

GMS TUTORIALS

Velocity and Mass Flux Calculators

This tutorial gives an overview of the *Velocity* and *Mass Flux* calculators. These calculators are in the 3D Grid module of GMS and were designed to be used with imported sample data – i.e. data obtained from borehole geophysical logs or cone penetrometer logs.

1 Velocity Calculator

The *Velocity* calculator takes three scalar data sets and from them creates a vector data set representing seepage velocity. The three input data sets are *head*, *porosity* and *hydraulic conductivity*. The calculations are based on Darcy's Law:

$$\mathbf{v}_s = \frac{\mathbf{v}_d}{n} = \frac{\mathbf{k}\mathbf{i}}{n}$$

Where \mathbf{v}_s is the seepage velocity, \mathbf{v}_d is the Darcy velocity, n is the effective porosity, \mathbf{k} is the hydraulic conductivity, and \mathbf{i} is the head gradient.

In 3D, the equation is:

$$\begin{bmatrix} v_x \\ v_y \\ v_z \end{bmatrix} = - \begin{bmatrix} k_{xx} & k_{xy} & k_{xz} \\ k_{yx} & k_{yy} & k_{yz} \\ k_{zx} & k_{zy} & k_{zz} \end{bmatrix} \begin{bmatrix} \partial h / \partial x \\ \partial h / \partial y \\ \partial h / \partial z \end{bmatrix}$$

If we assume $k_x = k_y = k_h$ and $k_z = (\text{anis factor}) * k_h$ then this equation simplifies to:

$$\begin{bmatrix} v_x \\ v_y \\ v_z \end{bmatrix} = - \begin{bmatrix} k_h & 0 & 0 \\ 0 & k_h & 0 \\ 0 & 0 & k_z \end{bmatrix} \begin{bmatrix} \partial h / \partial x \\ \partial h / \partial y \\ \partial h / \partial z \end{bmatrix}$$

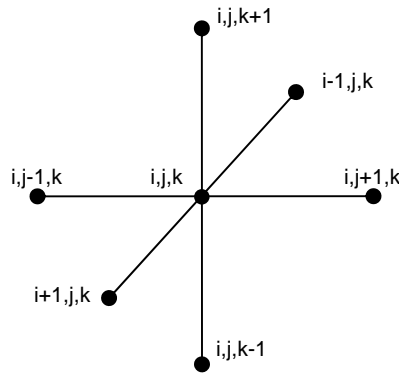
Or:

$$v_x = -k_h \frac{\partial h}{\partial x}$$

$$v_y = -k_h \frac{\partial h}{\partial y}$$

$$v_z = -k_z \frac{\partial h}{\partial z}$$

Thus, the first step is to calculate the hydraulic gradient vector. This is done using simple finite differences. For an interior node (ijk):



We can compute the dh/dx as:

$$\frac{\partial h}{\partial x} = \frac{\frac{h_{i+1,j,k} - h_{i,j,k}}{x_{i+1,j,k} - x_{i,j,k}} + \frac{h_{i,j,k} - h_{i-1,j,k}}{x_{i,j,k} - x_{i-1,j,k}}}{2}$$

The gradients in the other direction are computed in a similar fashion.

2 Mass Flux Calculator

The *Mass Flux* calculator multiplies a seepage velocity data set by a concentration data set to create a vector data set representing mass flux. The units for mass flux are mass per unit area per unit time, or:

$$\frac{M}{L^2 * T}$$

Multiplying the seepage velocity, which has units of length over time (L/T), by a concentration, which has units of mass per volume (M/L³), results in units of:

$$\frac{L}{T} * \frac{M}{L^3}$$

This reduces to $\frac{M}{L^2 * T}$ which are the correct units for mass flux.

2.1 Outline

This is what you will do:

1. Import SCAPS data.
2. Create 3D scatter points.
3. Create a bounding 3D Grid.
4. Interpolate to the 3D Grid.
5. Run the calculators.
6. View the results.

2.2 Required Modules/Interfaces

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

- Sub-surface characterization
- Grid
- Geostatistics

You can see if these components are enabled by selecting the *File / Register*. If you do not have these components enabled, you can complete the tutorial in *Demo Mode*. You can switch to *Demo Mode* by selecting the *File / Demo Mode* menu command.


3 Getting Started

Let's get started.

1. If necessary, launch GMS. If GMS is already running, select the *File / New* command to restore the program settings to their default state.

4 Import Sample Data

We will start by importing sample data.

1. Select the *Open* button .
2. In the *Open* dialog, locate and open the directory entitled **sampcalc**.
3. Change the *Files of type*: to **Text Files (*.txt,*.csv)**.
4. Select the file named **push data.txt** and click *Open*.
5. In step 1 of the *File Import Wizard*, turn **off** the *Space* toggle and turn **on** the *Heading row* toggle as shown in the figure below and click *Next*.

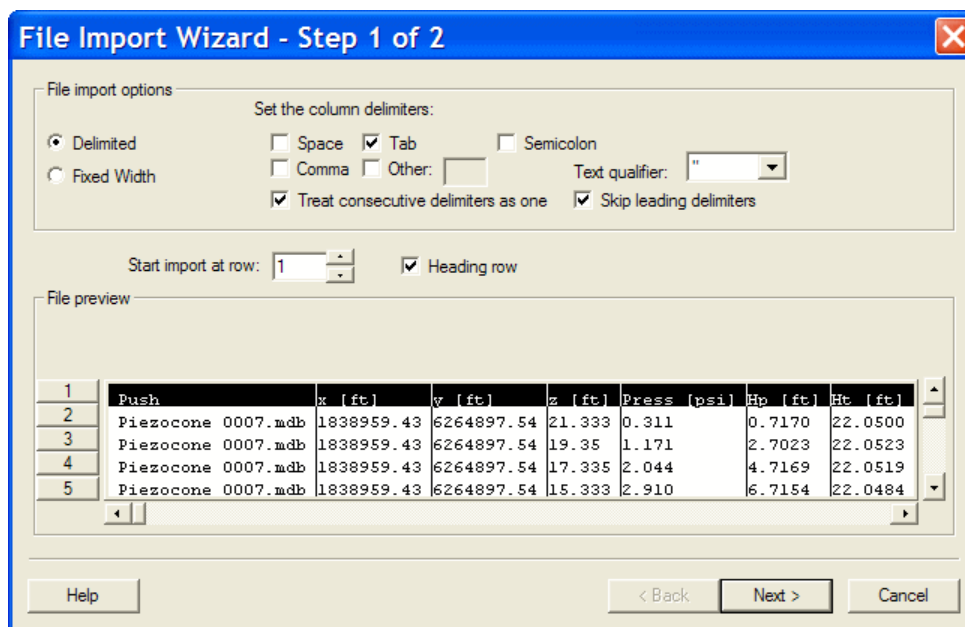


Figure 4.1 File Import Wizard step 1

6. In step 2 of the *File Import Wizard*, change the *GMS data type* to **Borehole sample data**. Change the first column *Type* to **Name**. Make sure everything else is as shown in the figure below and click *Finish*.

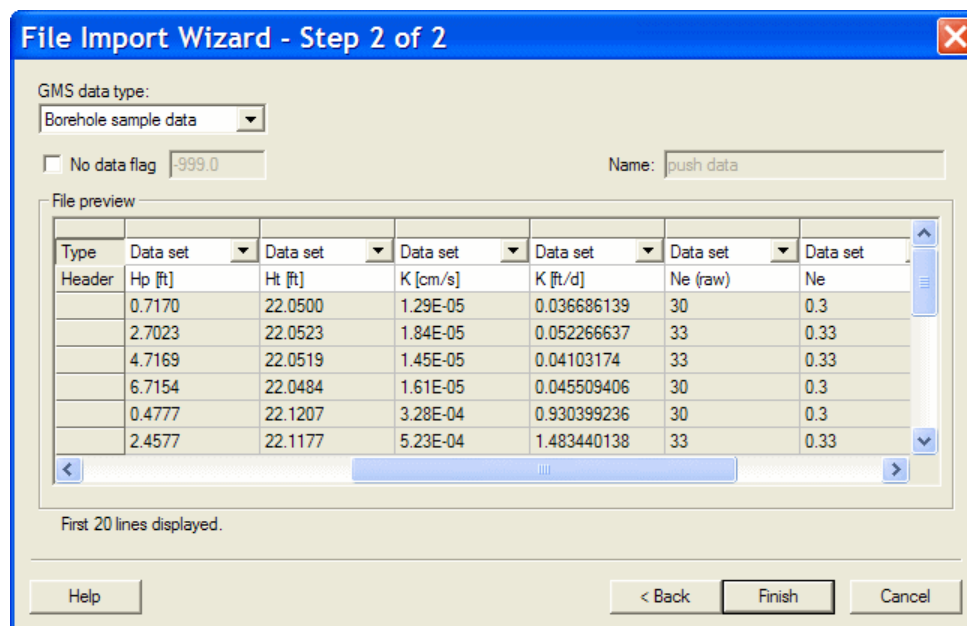




Figure 4.2 File Import Wizard step 2

By default, the imported data are shown in plan view. To better see the data:

7. Switch to oblique view by clicking the *Oblique View* button .

5 Changing the Display Options

Next, we'll adjust the display options so that the boreholes are more visible. Boreholes consist of two types of information: stratigraphy (sand, silt, clay, etc.) and sample data (data set values measured at point locations along the borehole). In this case, we wish to focus on the sample data, so we will turn off the display options related to the stratigraphy. We will also exaggerate the z scale.

1. Click on the *Display Options* button .
2. Turn **off** the *Borehole edges* option.
3. Turn **off** the *Borehole faces* option.
4. Change the *Z magnification* to **4**.
5. Click *OK*.
6. Select the *Frame* button  to center the data.

6 Convert to Scatter Points

We need to interpolate the sample data to a 3D grid. Interpolation is done using scatter points, so we must convert the borehole sample data to scatter points.


1. Select the *Boreholes/Advanced/Sample Data → 3D Scatter Points* menu command.

This dialog is used to filter borehole sample data. In many cases, the borehole sample data are densely sampled in the vertical direction. Since this can lead to difficulties with 3D interpolation, this dialog can be used to thin the sample data. However, our sample data are quite sparse and no filtering is needed.



2. Accept all the default settings and click *OK*.
3. Accept the default name for the new scatter point set and click *OK*.

7 Changing the Display Options

At this point, you should see a set of symbols appear at the location of the borehole sample data locations. Before proceeding, we will hide the borehole sample data.




1. In the *Project Explorer*, turn **off** the *Borehole Data*  folder.

We will also adjust the display of the scatter points so the data values are plotted and the point color is adjusted based on the data value.

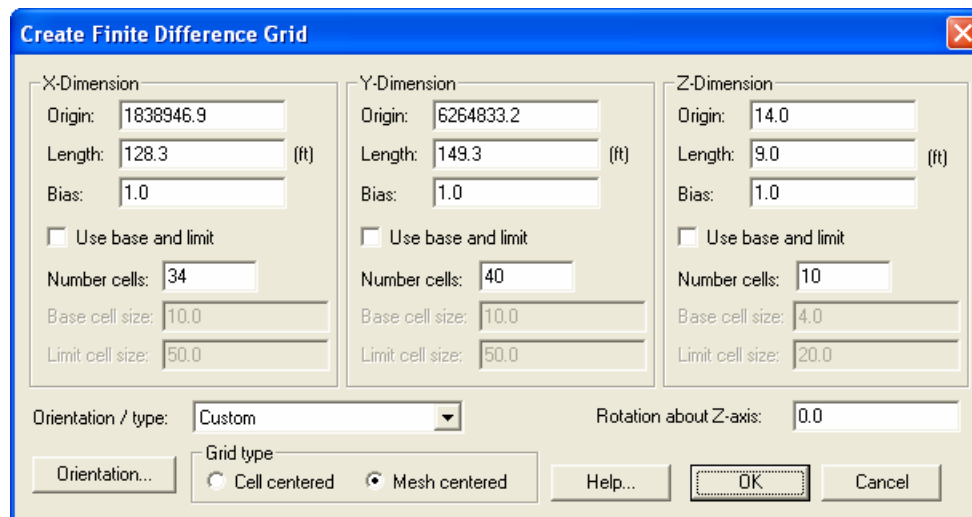
2. In the *Project Explorer*, click on the *3D Scatter Data*  folder.
3. Click on the *Display Options* button .
4. Under the *Scatter Point Symbols* option, change the *Color* option to **data**.
5. Click *OK*.

8 Creating the Bounding Grid

Now that we have scatter point data, we are ready to interpolate the measured values to a grid so that we can visualize the data in three dimensions. First we will create a 3D grid which bounds our scatter points. Two types of grids are supported in GMS: cell-centered (data values at cell centers) and mesh-centered (data values at cell corners). We will use a mesh-centered grid since this type of grid is best-suited for 3D visualization.

1. In the *Project Explorer*, expand the *3D Scatter Data*  folder if necessary so the *scatter*  object is visible.
2. Right-click on the *scatter*  object and select the *Bounding 3D Grid* command from the pop-up menu.

3. Change the values to be as shown in the dialog below and click *OK*.



The dialog box titled "Create Finite Difference Grid" has three main sections for X-Dimension, Y-Dimension, and Z-Dimension. Each section contains fields for Origin, Length (ft), Bias, a checkbox for "Use base and limit", Number cells, Base cell size, and Limit cell size. At the bottom, there is a dropdown for "Orientation / type" set to "Custom", a "Rotation about Z-axis" field set to "0.0", a "Grid type" section with radio buttons for "Cell centered" and "Mesh centered" (the latter is selected), and buttons for "Orientation...", "Help...", "OK", and "Cancel".


Dimension	Origin	Length (ft)	Bias	Use base and limit	Number cells	Base cell size	Limit cell size
X-Dimension	1838946.9	128.3	1.0	<input type="checkbox"/>	34	10.0	50.0
Y-Dimension	6264833.2	149.3	1.0	<input type="checkbox"/>	40	10.0	50.0
Z-Dimension	14.0	9.0	1.0	<input type="checkbox"/>	10	4.0	20.0

Orientation / type: Custom Rotation about Z-axis: 0.0

Grid type: ☐ Cell centered ☒ Mesh centered



Figure 8.1 Creating the Bounding Grid

You should now see a 3D grid.

4. Select the *Frame*  button to frame the data in the window.


9 Changing the Display Options



We'll change the display options so that only the outline of the grid is visible for now.

1. In the *Project Explorer*, select the *3D Grid Data*  object.
2. Click on the *Display Options* button .
3. Turn **off** the *Cell edges* option.
4. Turn **on** the *Grid shell* option.
5. Click *OK*.

10 Interpolating K to the 3D Grid



Next, we'll interpolate the hydraulic conductivity data from the scatter points to the 3D grid.

1. In the *Project Explorer*, select the *3D Scatter Data*  folder.
2. Select the *Interpolation/Interpolation Options* menu command.

3. In the *3D Interpolation Options* dialog, select the *Inverse distance weighted* method.
4. Select the *Options* button next to the *Inverse distance weighted* option.
5. Change the *Nodal function* to be *Quadratic* and click *OK*.
6. Click *OK* to exit the *3D Interpolation Options* dialog.
7. In the *Project Explorer*, expand the *scatter*  object so that you can see the data sets underneath it.
8. Select the *K [fid]* data set so that it's the active data set.
9. In the *Project Explorer*, right-click on the *scatter*  object and select the *Interpolate To/3D Grid* menu command.
10. Click *OK* to perform the interpolation.

11 Changing the Display Options

Now that the data values are interpolated to the 3D grid, we'll turn on grid contours to help visualize the data.




1. In the *Project Explorer*, select the *3D Grid Data*  object.
2. Click on the *Display Options* button .
3. Turn **on** the *Contours* option.
4. Select the *Grid contours* option.
5. Click *OK*.

Next we will try color-fill contours.

6. Select the *Data/Contour Options* menu command.
7. Change the *Contour method* option to **Linear and color fill**.
8. Click *OK*.




12 Interpolating Head to the 3D Grid

Now we'll interpolate the head data from the scatter points to the 3D grid.

1. In the *Project Explorer*, select the *Ht [ft]*  data set under the *scatter*  object. Note that this data set represents the total hydraulic head (pressure head + elevation head).
2. In the *Project Explorer*, right-click on the *scatter*  object and select the *Interpolate To/3D Grid* menu command.
3. Click *OK* to exit the dialog and perform the interpolation.





13 Interpolating Porosity to the 3D Grid

Now we'll interpolate the porosity data from the scatter points to the 3D grid.

1. In the *Project Explorer*, select the *Ne*  data set under the *scatter*  object. Note that this data set represents the effective porosity scaled between 0-1.
2. In the *Project Explorer*, right-click on the *scatter*  object and select the *Interpolate To/3D Grid* menu command.
3. Click *OK* to exit the dialog and perform the interpolation.


14 Computing Seepage Velocity

The 3D Grid now has all the data sets necessary to compute the seepage velocity.

1. In the *Project Explorer*, select the *3D Grid Data*  object.
2. Select the *Data/Velocity / Mass Flux Calculator* menu command.
3. In the tree of data sets on the left of the dialog, select the *Ht [ft]_idw_quad*  data set.
4. Click the first (top) *Map >* button. This puts the path to the head data set in the field.
5. Now select the *K [ftd]_idw_grad*  data set on the left and click the middle *Map >* button.
6. Now select the *Ne_idw_quad*  data set on the left and click the bottom *Map >* button.
7. Click the *Create Data Set* button.
8. Click *OK*.

15 Changing the Display Options

We'll turn on grid vector arrows to visualize the velocity field.

1. Click on the *Display Options* button .
2. Turn **off** the *Contours* option.
3. Turn **on** the *Vectors* option.
4. Select the *Options* button to the right of the *Vectors* option.
5. Change the settings to be as shown in Figure 15.1 below.

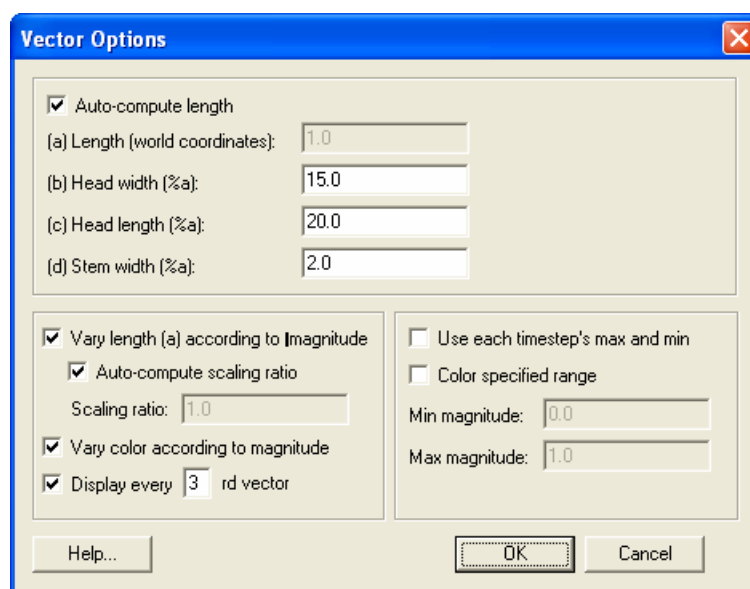







Figure 15.1 Vector Options Dialog

6. Click *OK* twice to exit both dialogs.
7. Use the zoom  and rotate  tools to examine the vectors at different places on the grid.

16 Interpolating Concentrations



The *Velocity/Mass Flux Calculator* can also be used to create a mass flux data set. We will use the concentration data set (Conc).

1. In the *Project Explorer*, select the *Conc*  data set under the *scatter*  object.
2. In the *Project Explorer*, right-click on the *scatter*  object and select the *Interpolate To/3D Grid* command from the pop-up menu.

3. Select the *Interpolation Options* button.
4. Turn **on** the *Truncate values* option.
5. Select the *Truncate to specified range* option.
6. For the *Min* enter **0.0** and for the *Max* enter **100.0**.
7. Click *OK* twice to exit both dialogs.

17 Changing the Display Options


We'll turn on grid iso-surfaces to see the concentration data.


1. In the *Project Explorer*, select the *3D Grid Data*  object.
2. Click on the *Display Options* button .
3. Turn **off** the *Vectors* option.
4. Turn **on** the *Iso-surfaces* option.
5. Select the *Options* button to the right of the *Iso-surfaces* option.
6. Change the *Number of iso-surfaces* value to **3**.
7. Click the *Default* button.
8. Click *OK* twice to exit both dialogs.

You should see three colored iso-surfaces representing the contaminant at three different concentrations.

18 Computing Mass Flux




The 3D Grid has all the data sets necessary to compute a mass flux data set so we'll do that now.

1. Select the *Data/Velocity/Mass Flux Calculator* menu command.
2. Select the *Create Contaminant Flux Data Set* tab.
3. In the tree of data sets on the left of the dialog, select the *velocity*  data set (make sure you don't select the *velocity_Mag* data set).
4. Click the top *Map >* button.

5. Now select the *Conc_idw_quad*  data set on the left and click the lower *Map >* button.
6. Click the *Create Data Set* button.
7. Click *OK*.

19 Changing the Display Options

We'll turn the vector arrows back on to see the mass flux data.

1. Click on the *Display Options* button .
2. Turn **on** the *Vectors* option.
3. Turn **off** the *Iso-surfaces* option.
4. Click *OK*.
5. Use the zoom  and rotate  tools to examine the vectors at different places on the grid.

20 Conclusion

This concludes the tutorial. Here are the things that you should have learned in this tutorial:

- The *Velocity/Mass Flux Calculator* can be used to create a vector data set representing seepage velocity.
- You must have a head data set, a hydraulic conductivity data set, and a porosity data set in order to create a seepage velocity data set.
- You can use the *Velocity/Mass Flux Calculator* to create a mass flux data set given a seepage velocity data set and a concentration data set.