



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

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

## Tutorial Manual

**ED-4B**

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- **SVFLUX Boundary Conditions**

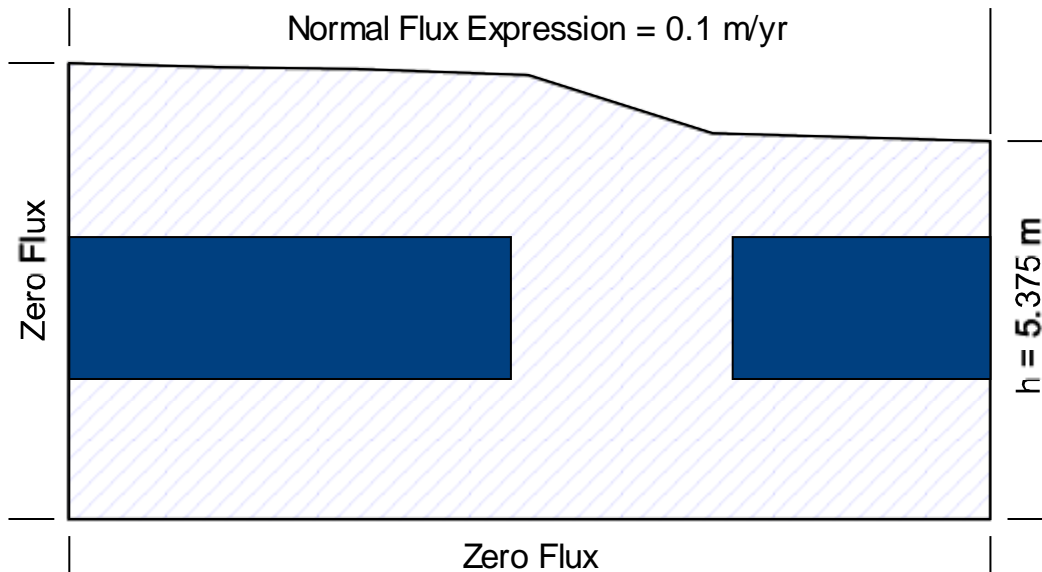



Figure 2: 2D example, seepage boundary conditions

- **SVFLUX Soil Properties**

	
<p>Ksat = 5.0e-06 m/s          ky-ratio = 1.0          Volumetric water content = 0.35</p>	<p>Ksat = 1.0e-04 m/s          ky-ratio = 1.0          Volumetric water content =</p>

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 problem.



**Tip!**

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 problems where the soil storage will change with time.

- **SVFLUX Flow Regime**

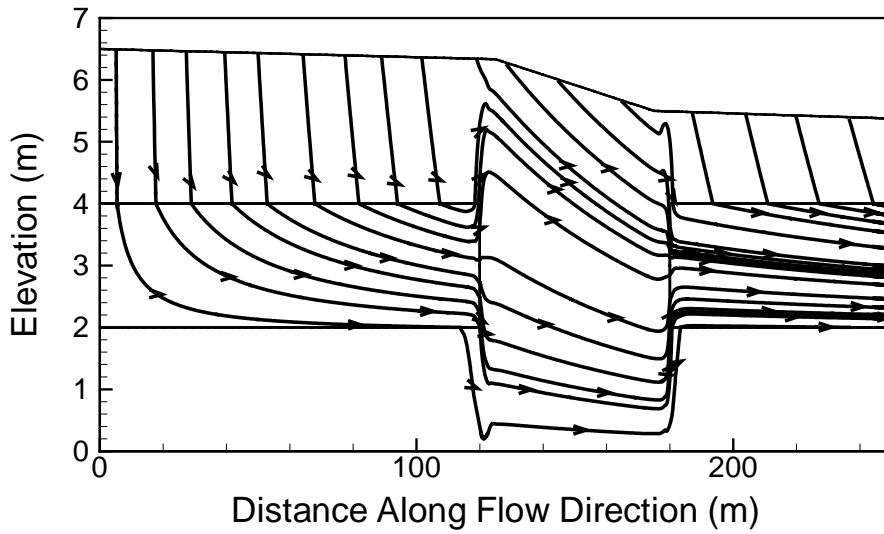


Figure 3: 2D example, flow regime



Note that the problem is completely saturated.

## 1.2 CHEMFLUX SOLUTION DATA

- **CHEMFLUX Boundary Conditions**

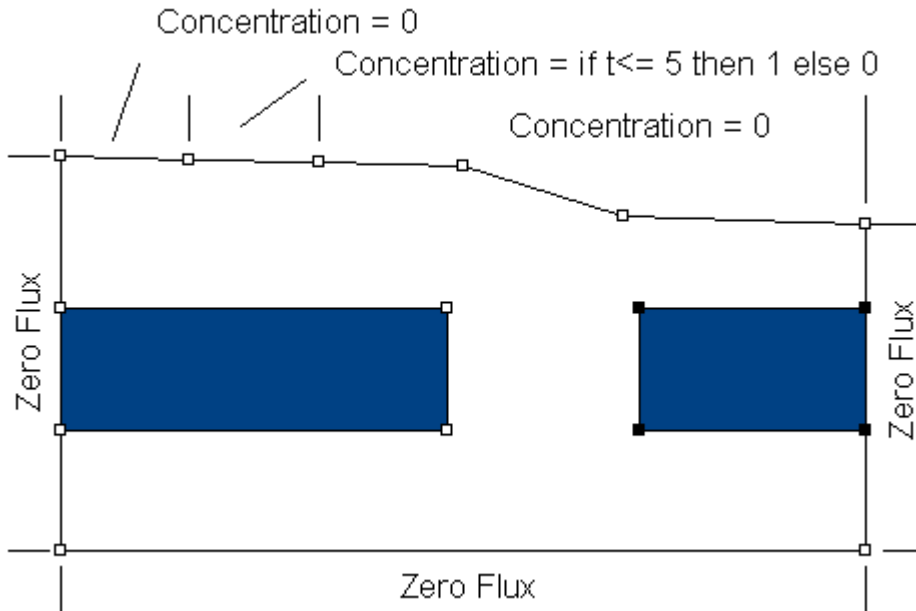


Figure 4: 2D example, CHEMFLUX boundary conditions

- **CHEMFLUX Soil Properties**

Only one soil is used for the problem 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 problem described above has been included in the database file distributed with the SVFLUX software. To generate the necessary seepage gradient file, follow these instructions.

1. Open the SVFLUX software.
2. From the menu select Model > Projects/Problems.
3. The Projects/Problems form should now be open. By clicking on plus signs (+) expand the tree under **Examples > 2D > Steady State**.
4. Click the problem name **ChemFlux2D**.
5. Click **OK**.

6. When the problem has opened click the analyze button to run the problem.

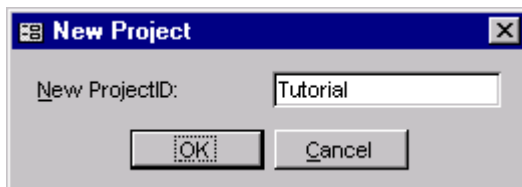
When the problem is finished, the necessary gradient file will be created in the solution folder automatically by SVFLUX. The file is called Examples\_ChemFlux2D.GRD (i.e. Project\_Problem.GRD). The file is given a .GRD extension to separate it as a gradient file.

## 1.4 ADDING A CHEMFLUX PROJECT

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

Follow these steps in order to add this project:

1. Select **Model > Projects/Problems...** from the menu to open the Projects / Problems form.
2. Click **New Project...** in the lower left of the form.
3. The Project Properties form is opened along with a prompt asking for a new ProjectID.



4. Type "Tutorial" as the new ProjectID and press OK.

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



**Tip!**

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

The form is opened ready to accept information.

The screenshot shows a 'Project Properties' dialog box with a blue title bar and a close button (X) in the top right corner. On the left, there is a list box titled 'Problems In Project:' containing the text 'Example2D'. The main area of the dialog is divided into several tabs: 'Project', 'Client', 'Phone', 'Client Address', 'Contractor', and 'Project Engineer'. The 'Project' tab is currently selected. Below the tabs, there are several input fields and a text area:

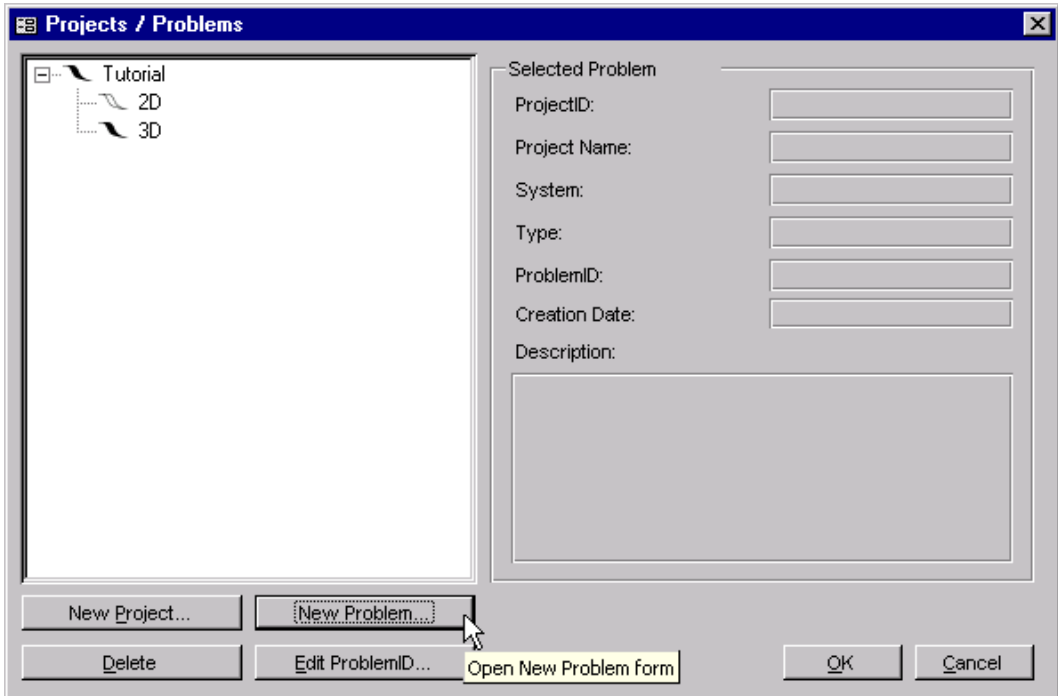
- Project ID:** Tutorial
- Project Name:** Tutorial Example problems for ChemFlux
- Project Location:** Saskatoon, SK Canada
- Project Start Date:** Jun 17/2003
- Project End Date:** Jun 17/2003
- Project Notes:** The tutorial example problems are stored under this projectid

At the bottom of the dialog, there are two buttons: 'Edit ProjectID...' on the left and 'OK' on the right.

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

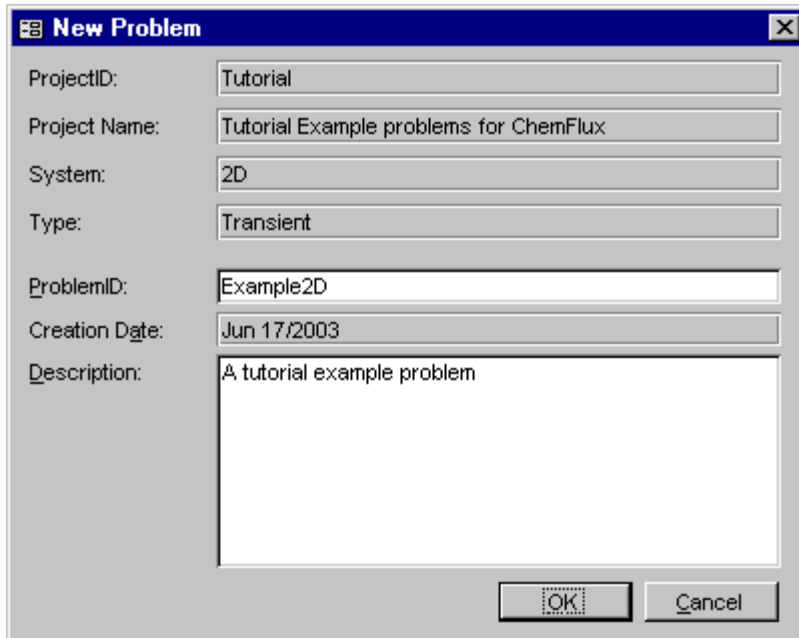
5. Fill out the form with the desired **information**.
6. To exit this form and return to Projects / Problems click **OK**. The project information is automatically saved upon entry.

## 1.5 ADDING A CHEMFLUX PROBLEM



Once a project has been created any number of problems may be stored in it. When the Projects/Problems form 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 problem:

1. Click on the plus sign and expand the project **Tutorial**.
2. Select **2D**.
3. Click the **New Problem** button. The New Problem form will open.



The screenshot shows a 'New Problem' dialog box with the following fields and values:

- ProjectID: Tutorial
- Project Name: Tutorial Example problems for ChemFlux
- System: 2D
- Type: Transient
- ProblemID: Example2D
- Creation Date: Jun 17/2003
- Description: A tutorial example problem

Buttons: OK, Cancel

4. Enter the **ProblemID: Example2D**. The description is optional.
5. Click the **OK** button to save the problem and close the New Problem form.
6. The new problem will automatically be opened in the workspace.

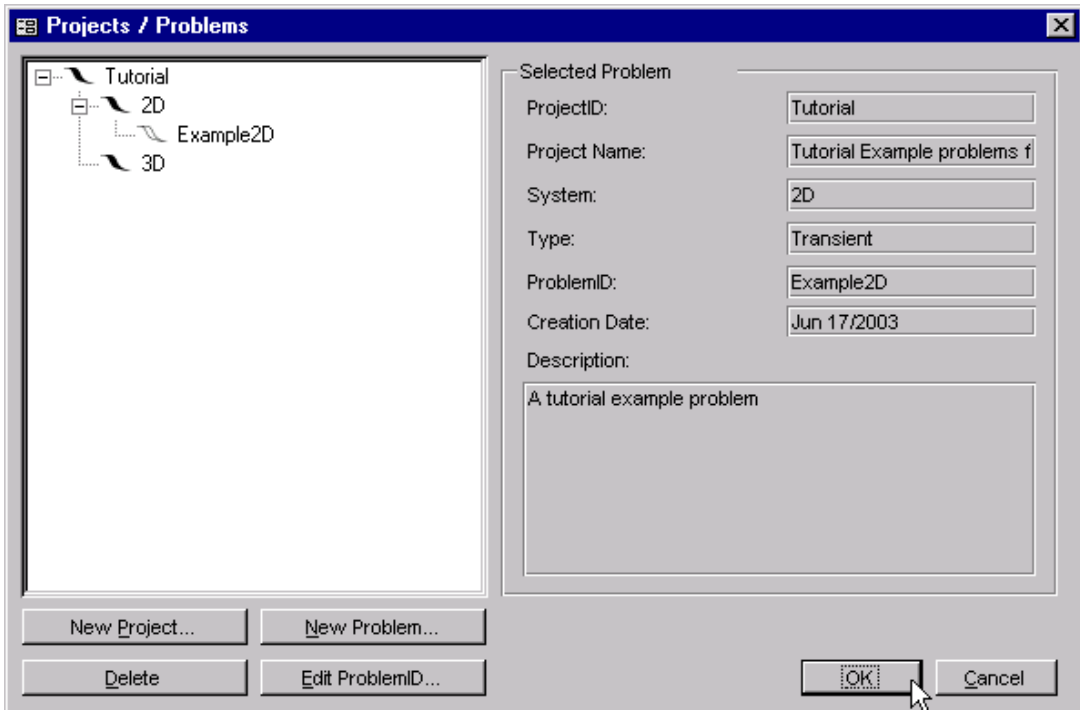


**Tip!**

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.

## 1.6 OPENING THE CHEMFLUX PROBLEM

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



1. **Navigate** back to the problem via Tutorial, 2D.
2. Select **Example2D**.
3. The problem may be opened by clicking the **OK** button or by double clicking on the ProblemID.

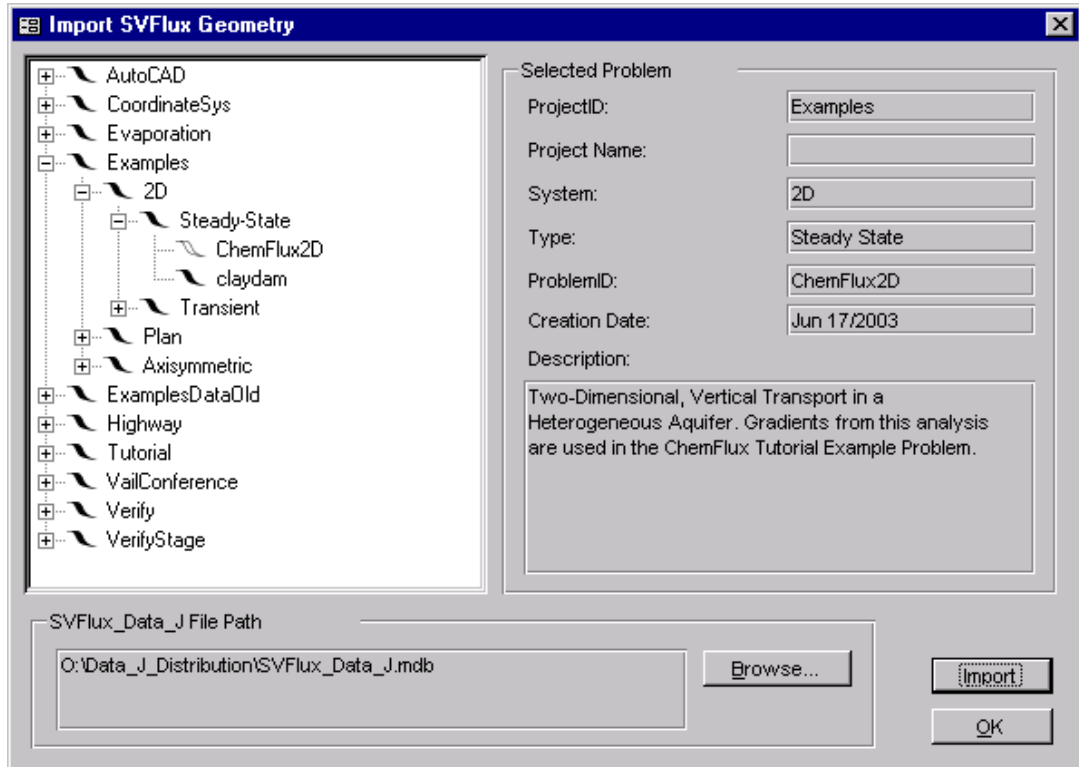
## 1.7 DEFINING THE CHEMFLUX PROBLEM

The following section provides instructions on how to begin defining the problem 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 **Model > SVFlux Geometry** from the menu.



2. Click **Browse**.
3. Select the **SVFlux\_Data\_J.mdb** file that contains the ChemFlux2D problem.
4. Expand the tree and select **ChemFlux2D**.
5. Press the **Import** button.
6. Once the import is complete press **OK** to close the form.

The import includes any regions, region shapes, surfaces, surface grids and elevations. These parts of the problem 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 next step in defining the problem is to specify the settings that will be used for the problem.

The screenshot shows the 'Settings' dialog box with the following configuration:

- System:** 2D (selected), Plan, Axisymmetric, 3D.
- Units:** Metric (selected), Imperial. Length: m, Time: yr, Concentration: g/m<sup>3</sup>. A note states: 'Units set to the SVFlux geometry import problem units.'
- Processes:** Advection (checked), Dispersion (checked), Adsorption (unchecked), Decay (unchecked).
- Time:** Start Time: 0 yr, Increment: 1 yr, End Time: 20 yr.

Buttons at the bottom: FEM Options..., Solution Files Path..., OK.

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

1. To open the Settings form 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 **1 yr**, and an End Time of **20 yr**.
4. Select the **Advection** tab.

**Settings**

General | **Advection** | Adsorption | Initial Conditions

Advection Control - Gradients

Import from SVFlux     Defined

Gradient File Path

O:\Data\_H\My\_Problems\Examples\2D\SteadyState\ChemFlux2D\Examples\_ChemFlux2D\_2.grd

vwc present in file

Gradient Definition

V<sub>x</sub>:

V<sub>y</sub>:

V<sub>z</sub>:

Provide constants or functions in terms of x,y,z, or t. Place () around negative values.

5. Choose **Import from SVFlux** from the Advection Control option.
6. Click **Browse**.
7. Specify the file **Examples\_ChemFlux2D\_2.grd** that was generated by SVFLUX.
8. Press **OK** to close the Settings form.

**Tip!**

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


### 1.7.3 Define Material Properties

Soil Index	Soil Name	USCS Texture	D* (m <sup>2</sup> /yr)
530989	Soil#1		4.23E-02

Suppress Warning Messages

Buttons: New Soil, Import Soil..., Delete Soil, Properties..., OK

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

1. Open the Soils form by selecting **Model > Soils** from the menu or click the soils button,  in the Tools toolbar.
2. Click the **New Soil** button to create a soil in the database. A unique Soil Index is generated that is used to reference the soil in other CHEMFLUX forms.
3. Double-click on the new soil to open the **Soil Properties** form.

Soil Properties

Description | Dispersion | Adsorption | Decay

Soil Index: 530989

Soil Name: Soil#1

USCS Texture: [dropdown]

Soil Description: [text area]

Geologic Description: [text area]

Notes: This soil is for the tutorial example problem.

OK


4. Enter the information above into the appropriate fields on the **Description** tab
5. Move to the **Dispersion** tab.

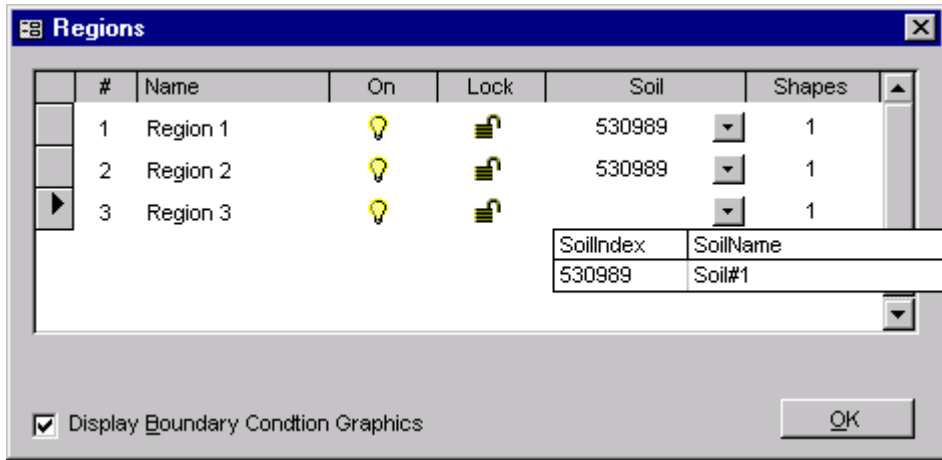
6. Refer to the data provided at the beginning of this tutorial. Enter the Longitudinal Dispersivity,  $\alpha_L = 0.5\text{m}$ .
7. Enter the Transverse Dispersivity,  $\alpha_T = 0.005\text{m}$ .
8. Select Constant as the Diffusion option.
9. Enter the Diffusion Coefficient,  $D^* = 0.0423\text{m}^2/\text{yr}$ .
10. Close the Soil Properties and Soil Manager forms.

#### 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 problem 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 form by clicking the Regions button,  at the top of the workspace.



2. Select the **Soil Index** from the drop-down corresponding to Soil#1 for Region 1.
3. **Repeat** for Region 2 and Region 3.
4. Click **OK** to close the form.

### 1.7.5 Specify Boundary Conditions

The next step is to specify the boundary conditions. Refer to the diagram at the beginning of this tutorial. A zero flux condition will be defined on sides and base of the problem 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 the “Region 1” region in the drawing space with the mouse.
2. From the menu select **Model > Boundaries**. The boundary conditions form will open.

**Boundaries**

Region: Region 1      Select Shape Index: 515490002

X	Y	Boundary Condition	Expression	Units
0	0	Zero Flux		
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>

**Update Selected Segment**      Segment Length: 40 m

1. Select Boundary Condition: Concentration Expression      g/m<sup>3</sup>

2. Provide: Expression: if t<= 5 then 1 else 0

3. Update

Build Equation...  
Expr Reference...

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

OK

3. Select the **point** (0,0) from the list.
4. From the **Boundary Condition** drop down select a **Zero Flux** boundary condition.
5. Click the **Update** button to save the boundary condition to the list.
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)

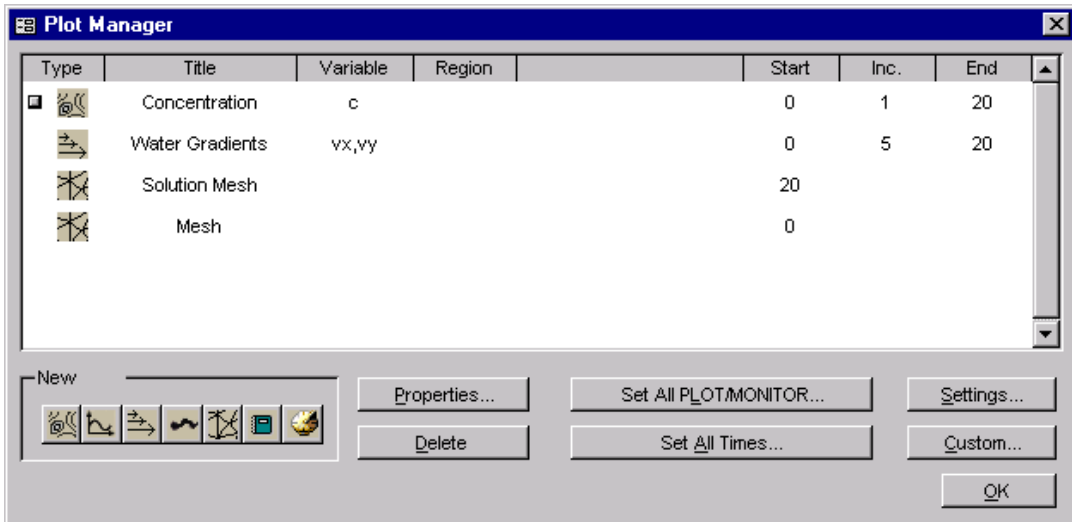


Any boundary condition becomes the boundary condition for the following line segments that have a Continue boundary condition until a new boundary condition is specified.

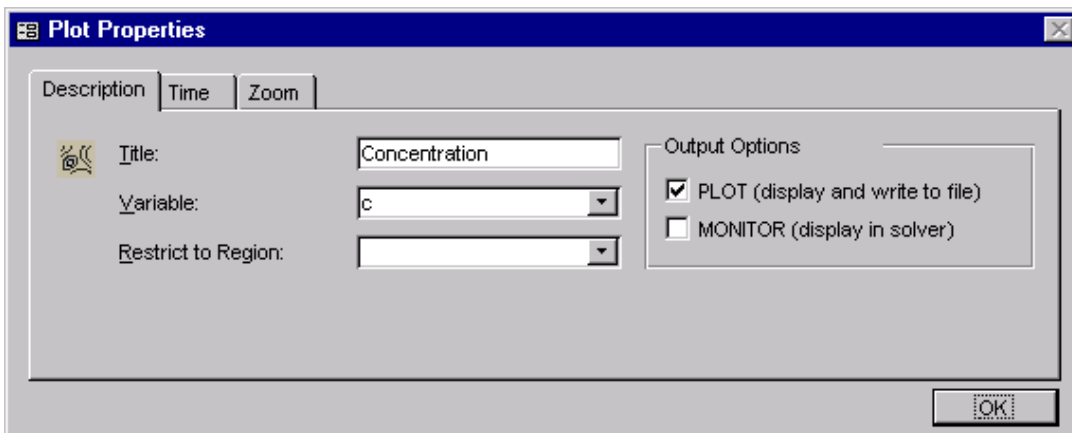
## 1.8 SPECIFY PLOTS

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 problem including a plot of the solution mesh, concentration contours, and water gradient vectors.

1. Open the Plot Manager form by selecting **Model > Plot Manager** from the menu.



- The toolbar at the bottom left of the form contains a button for each plot type. Click on the Contour button to begin adding the first contour plot. The Plot Properties form will open.



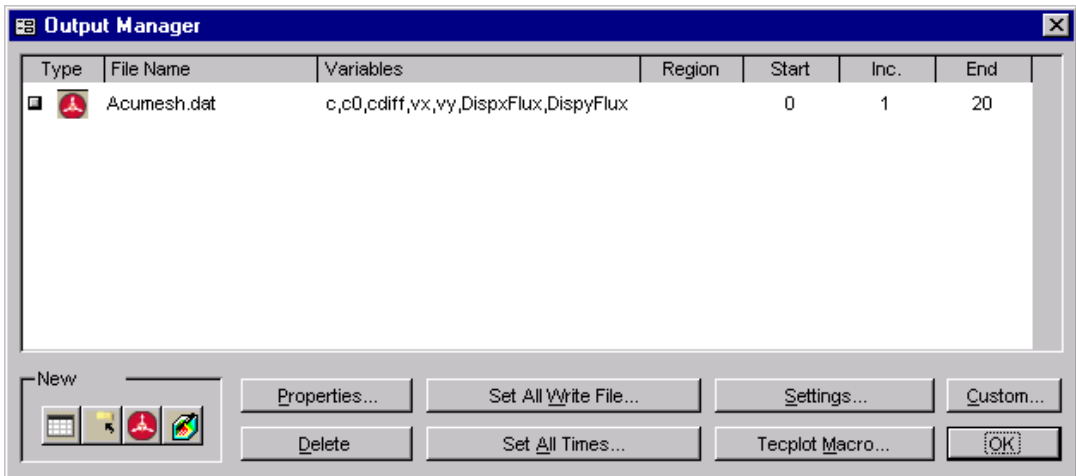
- Enter the title **Concentration**.
- Select **c** as the variable to plot from the drop-down.
- Select the **PLOT** output option.
- Move to the **Time** tab and enter a Start Time = 0, a Time Increment = 1, and an End Time = 20.
- Move to the **Zoom** tab and enter X = 100, Y = 0.1, Width = 100, and Height = 6.6.
- Click OK to close the form and add the plot to the list.
- Repeat steps 2 – 8 to create the plots shown above. 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.

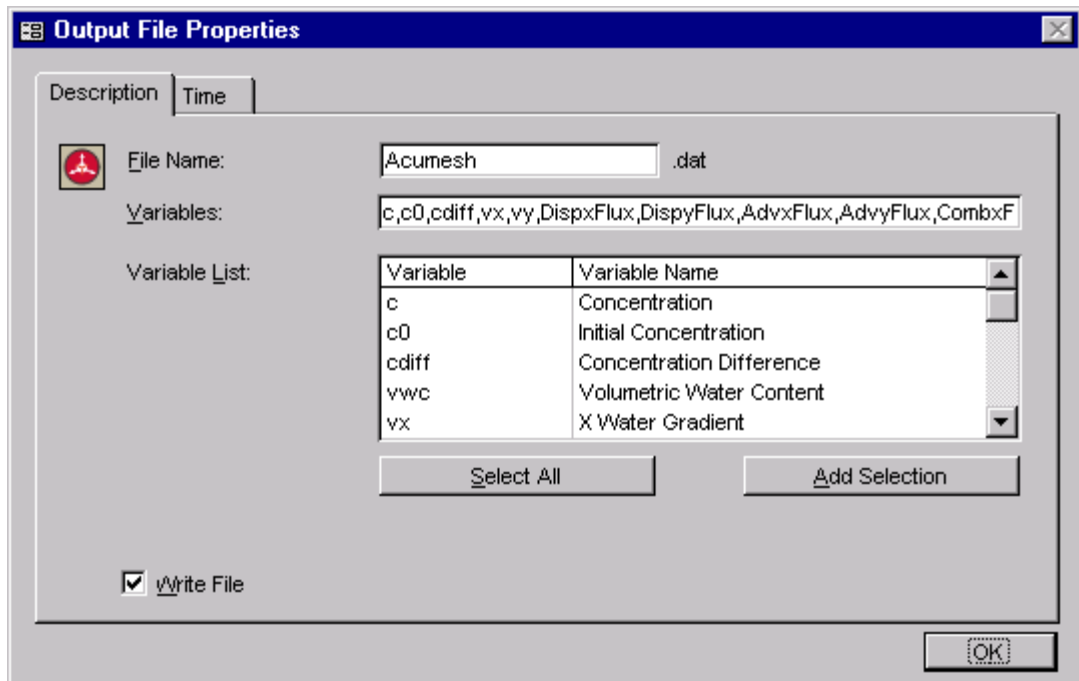
## 1.9 SPECIFY OUTPUT FILES

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

1. Open the Output Manager form by selecting **Model > Output Manager** from the menu.



2. The toolbar at the bottom left of the form contains a button for each output file type. Click on the AcuMesh button to begin adding the output file. The Output File Properties form 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.
7. Click OK to close the form and add the output file to the list.
8. Click **OK** to close the Output Manager and return to the workspace.

## 1.10 ANALYZE

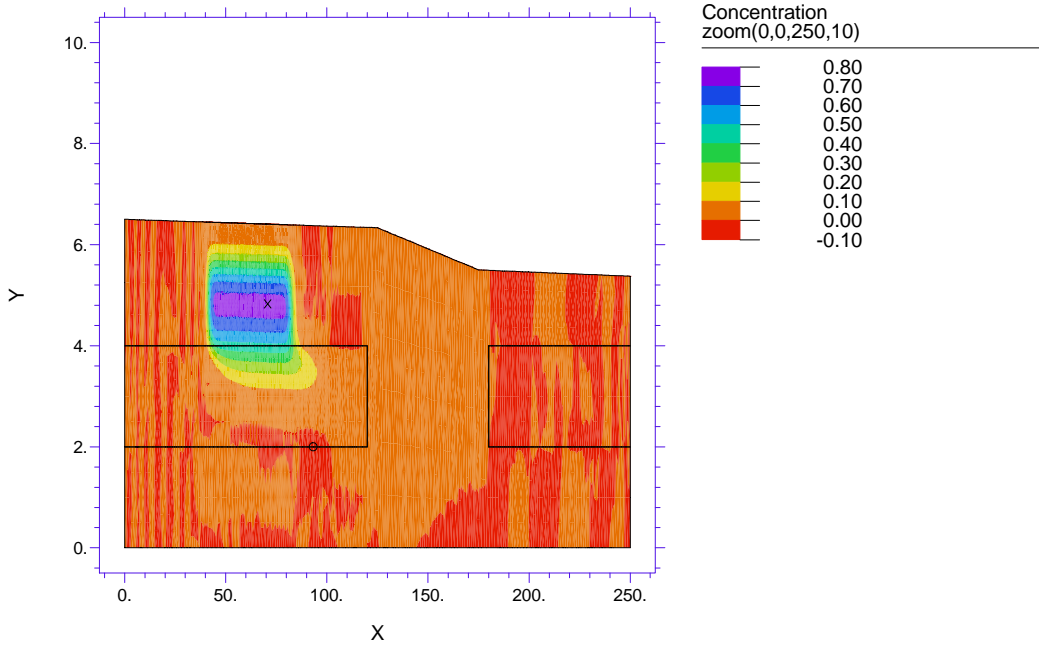
The next step is to analyze the problem. Click the Analyze button located in the left toolbar. This action will write the descriptor file and open the CHEMFLUX solver. The solver will automatically begin solving the problem.

## 1.11 RESULTS

After the problem has finished solving, the results will be displayed in the form 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 problem for times of 8 years, 12 years, and 20 years.

- Time = 8 years

16:36:05 2/20/02  
FlexPDE 2.22

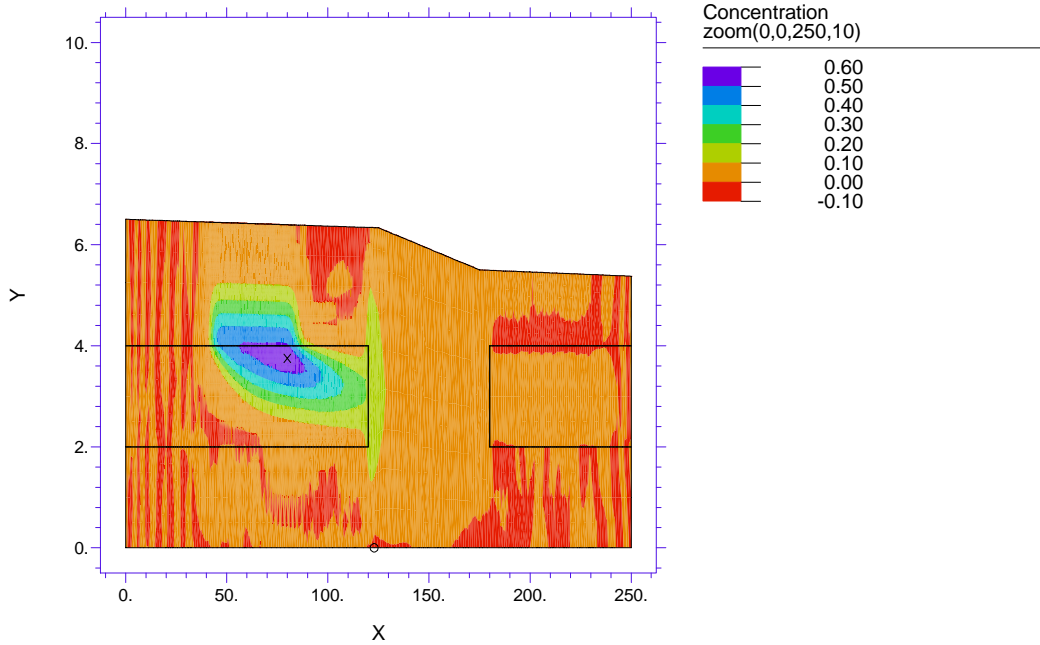


Examples\_2DExample: Cycle=96 Time= 8.0000 dt= 0.1961 p2 Nodes=6375 Cells=3068 RMS Err= 2.9e-4  
Integral= 56.74936

The source has been shut off for 3 years

- Time = 12 years

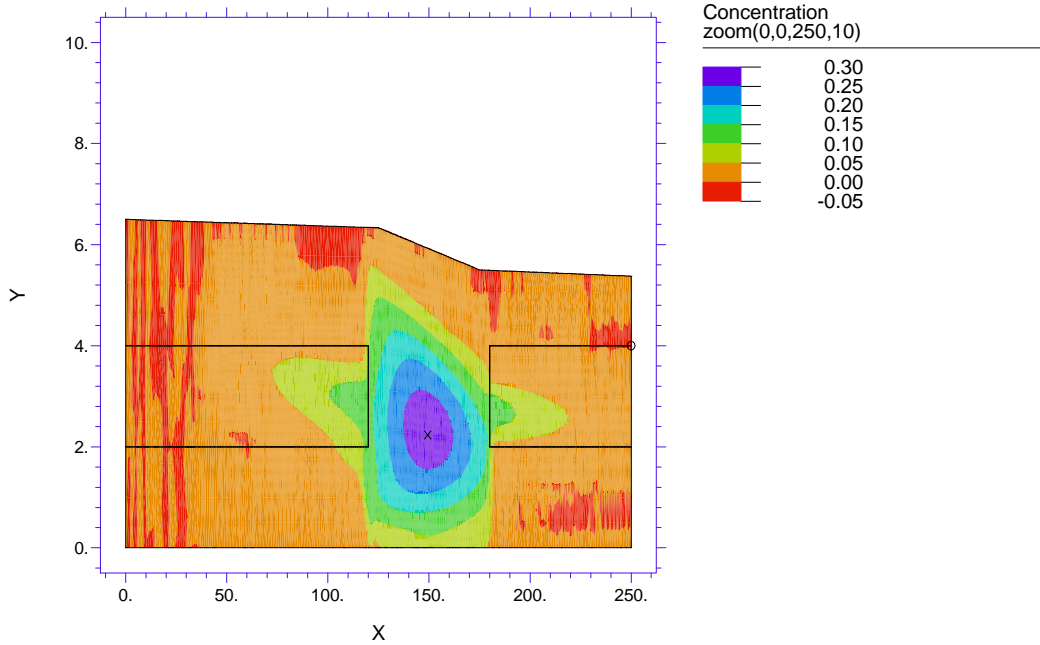
16:36:05 2/20/02  
FlexPDE 2.22



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

16:36:05 2/20/02  
FlexPDE 2.22



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 PROBLEM

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 problem 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 problem.

ProjectID: Tutorial

ProblemID: Example3D

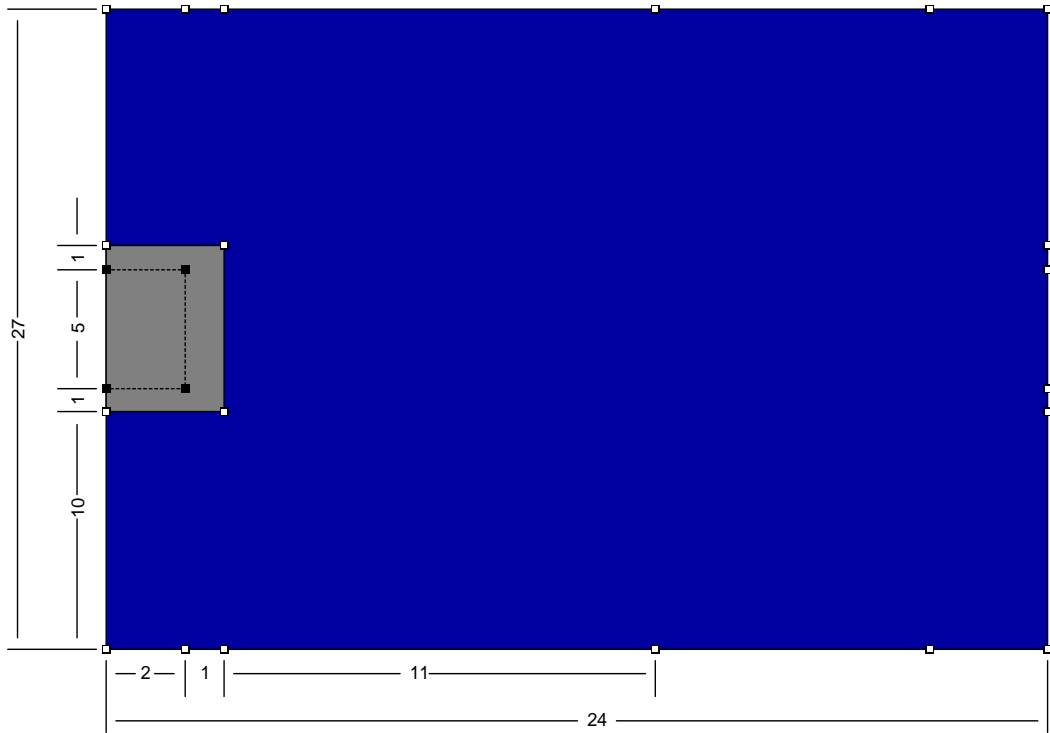
### 2.1 STEADY STATE SVFLUX SOLUTION

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 problem solved by SVFLUX.

ProjectID: Examples

ProblemID: ChemFlux3D

- **Problem Dimensions**



**Figure 5: 3D Example; Problem Dimensions**

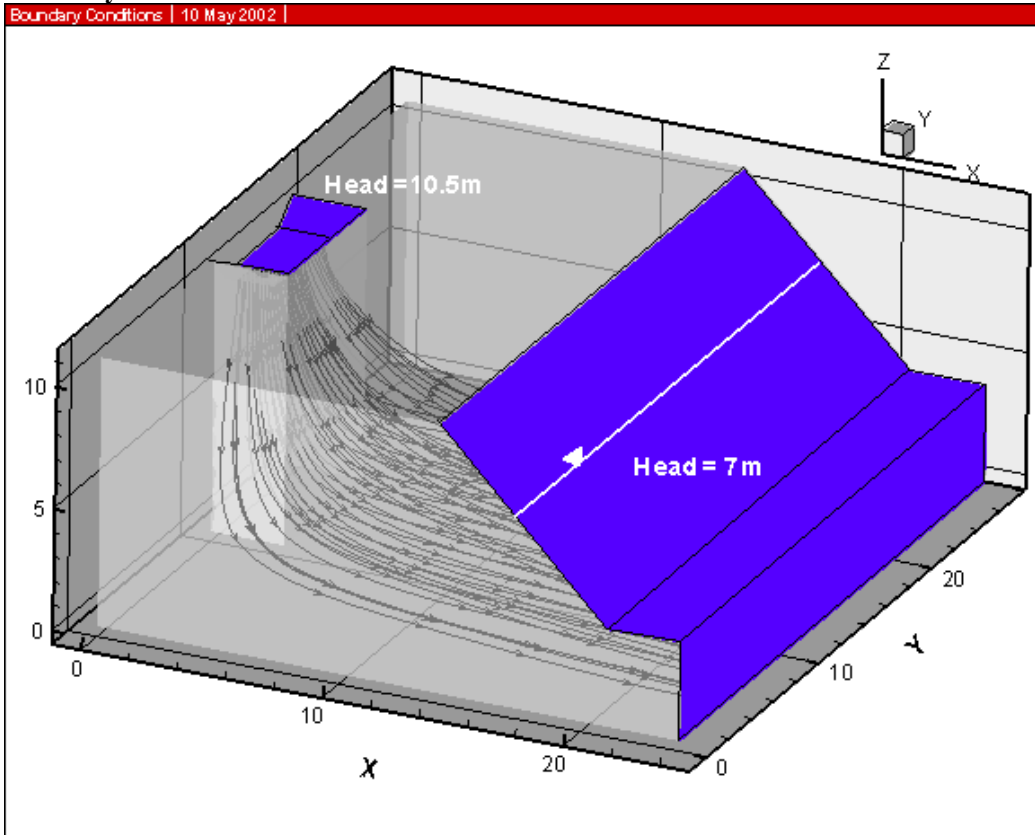
- Surface 1 Grid

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**

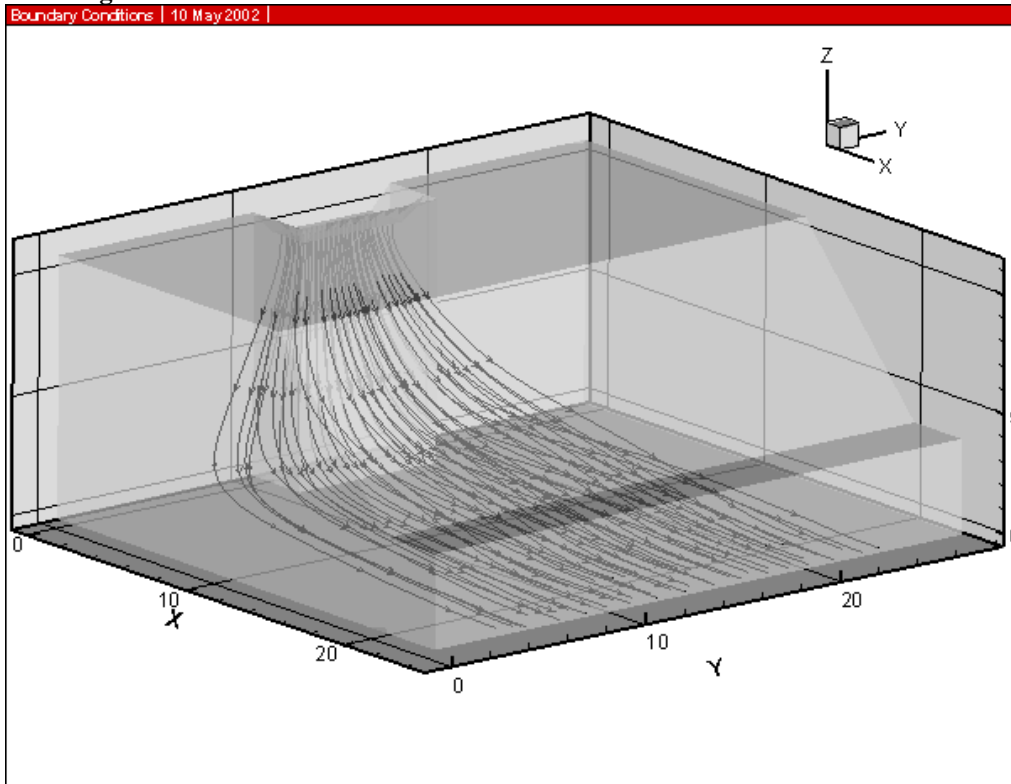
The steady state seepage model is set up to simulate a pond or reservoir a certain distance from a river channel. The water levels in the reservoir and river channel are set using head boundary conditions. The level of water in the reservoir is set using a **Head Expression = 10.5m** set on surface 2 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 problem despite the presence of separate colors for the two regions. Two regions have been implemented in this problem in order to apply the necessary boundary conditions. The soil in the problem 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 problem 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**

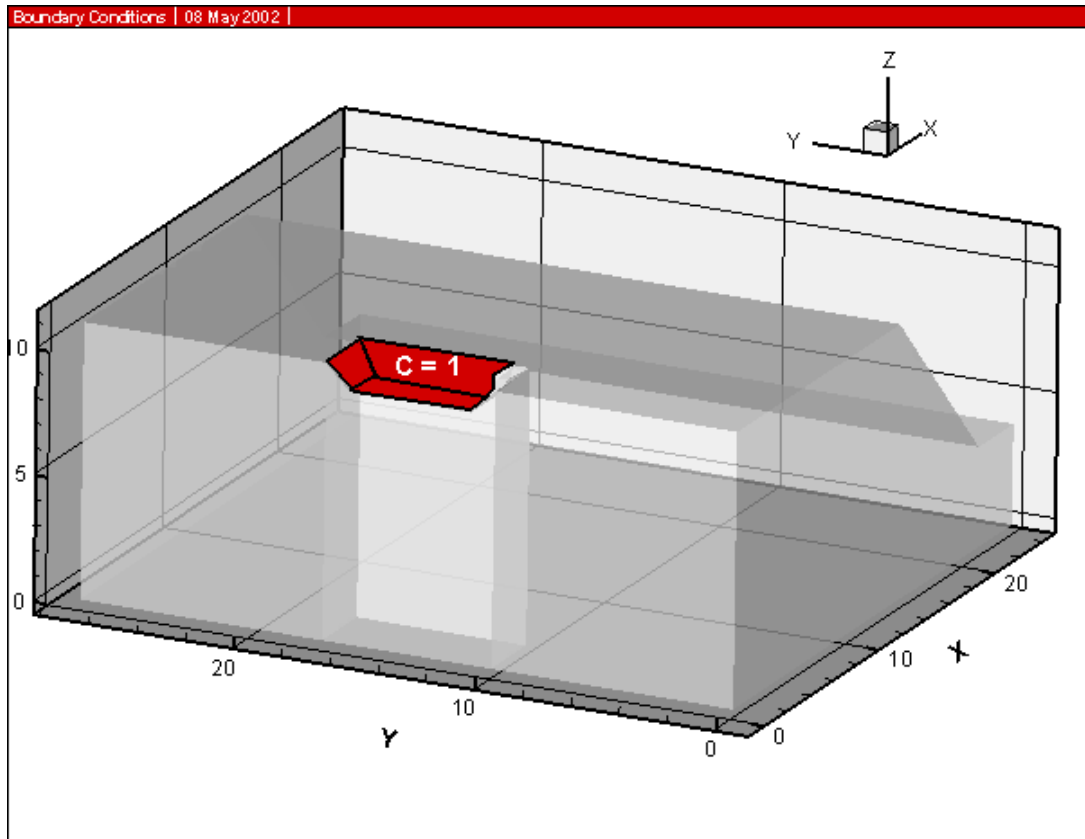


Figure 8: 3D example, CHEMFLUX boundary conditions

- **CHEMFLUX Soil Properties**

Only one soil is used for the problem 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 problem described above has been included in the database file distributed with the SVFLUX software. To generate the necessary seepage gradient file, follow these instructions.

1. Open the SVFLUX software.
2. From the menu select **Model > Projects/Problems**.
3. The Projects/Problems form should now be open. By clicking on plus signs (+) expand the tree under **Examples > 3D > Steady State**.
4. Click the problem name **ChemFlux3D**.
5. Click **OK**.
6. When the problem has opened click the analyze button to run the problem.

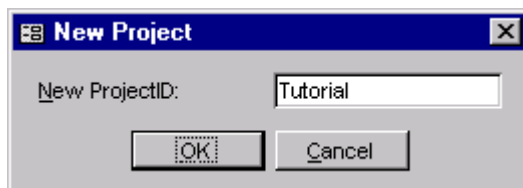
When the problem is finished, the necessary gradient file will be created in the solution folder automatically by SVFLUX. The file is called `Examples_ChemFlux3D.GRD` (i.e. `Project_Problem.GRD`). The file is given a `.GRD` extension to separate it as a gradient file.

## 2.4 ADDING A CHEMFLUX PROJECT

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

Follow these steps in order to add this project:

1. Select **Model > Projects/Problems...** from the menu to open the Projects / Problems form.
2. Click **New Project...** in the lower left of the form.
3. The Project Properties form is opened along with a prompt asking for a new ProjectID.



4. Type "Tutorial" as the new ProjectID and press OK.

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



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

The form is opened ready to accept information.

**Project Properties**

Problems In Project:  
Example2D

Project | Client | Phone | Client Address | Contractor | Project Engineer

Project ID: Tutorial

Project Name: Tutorial Example problems for ChemFlux

Project Location: Saskatoon, SK Canada

Project Start Date: Jun 17/2003

Project End Date: Jun 17/2003

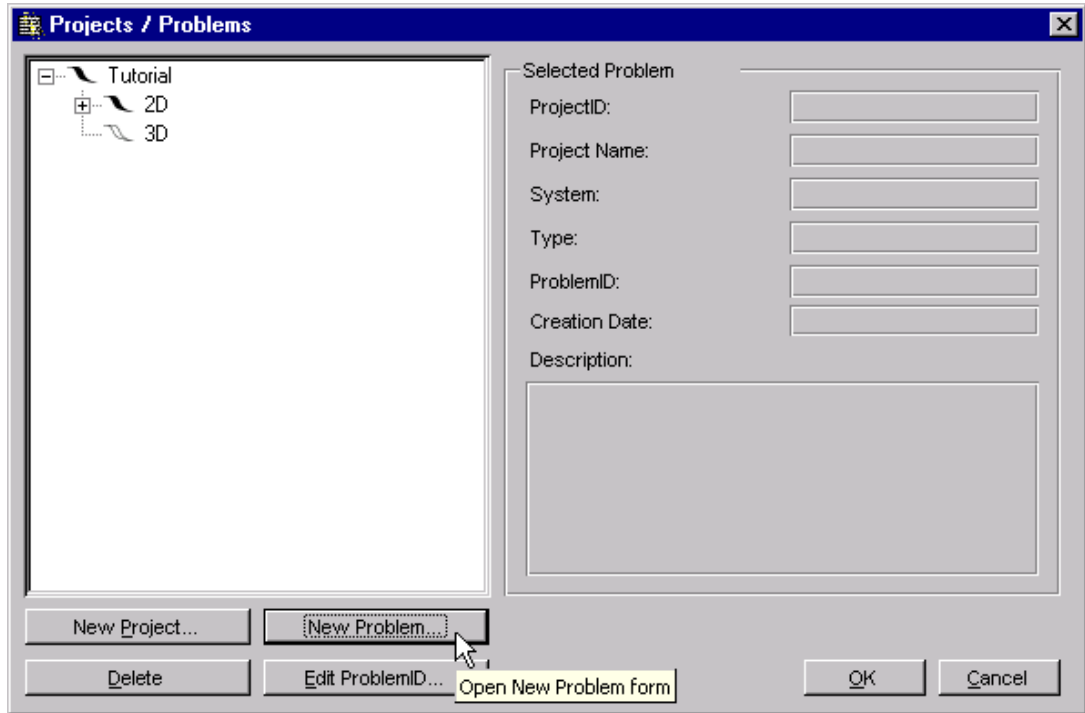
Project Notes: The tutorial example problems are stored under this projectid

Edit ProjectID... OK

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

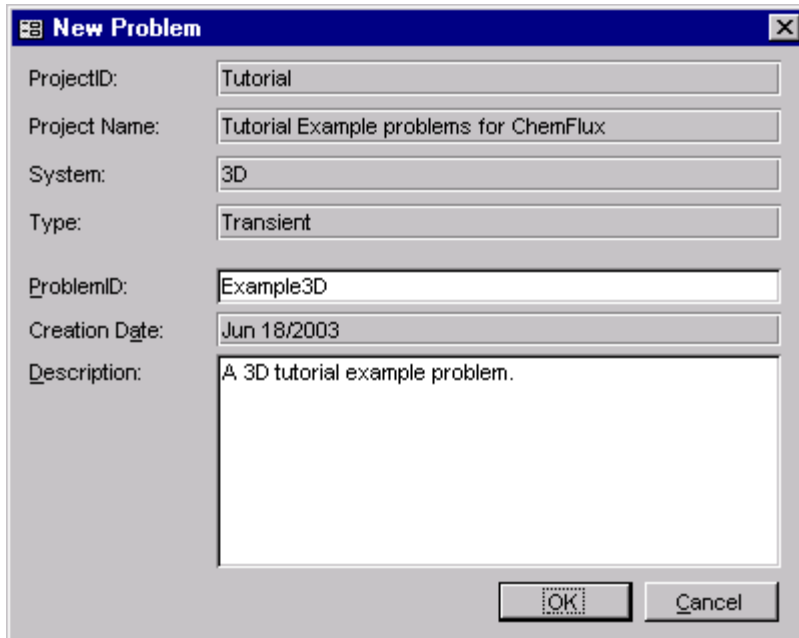
5. Fill out the form with the desired **information**.
6. To exit this form and return to Projects / Problems click **OK**. The project information is automatically saved upon entry.

## 2.5 ADDING A CHEMFLUX PROBLEM



Once a project has been created any number of problems may be stored in it. When the Projects/Problems form 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 problem:

1. Click on the plus sign and expand the project **Tutorial**.
2. Select **3D**.
3. Click the **New Problem** button. The New Problem form will open.



**New Problem**

ProjectID: Tutorial

Project Name: Tutorial Example problems for ChemFlux

System: 3D

Type: Transient

ProblemID: Example3D

Creation Date: Jun 18/2003

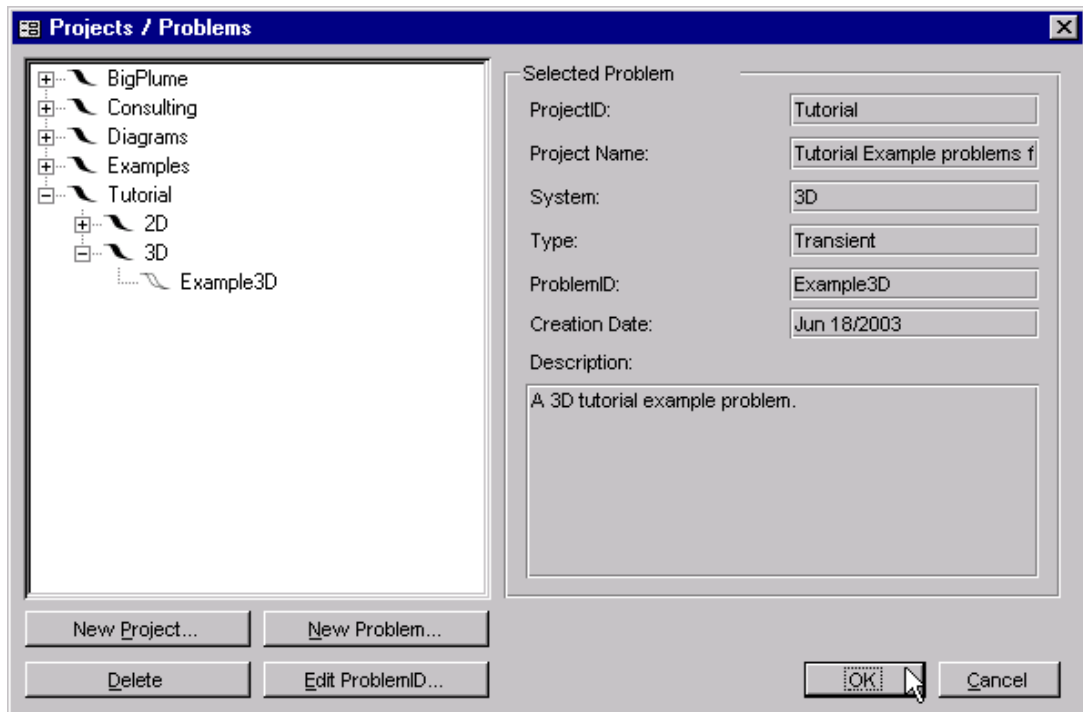
Description: A 3D tutorial example problem.

OK Cancel

4. Enter the **ProblemID: Example3D**. The description is optional.
5. Click the **OK** button to save the problem and close the New Problem form.
6. The new problem will automatically be opened in the workspace.

## 2.6 OPENING THE PROBLEM

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



1. **Navigate** back to the problem via Tutorial, 3D.
2. Select **Example3D**.
3. The problem may be opened by clicking the **OK** button or by double clicking on the ProblemID.

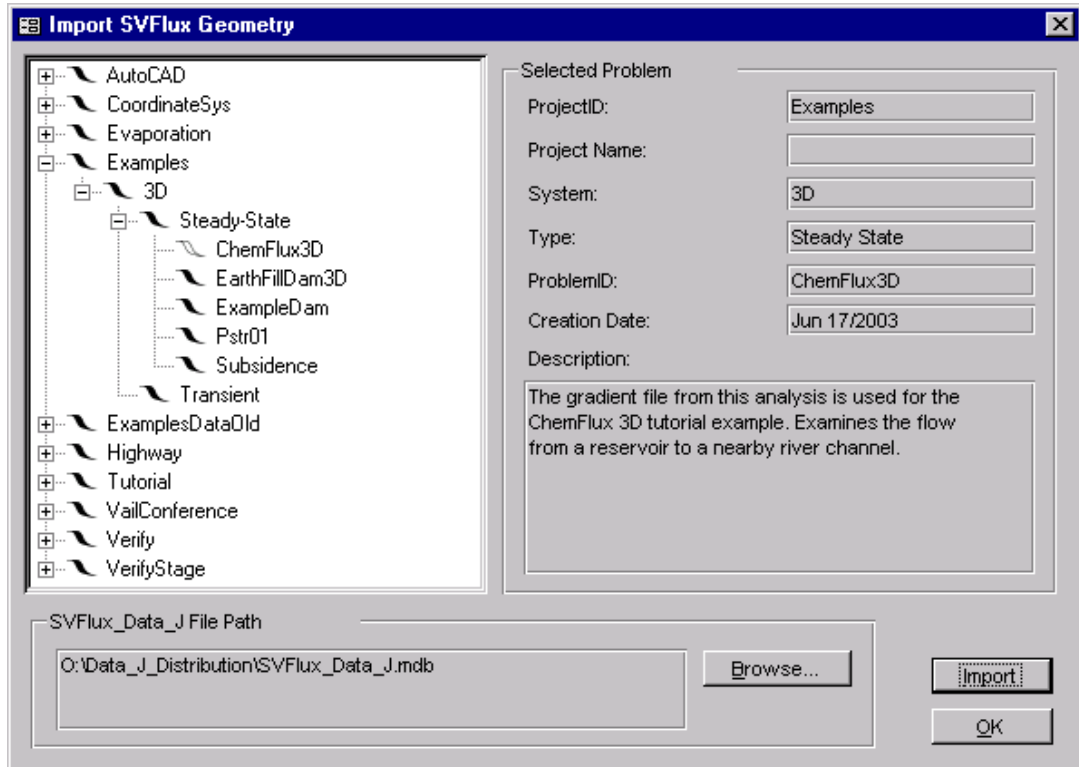
## 2.7 DEFINING THE PROBLEM

The following section provides instructions on how to begin defining the problem 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 **Model > SVFlux Geometry** from the menu.



2. Click **Browse**.
3. Select the **SVFlux\_Data\_J.mdb** file that contains the ChemFlux3D problem.
4. Expand the tree and select **ChemFlux3D**.
5. Press the **Import** button.
6. Once the import is complete press **OK** to close the form.

The import includes any regions, region shapes, surfaces, surface grids and elevations. These parts of the problem 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 problem is to specify the settings that will be used for the problem.

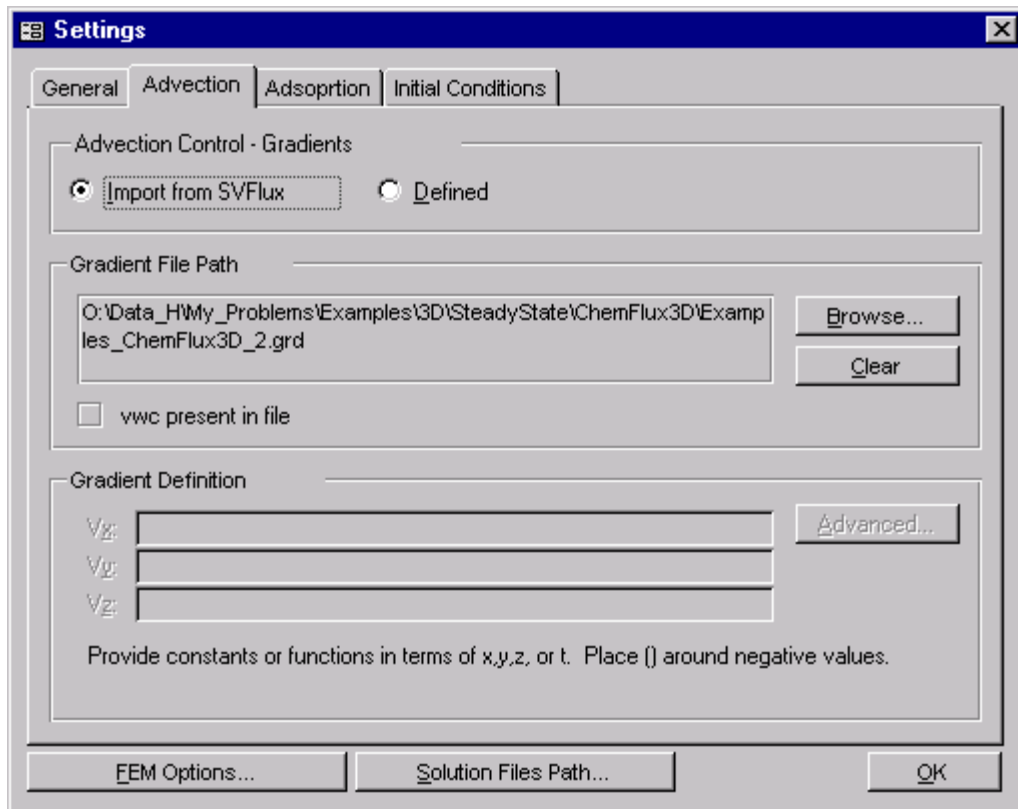
The screenshot shows the 'Settings' dialog box with the following configuration:

- System:** 3D (selected)
- Units:** Metric (selected), Length: m, Time: day, Concentration: g/m<sup>3</sup>. A note states: 'Units set to the SVFlux geometry import problem units.'
- Processes:** Advection (checked), Dispersion (checked), Adsorption (unchecked), Decay (unchecked)
- Time:** Start Time: 0 day, Increment: 50 day, End Time: 400 day

Buttons at the bottom: FEM Options..., Solution Files Path..., OK

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

1. To open the Settings form 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.

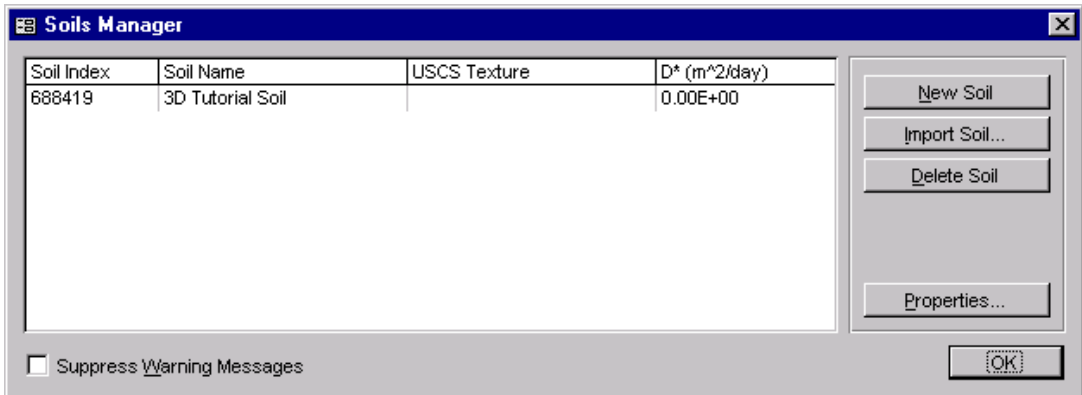
**Tip!**

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


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.

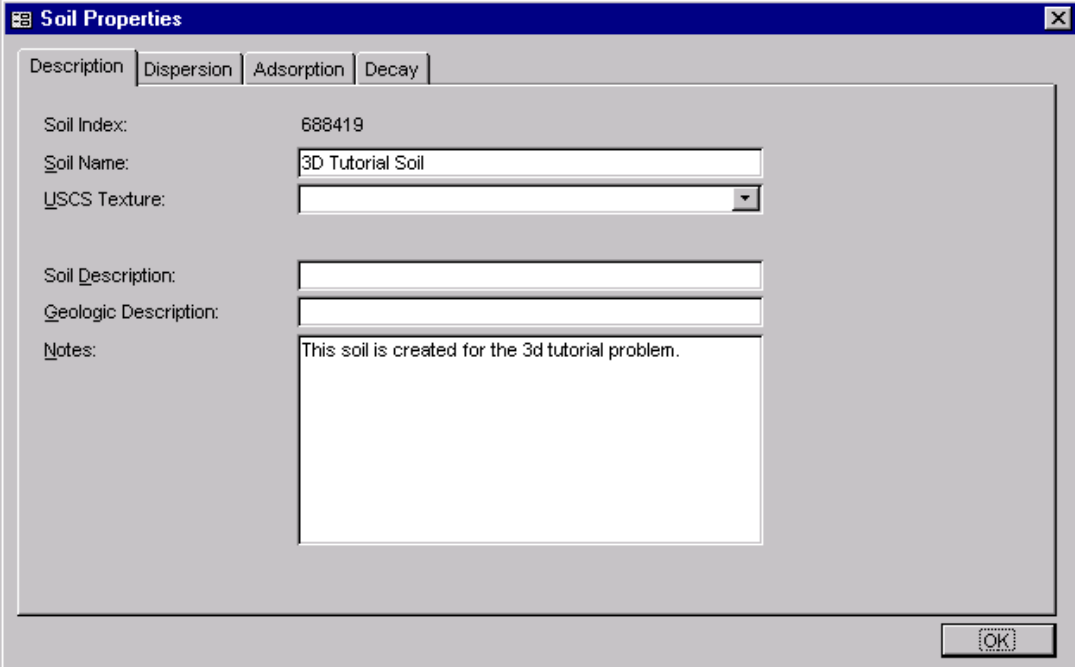
8. Press the **FEM Options** button to open the FEM Options form.
9. Set the **NODELIMIT** as 800. (This is the student version maximum)
10. Set the **NGRID** parameter to 5. (This is the student version maximum)
11. Press **OK** to close the FEM Options form.
12. Press **OK** to close the Settings form.

### 2.7.3 Define Material Properties



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

1. Open the Soils form by selecting **Model > Soils** from the menu or click the soils button,  in the Tools toolbar.
2. Click the **New Soil** button to create a soil in the database. A unique Soil Index is generated that is used to reference the soil in other CHEMFLUX forms.
3. Double-click on the new soil to open the **Soil Properties** form.



The screenshot shows a software window titled "Soil Properties" with a blue title bar and a close button (X) in the top right corner. The window contains four tabs: "Description", "Dispersion", "Adsorption", and "Decay". The "Description" tab is currently selected. The form fields are as follows:

- Soil Index:** 688419
- Soil Name:** 3D Tutorial Soil
- USCS Texture:** [Empty dropdown menu]
- Soil Description:** [Empty text box]
- Geologic Description:** [Empty text box]
- Notes:** This soil is created for the 3d tutorial problem.

An "OK" button is located in the bottom right corner of the dialog box.


4. Enter the information above into the appropriate fields on the **Description** tab
5. Move to the **Dispersion** tab.

The screenshot shows the 'Soil Properties' dialog box with the 'Dispersion' tab selected. The 'Dispersion' section contains two input fields: 'Longitudinal:  $\alpha_L = 1.000E+00$  m' and 'Transverse:  $\alpha_T = 1.000E+00$  m'. The 'Diffusion' section has two radio buttons: 'Constant' (selected) and 'Function - Laboratory Data'. Below the radio buttons is an input field for 'D\* = 0.000E+00 m<sup>2</sup>/day'. The 'Laboratory Data' section features a table with two columns: 'Volumetric Water Content' and 'D\* (m<sup>2</sup>/day)'. The table is currently empty. Below the table are buttons for 'Paste Points...' and 'Graph...'. A 'Total Points:' label is followed by an input field containing '0'. The dialog box has an 'OK' button at the bottom right.

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 forms.

#### 2.7.4 Specifying a Soil by Region and Layer


Each region will cut through all the layers in a problem 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 problem all “blocks” will be assigned a soil.

1. Select “**Slope**” in the Region Selector.
2. Press the **Region Soils** button,  at the top of the workspace to open the Region Soils form.

Region Soils

Region:

	Bound By	Layer	Soil
▶	Surface 2	1	3D Tutorial Soil ▼
	Surface 1		

3. Select the soil from the drop-down for **Layer 1**.
4. Close the form using the **OK** button.
5. Select “**Reservoir**” in the Region Selector.
6. Press the **Region Soils** button,  at the top of the workspace to open the Region Soils form.
7. Select the soil from the drop-down for **Layer 1**.
8. Close the form using the OK button.

### 2.7.5 Specify Boundary Conditions

The next step is to specify the boundary conditions on the region shapes. The only boundary condition that is required for this problem 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**. The boundary conditions form will open and display the boundary conditions for Surface 1.
3. Select Surface 2 from the Surface option box.

**Boundaries**

Location

Region: Reservoir

Surface: Surface 2

Surface Boundary Condition

1. Select Boundary Condition: Concentration Expression g/m<sup>3</sup>

2. Expression: 1

Segment Boundary Conditions

X	Y	Boundary Condition	Expression	Units
0	10	Zero Flux		
3	10	Continue		
3	17	Continue		
0	17	Continue		

Update Selected Segment Segment Length: 3 m

1. Select Boundary Condition: Zero Flux

2. Provide: Expression:

Build Equation...  
Expr Reference...

3. Update

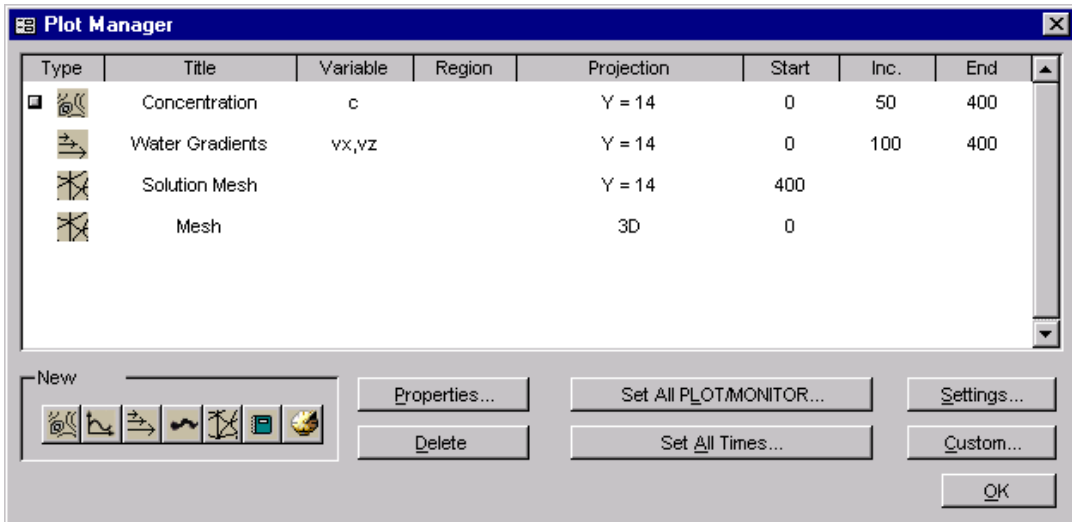
Copy To Surface... Notes... OK

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 form.

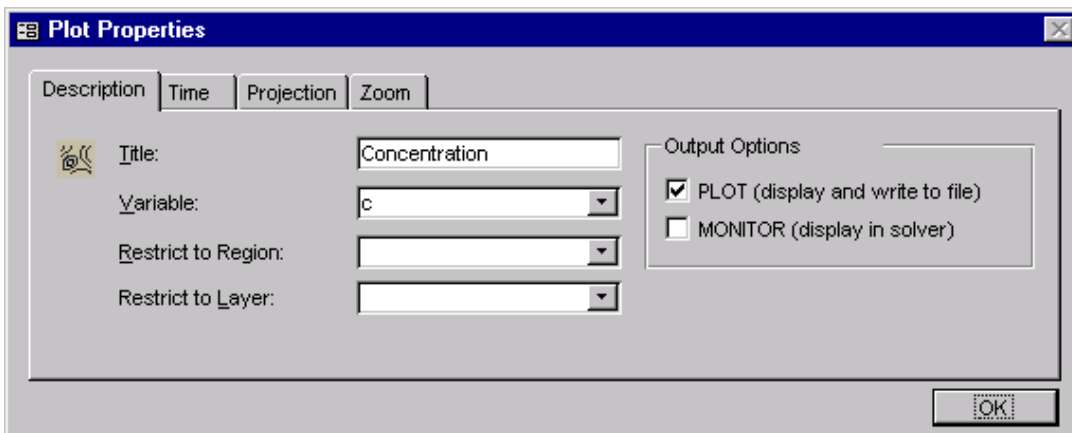
## 2.8 SPECIFY PLOTS

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 problem including a plot of the concentration contours, solution mesh, and water gradient vectors.

1. Open the Plot Manager form by selecting **Model > Plot Manager** from the menu.



- The toolbar at the bottom left of the form contains a button for each plot type. Click on the Contour button to begin adding the first contour plot. The **Plot Properties** form will open.



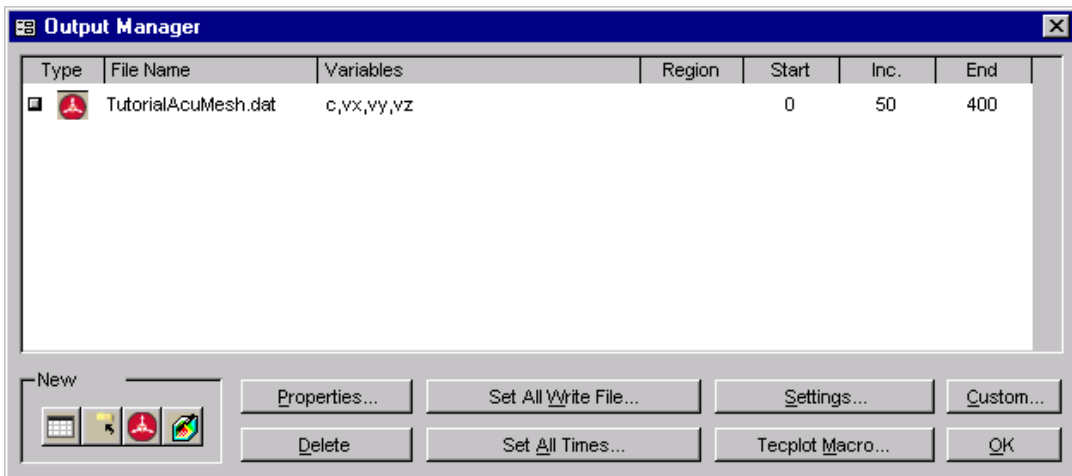
- Enter the title **Concentration**.
- Select **c** as the variable to plot from the drop-down.
- Select the **PLOT** output option.
- Move to the **Time** tab.
- Press the Arrow to put the problem times in the plot time fields.
- Move to the **Projection** tab.
- Select **Plane** Projection option.
- Select **Y** from the Coordinate Direction drop-down.

11. Enter **14** in the Coordinate field. This will generate a 2D slice at  $Y = 14\text{m}$  on which the concentration contours will be plotted.
12. Click **OK** to close the form and add the plot to the list.
13. Repeat these steps 2 – 12 to create the plots shown above. Note that the Mesh plot does not require entry of a variable.
14. Click **OK** to close the Plot Manager and return to the workspace.

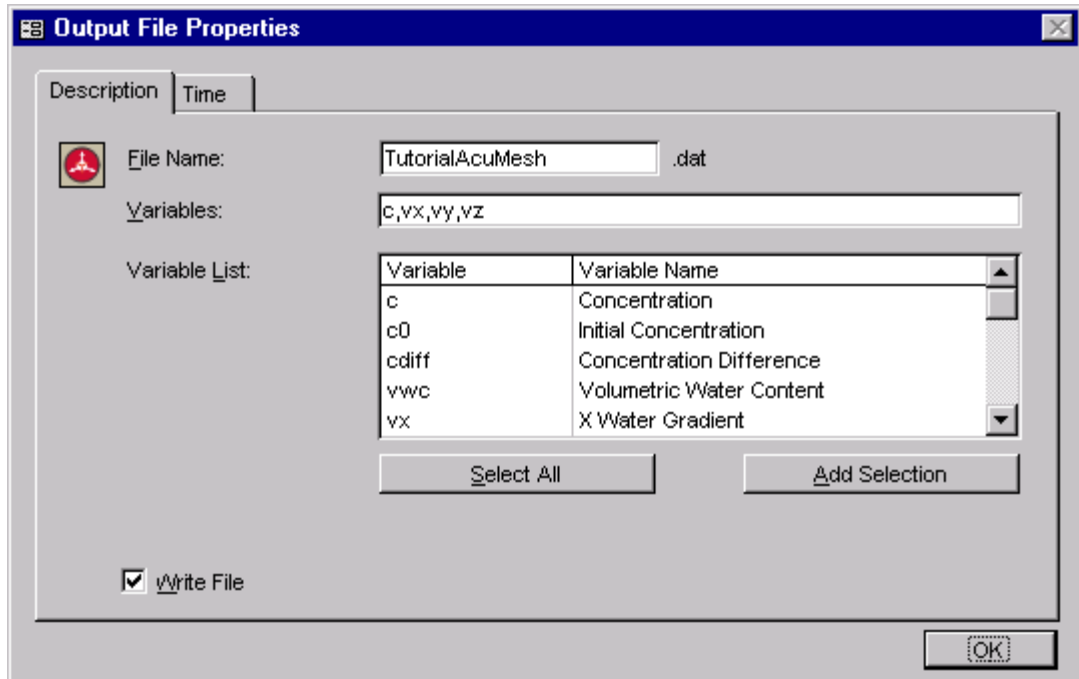
## 2.9 SPECIFY OUTPUT FILES

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 problem: a file to output the results to AcuMesh for advanced visualization.

1. Open the Output Manager form by selecting **Model > Output Manager** from the menu.



2. The toolbar at the bottom left of the form contains a button for each output file type. Click on the AcuMesh button to begin adding the output file. The Output File Properties form will open.



3. Enter the title TutorialAcuMesh.
4. Select variables **c**, **vx**, **vy**, and **vz** in the list.
5. Press the **Add Selection** button.
6. Check the **Write File** box.
7. Click **OK** to close the form and add the output file to the list.
8. Click **OK** to close the Output Manager and return to the workspace.

## 2.10 ANALYZE

The next step is to analyze the problem. Click the Analyze button located in the left toolbar. This action will write the descriptor file and open the CHEMFLUX solver. The solver will automatically begin solving the problem.

## 2.11 RESULTS

After the problem has finished solving, the results will be displayed in the form 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.

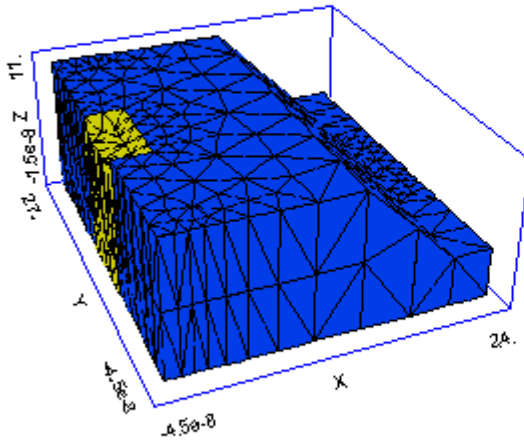
### 2.11.1 Solution Mesh

15:07:36 6/18/03

FlexPDE 3.10.1

Mesh  
(-31.4,-91.2, 30.)

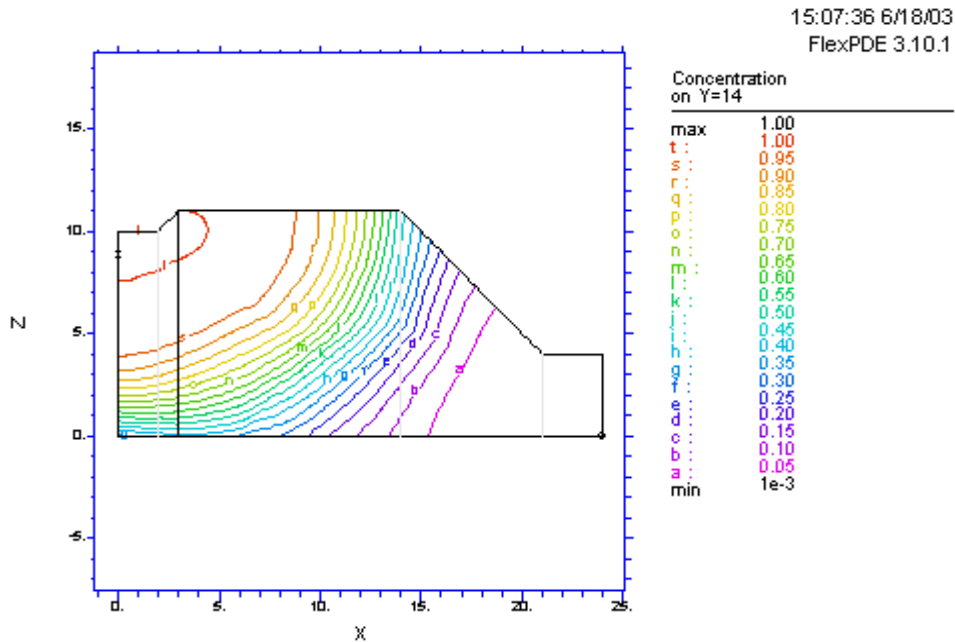
---



Tutorial\_Example3D: Cycle=66 Time= 400.00 dt= 39.233 p2 Nodes=2683 Cells=1411 RMS Err= 0.00

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.

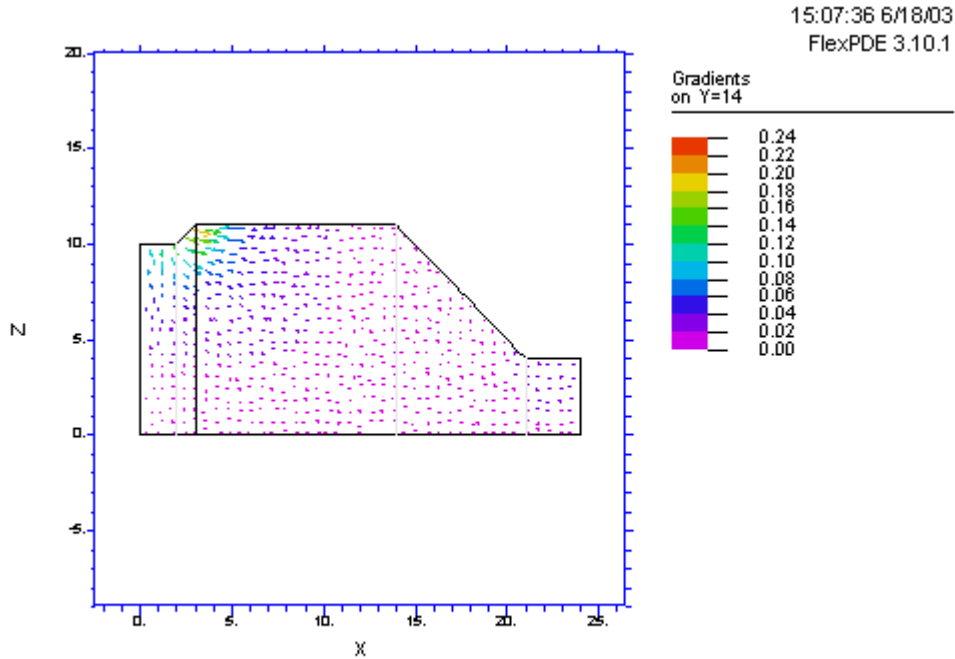
2.11.2 Concentration Contours



Tutorial\_Example3D: Cycle=66 Time= 400.00 dt= 39.233 p2 Nodes=2683 Cells=1411 RMS Err= 0.00  
Integral= 114.7896

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



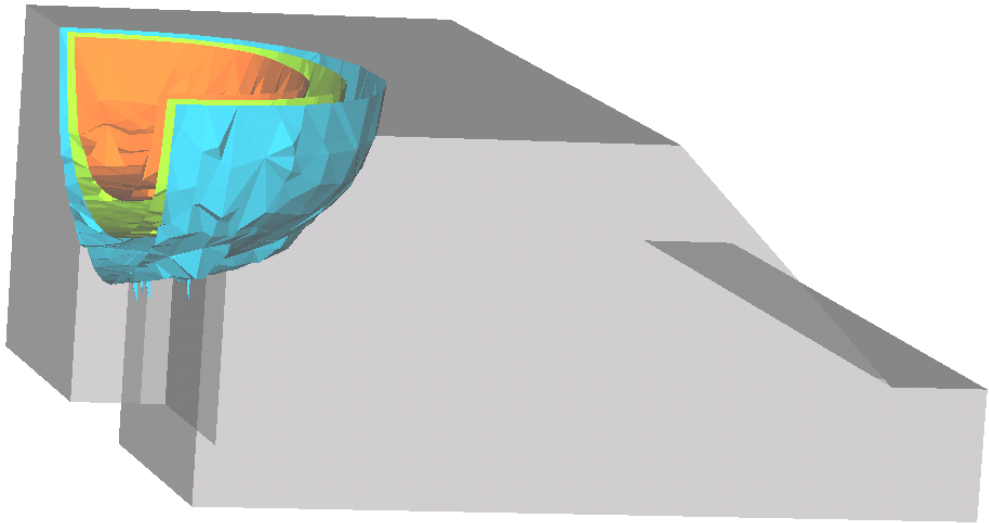
Tutorial\_Example3D: Cycle=66 Time= 400.00 dt= 39.233 p2 Nodes=2683 Cells=1411 RMS Err= 0.00

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

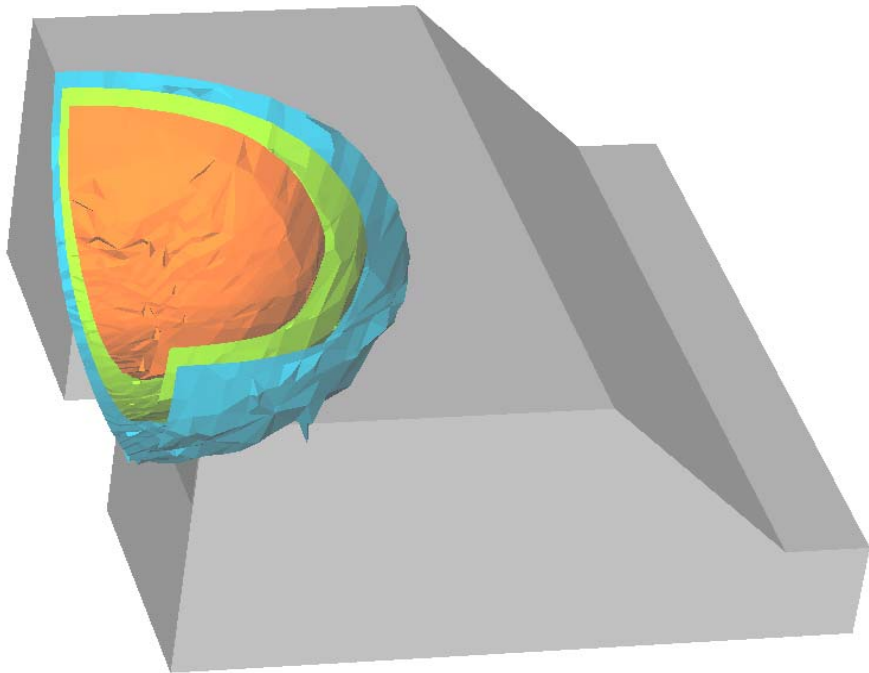
### 2.11.4 AcuMesh

The following is a short summary of plots created in AcuMesh illustrating the movement of the plume through the problem 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.

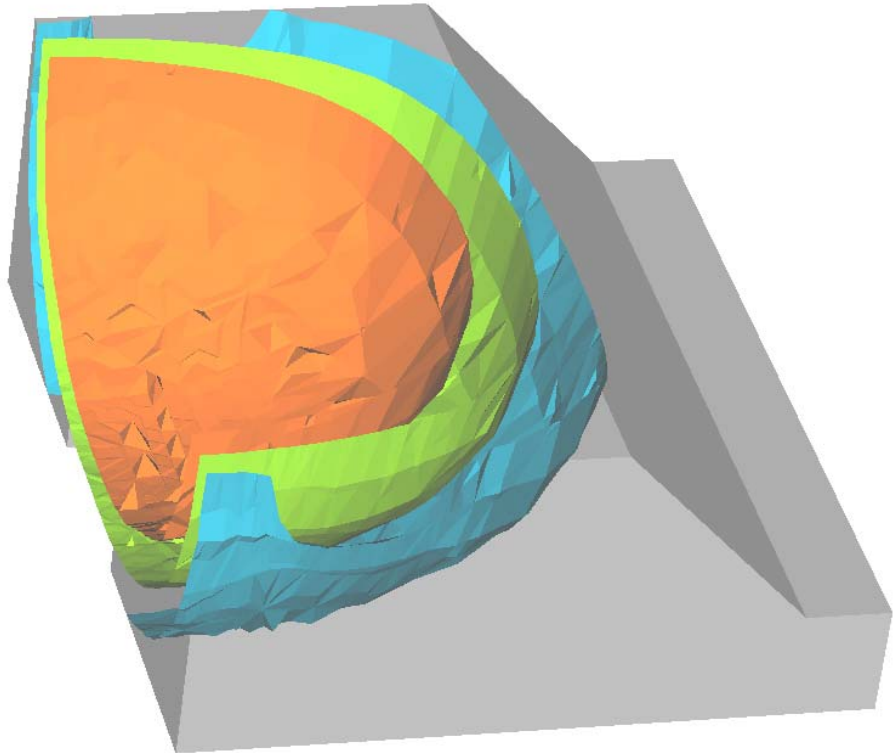
- Time = 50 days



- **Time = 100 days**



- **Time = 400 days**



### 3 REFERENCES

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- Tecplot User’s Manual, version 8.0, 1999. Amtec Engineering Inc. Bellevue, WA 98009-3633

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