 3 | 17 | 11 |  | 24 | 17 | 4  |
| 3 | 27 | 11 |  | 24 | 27 | 4  |

- Boundary Conditions**



**Figure 6: 3D Example; Boundary Conditions**

The steady state seepage model is set up to simulate a pond or reservoir a certain distance from a river channel. The water levels in the reservoir and river channel are set using head boundary conditions. The level of water in the reservoir is set using a Head Expression = 10.5m set on surface 2 for the reservoir region. The level of water in the river channel is set using a Head Expression = 7m set on the line segment extending from point (14,0) to (14,27) on surface 1.

- Soil Properties**



There is only one soil in the saturated 3D example model despite the presence of separate colors for the two regions. Two regions have been implemented in this model in order to apply the necessary boundary conditions. The soil in the model has a hydraulic conductivity,  $ksat = 2.17e-01$  m/d.

- **Flow Regime**

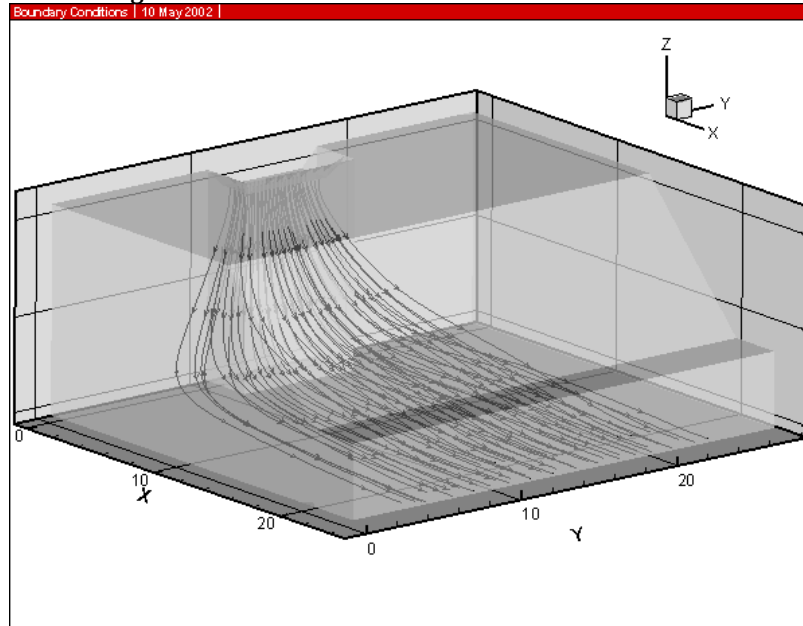


Figure 7: 3D Example; Flow Regime

Flow lines show that groundwater is flowing from the reservoir toward the adjacent river channel. The presence of unsaturated soil near the surface of the model is causing water to first flow down to the saturated zone and then move toward the river channel.

## 2.2 CHEMFLUX Solution Data

- **CHEMFLUX Boundary Conditions**

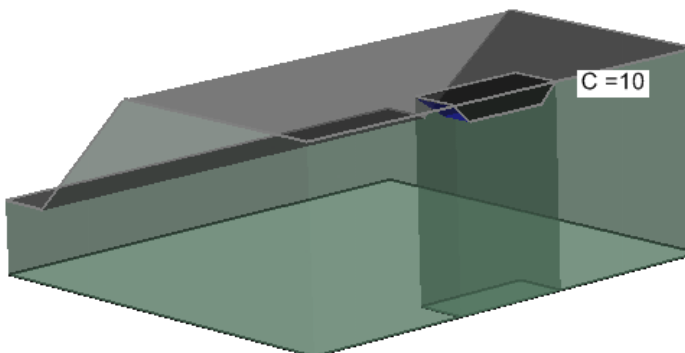


Figure 8: 3D example, CHEMFLUX boundary conditions

- **CHEMFLUX Soil Properties**

Only one soil is used for the model with these properties:

Longitudinal Dispersivity,  $\alpha_L = 1\text{m}$

Transverse Dispersivity,  $\alpha_T = 1\text{m}$

Diffusion Coefficient,  $D^* = 0\text{m}^2/\text{day}$

## 2.3 SVFLUX Gradients File

A gradient file generated by SVFLUX is required for this example. The seepage model described above has been included in the model files distributed with the SVFLUX software. To generate the necessary seepage gradient file, follow these instructions.

1. Open the SVOOffice 2006 software.
2. From SVOOffice 2006 Manager select Examples as the Project.
3. Ensure that "SVFlux" is in the Application drop-down.
4. Select the model name ChemFlux3D.
5. Press the Open button.
6. Select Model > Reporting > Output Manager from the menu.
7. Add a transfer file to the Output Manager by pressing the Add Transfer Output File button in the lower left in the New box.
8. Enter gradient3D as the file name. Select gradx, grady, and gradz and press the Add Selection button.
9. Click OK to close the dialog.
10. Select Solve > Analyze from the menu to run the model.

When the model is finished, the necessary gradient file will be created in the solution folder automatically by SVFLUX. The file is called gradient3D.trn.

## 2.4 Adding a CHEMFLUX Project

The first step in defining a model is to decide the project under which the model is going to be organized. If the project is not yet included you must add the project before proceeding with the model. In this case, the model is placed under a project called Tutorial.

Follow these steps in order to add this project:

1. Access the SVOOffice 2006 Manager dialog. If a project named Tutorial already exists skip to the Adding a ChemFlux Model section.
2. Click New in the upper right of the Projects section.
3. The Create New Project dialog is opened along with a prompt asking for a new Project Name.
4. Type "Tutorial" as the new Project Name and press OK.

The Project Properties dialog is where you information specific to each project is stored. This will include the Project Name, Location, Start Date, End Date, Project Notes, client information, contractor and project engineer information.



**Tip!**

The Project Name is the only required information needed to define a project. The rest of the fields are optional.

The dialog is opened ready to accept information.

Note that once the project is defined it will be identified by the Project Name throughout the rest of the program. Also, CHEMFLUX does not allow you to specify two projects with the same Project Name.

5. Fill out the Project Properties dialog with the desired information.
6. To exit this dialog and return to Projects / Models click OK. The project information is automatically saved upon entry.

## 2.5 Adding a CHEMFLUX Model

Once a project has been created any number of models may be stored in it. When the Projects/Models dialog is opened there will be a list of the projects that have been defined. In this case there is only the Tutorial project. To add a model:

1. Press the "New..." button under the 'Models' heading.
2. Enter Example3D in the Model Name box.
3. Select 3D for System, Transient for Type, Metric for Units, and Days for Time Units.
4. Click the OK button to save the model and close the New Model dialog.
5. The new model will automatically be opened in the workspace.

## 2.6 Opening the Model

If the model was just added it will already be open in the workspace. When returning to the model, follow these steps to open it in the workspace:

1. Select the Tutorial project in the SVOOffice 2006 Manager dialog.
2. Ensure that ChemFlux is selected in the Application drop-down.
3. Select Example3D from the Models list.
4. The model may be opened by clicking the Open button or by double clicking on the model name.

## 2.7 Defining the Model

The following section provides instructions on how to begin defining the model in the workspace.

### 2.7.1 Import SVFLUX Geometry

Geometry must be imported from SVFLUX before any other modeling can be done in CHEMFLUX.

1. Select the Model > Geometry > Import Geometry > From Existing Model... menu.
2. The Import Geometries menu will pop up. Select the appropriate project name Examples.
3. Select the ChemFlux3D model.
4. Press the Import button.

The import includes any regions, region shapes, surfaces, surface grids and elevations. These parts of the model definition are fixed in CHEMFLUX. World coordinate system settings and features are also imported if present, but may be edited in CHEMFLUX.

## 2.7.2 Specify Settings

The next step in defining the model is to specify the settings that will be used for the model.

The Settings dialog will contain information about the current model System, Units, Time, and contaminant transport processes.

1. To open the Settings dialog select Model > Settings in the workspace menu.
2. Check Advection and Dispersion in the Processes section.
3. Enter a Start Time of 0, a Time Increment of 50 days, and an End Time of 400 days.
4. Select the Advection tab.
5. Choose Import from SVFlux from the Advection Control option.
6. Click Browse.
7. Specify the file Examples\_ChemFlux3D\_2.grd that was generated by SVFLUX.



It is very important that the .GRD file and the geometry are obtained from the same SVFLUX model.

In order to improve solution time for the purposes of this tutorial certain finite-element options will be set. The finite element mesh node limit and grid spacing will be set to generate a simpler mesh that will increase the solution time.

8. Select Model > FEM Options from the menu to open the FEM Options dialog.
9. Set the NODELIMIT as 800. (This is the student version maximum)
10. Set the NGRID parameter to 5. (This is the student version maximum)
11. Press OK to close the FEM Options dialog.
12. Press OK to close the Settings dialog.

## 2.7.3 Define Material Properties

The next step in defining the model is to enter the material properties for the single soil that will be used in the model.

1. Open the Soils Manager dialog by selecting Model > Soils > Manager... from the menu.
2. Click the New Soil button to create a soil. The Soil Properties dialog will open automatically.
3. Double-click on the new soil to open the Soil Properties dialog.
4. Enter the information above into the appropriate fields on the Description tab.
5. Move to the Dispersion tab.
6. Refer to the data provided at the beginning of this tutorial. Enter the Longitudinal Dispersivity,  $\alpha_L = 1\text{m}$ .
7. Enter the Transverse Dispersivity,  $\alpha_T = 1\text{m}$ .
8. The Diffusion option is set to Constant as the gradient file specified does not contain volumetric water content, which is required to define a diffusion curve.
9. Enter the Diffusion Coefficient,  $D^* = 0\text{m}^2/\text{day}$ .
10. Close the Soil Properties and Soil Manager dialogs.

## 2.7.4 Specifying a Soil by Region and Layer

Each region will cut through all the layers in a model creating a separate “block” on each layer. Each block can be assigned a soil or be left as void. A void area is essentially air space. In this model all “blocks” will be assigned a soil.

1. Select “Slope” in the Region Selector.
2. Select Model > Soils > Region Soils from the menu to open the Region Soils dialog.
3. Select the 3D Tutorial Soil soil from the drop-down for Layer 1.
4. Close the dialog using the OK button.
5. Select “Reservoir” in the Region Selector.
6. Select Model > Soils > Region Soils from the menu to open the Region Soils dialog.
7. Select the 3D Tutorial Soil soil from the drop-down for Layer 1.
8. Close the dialog using the OK button.

### 2.7.5 Specify Boundary Conditions

Boundary conditions must be applied to region points. Once a boundary condition is applied to a boundary point this defines the starting point for that particular boundary condition. The boundary condition will then extend over subsequent line segments around the edge of the region in the direction in which the region shape was originally entered. Boundary conditions remain in effect around a shape until re-defined. The user may not define two different boundary conditions over the same line segment.

More information on boundary conditions can be found in Menu System > Model Menu > Boundary Conditions > 2D Boundary Conditions in your User's Manual.

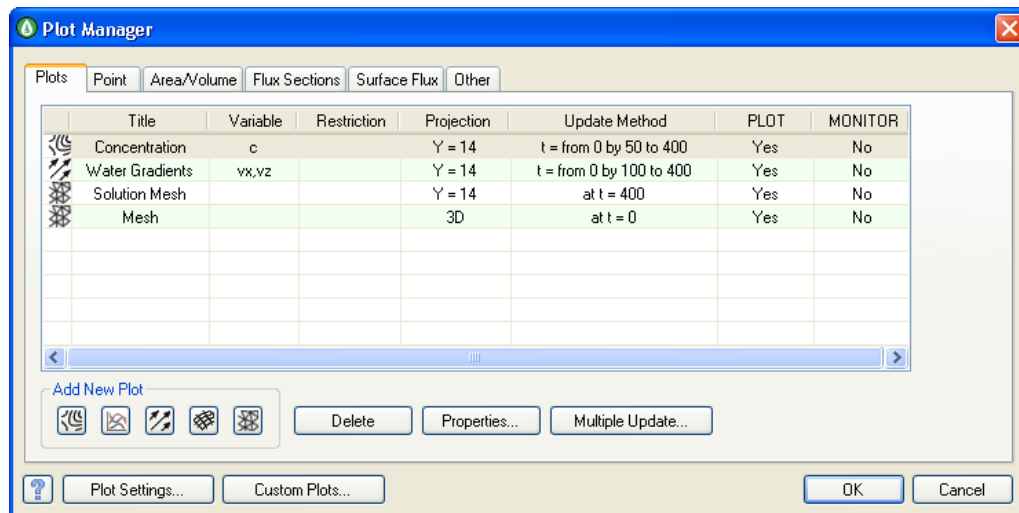
The next step is to specify the boundary conditions on the region shapes. The only boundary condition that is required for this model is to set a Concentration Expression condition for the reservoir region on Surface 2. The steps for specifying the boundary condition are thus:

1. Select the “Reservoir” region in the drawing space.
2. From the menu select Model > Boundaries > Boundary Manager. The boundary conditions dialog will open and display the boundary conditions for Surface 1.
3. Select Surface 2 from the Surface option box.
4. Select Concentration Expression from the Boundary Condition combo box under the Surface Boundary Condition section. This will cause the Concentration Expression box to be enabled.
5. In the Expression box enter a concentration of 1.
6. Click the OK button to close the dialog.

## 2.8 Specify Plots

There are many plot types that can be specified to visualize the results of the model. A few will be generated for this tutorial example model including a plot of the concentration contours, solution mesh, and water gradient vectors.

1. Open the Plot Manager dialog by selecting Model > Reporting > Plot Manager from the menu.



- The toolbar at the bottom left of the dialog contains a button for each plot type. Click on the Contour button to begin adding the first contour plot. The Plot Properties dialog will open.
- Enter the title Concentration.
- Select c as the variable to plot from the drop-down.
- Move to the Update Method tab.
- Press the Arrow to put the model times in the plot time fields.
- Move to the Projection tab.
- Select Plane Projection option.
- Select Y from the Coordinate Direction drop-down.
- Enter 14 in the Coordinate field. This will generate a 2D slice at Y = 14m on which the concentration contours will be plotted.
- Move to the Output Options tab.
- Select the PLOT output option.
- Click OK to close the dialog and add the plot to the list.
- Repeat these steps 2 – 12 to create the plots shown above. Note that the Mesh plot does not require entry of a variable.
- Click OK to close the Plot Manager and return to the workspace.

## 2.9 Specify Output Files

There are 4 output file types that can be specified to export the results of the model. One will be generated for this tutorial example model: a file to output the results to AcuMesh for advanced visualization.

- Open the Output Manager dialog by selecting selecting Model > Reporting > Plot Manager from the menu.
- The toolbar at the bottom left of the dialog contains a button for each output file type. Click on the AcuMesh button to begin adding the output file. The Output File Properties dialog will open.
- Enter the title TutorialAcuMesh.
- Select variables c, vx, vy, and vz in the list.
- Press the Add Selection button.
- Make sure the Write File box contains a check mark.
- Click OK to close the dialog and add the output file to the list.
- Click OK to close the Output Manager and return to the workspace.

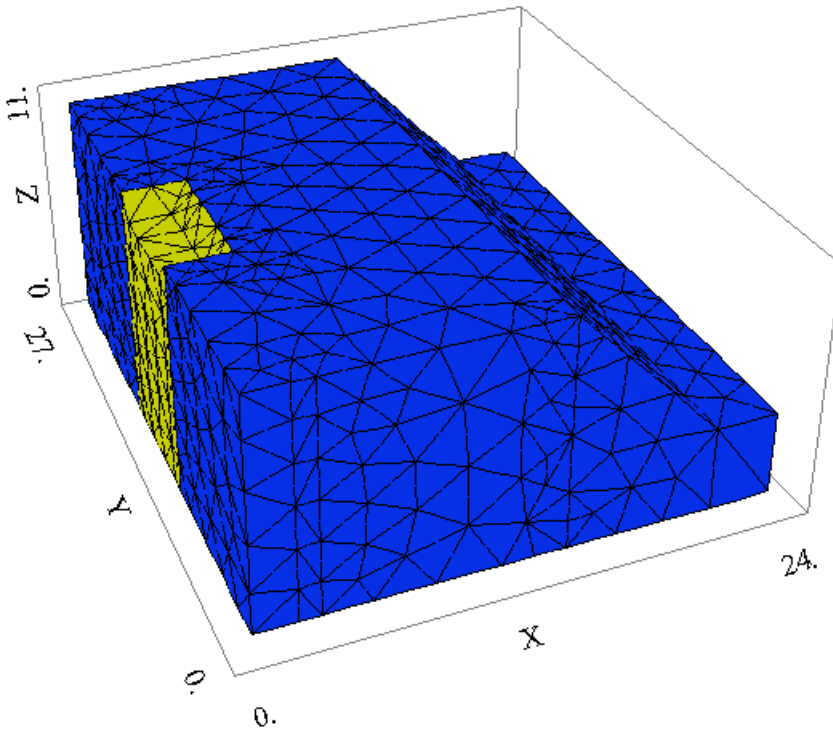
## 2.10 Analyze

The next step is to analyze the model. Select Solve > Analyze from the menu. This action will write the descriptor file and open the CHEMFLUX solver. The solver will automatically begin solving the model.

## 2.11 Results

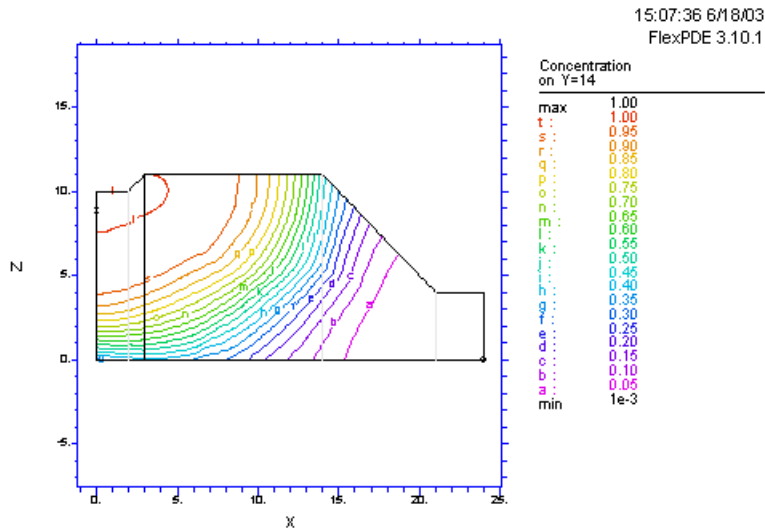
After the model has finished solving, the results will be displayed in the dialog of thumbnail plots within the CHEMFLUX solver. Right-click the mouse and select Maximize to enlarge any of the thumbnail plots. This section will give a brief analysis for each plot that was generated.

### 2.11.1 Solution Mesh



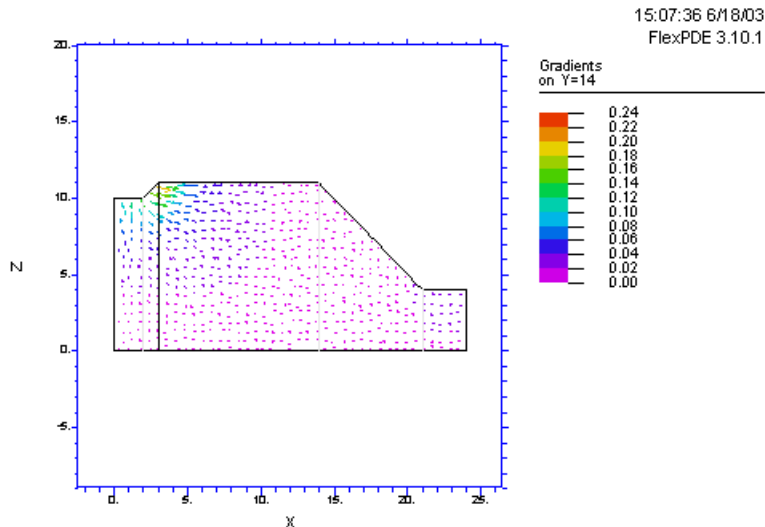
The Mesh plot displays the finite-element mesh generated by the solver. The mesh is automatically refined in critical areas. Right-click on the plot and select Rotate to enable the rotate window.

## 2.11.2 Concentration Contours



In this contour plot it can be seen the concentration is equal to 1 at the reservoir and decreases to 0 at the river.

## 2.11.3 Flow Vectors

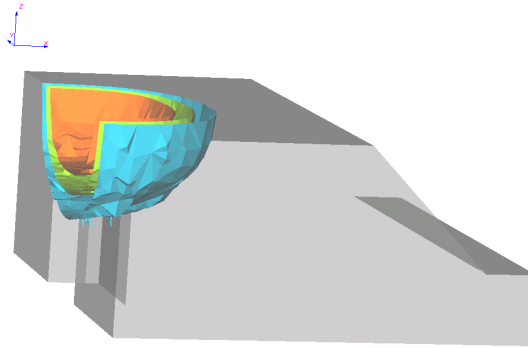


Gradient Vectors show both the direction and the magnitude of the flow at specific points in the model. Vectors illustrate that flow is from right to left towards the river in this view with higher gradients near the reservoir.

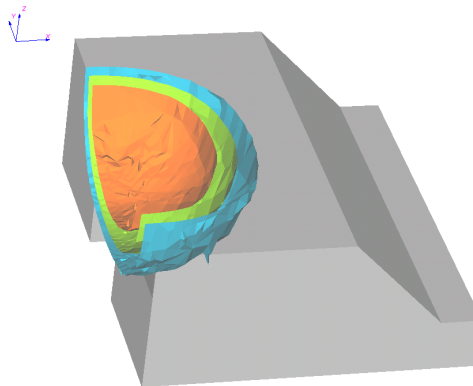
### 2.11.4 AcuMesh

The following is a short summary of plots created in AcuMesh illustrating the movement of the plume through the model for times of 50 days, 100 days, and 400 days. Note that the plume does not reach the river channel in within the 400 day time period.

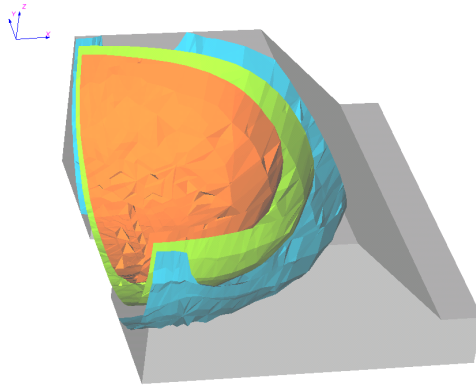
- **Time = 50 days**



- **Time = 100 days**



- Time = 400 days



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