GIFMod Applications Manual

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About the companion websites

- The examples presented in this manual can be downloaded as part of the installation package at www.GIFMod.com.
- The source code of the program is available at https://github.com/USEPA/GIFMod.

Abstract

In this, manual a few examples showing the steps needed to build hydraulic and water quality models using the GIFMod framework have been provided.

1

One dimensional flow in a confined aquifer

This example shows the steps needed to create and run a one-dimensional hydraulic model of a confined aquifer with a single pumping location. The assumption is that all the conditions are uniform over the horizontal axis, perpendicular to the main direction of flow. Note that the example is solely for instructional purposes and does not represent a real-world problem.

It is assumed that a withdrawal of 1m/day/m occurs at the center of the aquifer and that a constant recharge of 0.00181m/d occurs over the entire duration of the simulation (1000days). We will discretize the aquifer into 11 blocks so each block will have an area of $50m \times 1m$. The aquifer's porosity is assumed to be 0.35 and its thickness is assumed to be 4m. The aquifer's hydraulic conductivity is 1m/day. Figure 1.1 shows the schematic of the model. A no-flow boundary condition is assumed at the two boundaries of the aquifer. The steps needed to construct the model are presented below.

- Start GIFMod

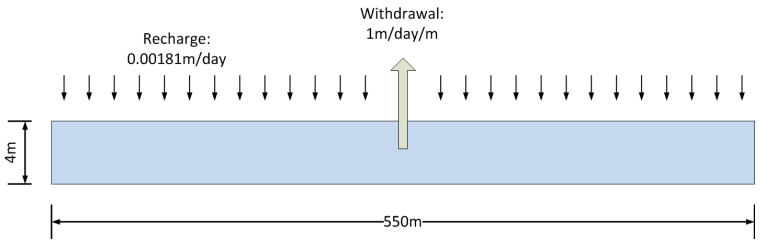


Figure 1.1: The schematic of the 1-D confined aquifer model

- **Create a single Darcy block:**

  From the top ribbon click on the Darcy icon  . Set the following properties:

  - Bottom area: *50*m^2.
  - Initial moisture content: *0.35* (assuming the initial hydraulic head is zero)
  - Saturated moisture content: *0.35*
  - Saturated hydraulic conductivity: *1m/day*
  - Precipitation: *Yes* (allows introducing recharge using the precipitation feature)
  - Storage coefficient *under* ***Specific Storage***: 0.01m^{-1}
  - Bottom elevation: *-4m* (this sets the datum on the interface between the confined aquifer and the top confining layer.)
  - Depth: *4m*

  Leave the rest of the properties unchanged. Default values will be used.

- **Create an array of blocks:**
  In this step we create a array of the Darcy block created in the previous step. The array will be composed of 11 blocks.

  - Right-click on the Darcy block created in the previous step and select **Make array of blocks** from the drop-down menu.
  - Select the **Horizontal 2D array** option and enter the number 11 in the text box labeled **Number of columns**.
  - For the **Horizontal distance between cell grids**, enter 50m.
  - Click on **Ok** button.

  The array should appear on your screen as shown in Figure 1.2.

- Setting the properties of the connectors:
  When an array of blocks are created GIFMod automatically connects the blocks sequentially and assign some of the relevant properties from the blocks to the connectors. For example in this case the values of saturate hydraulic conductivity from the initial block is assigned to the connectors. Also the length of the connectors are assigned based on the horizontal distance indicated in the array dialog. However, some

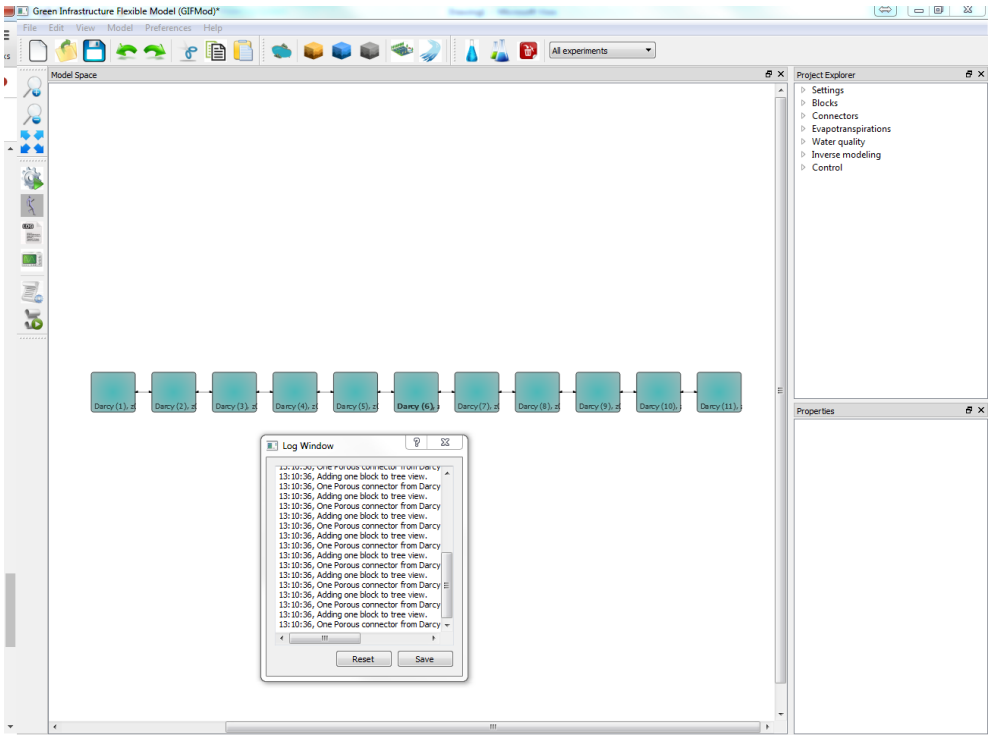


Figure 1.2: 1-D confined aquifer model representation in GIFMod

other properties of the connectors still need to be assigned. In this case the only property that needs to be specified for the connectors is **Interface/cross sectional area**.

- select each connector and from the **Properties** window set the interface area to $4m^2$ (i.e. 4m thickness$\times$ 1m horizontal depth in the axis perpendicular to the screen.

- **Adding recharge:**
  The recharge will be added using the precipitation feature of the program. First a text file containing the precipitation data should be created. The duration of the simulation is assumed to be 1000days starting from day zero until day 1000.

  - The precipitation data file is a file containing three columns the first representing the start time of an event, the second representing the end time of an event and the third one the volume (in meters) of precipitation during the event period. The precipitation file for a uniform precipitation of 0.00181m/d will look like Figure 1.3. It should be noted that the time-intervals in the precipitation data file do not have to be uniform (or daily) but the daily intervals are used here for convenience. Save the text file as "precipitation.txt".
  - Choose the **Climate setting** item from the **Settings** menu in **Project explorer** and then click on the box in front of **Precipitation** and from the open dialog box that appear select "precipitation.txt" that was created in the previous step.

- **Adding withdrawal:**
  The pumping/withdrawal will occur on the middle black named "Darcy (6)".

  - The flow file contain a heading showing the nature of the quantity it represent in this case flow. This is the top most row of the file. Create a new text file. Type "names, flow" (without quotation marks) as the first row. This file will have two columns separated by comma. The first column is the time and the second is the flow rate in m^3/day. The file should look like figure 1.4. The negative rates indicate withdrawal. Save the file as "pumping.txt".
  - Click on the block labeled "Darcy (6)" and from the properties window find **Inflow time series** and select "pumping.txt".

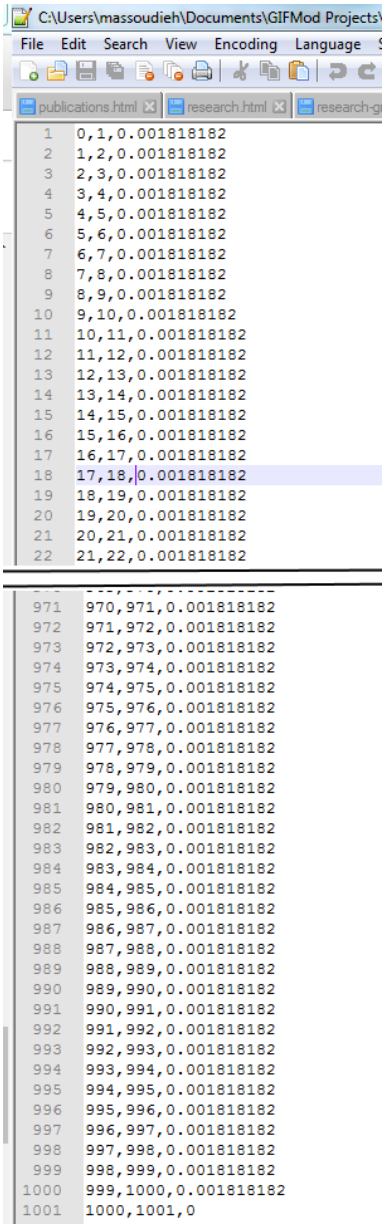


Figure 1.3: Precipitation data file for the 1-D confined aquifer model

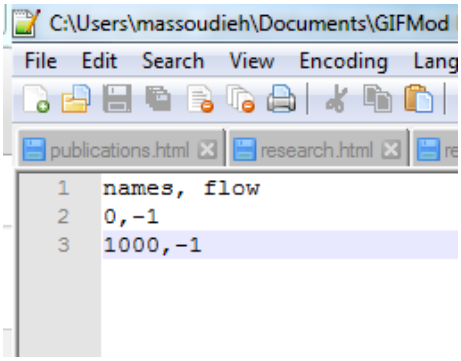


Figure 1.4: Pumping file for the 1-D confined aquifer example

- **Setting the duration of the simulation:**
  The duration of the simulation is from day zero to day 1000. From the **Project Explorer** select **Setting→Project settings**. From the property window fine right-click in the label **Simulation end time** and click on **Input Number**. Enter 1000 in the input box that appear.
- Save the project.
- **Adding a recharge gage:**
  Here we just add a pond to keep track of cumulative precipitation.
  - From the top ribbon click on the pond button to add a pond to the model.
  - Set the area of the pond to 1m.
- **Running the model:** The model is now ready for running. From the left hand ribbon click on the run button and wait until the simulation ends.
- **Inspecting the results**
  - Right-click on blocks Darcy(1) to Darcy(6) and choose **Plot Hydraulic results→Plot head** from the drop-down menu. You can copy and paste all the graphs onto a single one and color each differently. The final results should look like figure 1.5.
  - Right-click on each of the connectors connecting blocks Darcy (1)-(6) and choose **Plot flow**. Copy all the curves into the same

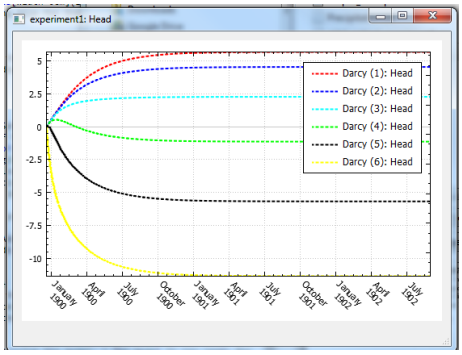


Figure 1.5: Temporal variation of hydraulic head in blocks Darcy (1)-(6) in the 1-D unconfined aquifer example

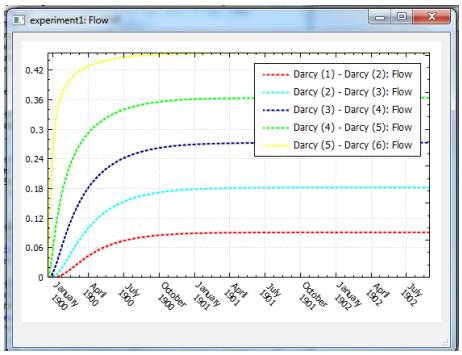


Figure 1.6: Temporal variation of flow rates in connectors connecting blocks Darcy (1)-(6) in the 1-D unconfined aquifer example

window and color each curve as you desire. The result should look like figure 1.6

2

Two dimensional flow in a confined aquifer

This example demonstrates how to create a model of a two dimensional groundwater flow system in a confined aquifer. The groundwater system is composed on three no-flow boundary conditions, one fixed head boundary, and two wells. The aquifer has a depth of 10m, a hydraulic conductivity of 1m/day, and a porosity of 0.35. Refer to figure 4.1 for a representation of the modeled system.

- Start GIFMod
- **Create a single Darcy block:**

  Click on the Darcy icon  on the top ribbon. Set the following properties:

  - Bottom area: *4000*m^2.
  - Initial moisture content: *0.35* (this assumes that the initial hydraulic head is zero.)
  - Saturated moisture content: *0.35*
  - Saturated hydraulic conductivity: *1m/day*
  - Precipitation: *Yes* (This allows introducing recharge using the precipitation feature.)
  - Storage coefficient: 0.0001m^{-1}
  - Bottom elevation: *-11m* (this sets the datum on the interface between the confined aquifer and the top confining layer.)

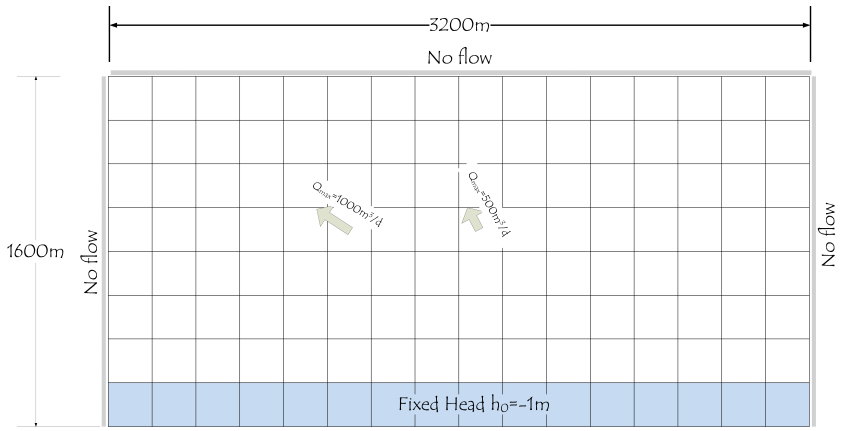


Figure 2.1: The schematic of he 2-D confined aquifer system

  - Depth: *10m*
  - Width: *200m*
  - Length: *200m*

  Leave the rest of the properties unchanged. Default values will be used.

- **Create an array of blocks:**
  In this step, we create an array of the Darcy block created in the previous step. The array will be composed of 8 rows and 16 columns.

  - Right-click on the Darcy block created in the previous step and choose **Make array of blocks** from the drop-down menu.
  - Choose the **Horizontal 2D array** option and enter the number 16 in the text box labeled **Number of columns** and 8 in the text box labeled **Number of rows**.
  - For the **Horizontal distance between cell grids**, enter 200m.
  - For the **Vertical distance between cell grids**, enter 200m.
  - Click on **Ok** button.

  Once you have created the array, your screen should look like Figure 1.2.

- **Imposition the fixed-head boundary condition:** To impose the fixed head boundary condition at $h_0 = -1m$ select the storage blocks on the bottom row.

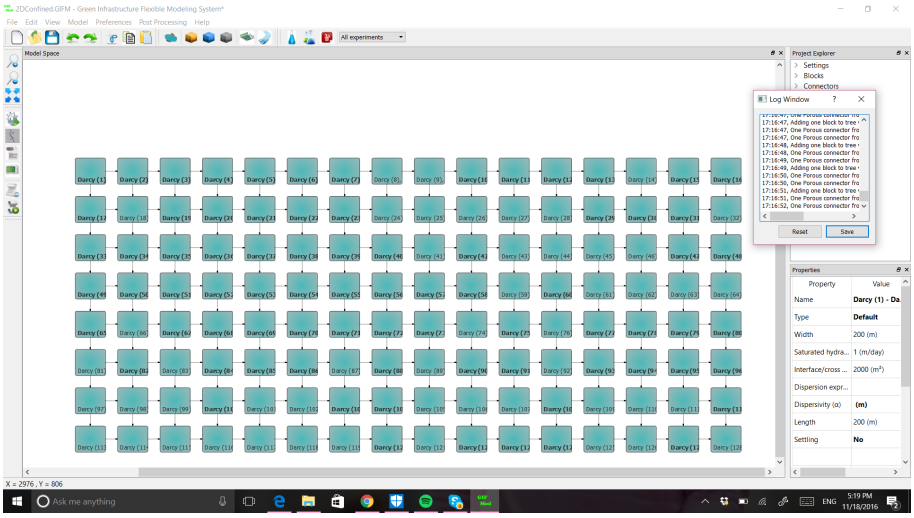


Figure 2.2: 2-D confined aquifer model representation

- Select the Darcy block labeled "Darcy (113)" and type "-1" in the property **Head-storage relationship**.
- Repeat the previous step for all block in the lowest row (Darcy (114)-Darcy (128)).

- **Introducing the pumping wells:**

  At the time we consider a constant pumping from storage block *Darcy (54)* at $1000m^3/day$ and storage block *Darcy (57)* at $500m^3/day$ over a 1000days period. The inflow time-series files should look like Figure 4.3. Create the files and save them respectively as "pumping1000.txt" and "pumping500.txt". Select the block labeled *Storage(54)* and from the properties window find the property called **Inflow time series** and choose *pumping1000.txt*. Repeat the previous task for *Darcy (57)* block and select *pumping500.txt*.

- **Setting the duration of the simulation:**
  The duration of the simulation is from day zero to day 1000. From the **Project Explorer** select **Setting→Project settings**. From the property window fine right-click in the label **Simulation end time** and click on **Input Number**. Enter 1000 in the input box that appear.

- **Changing the initial time-step:** The final results will be stored at

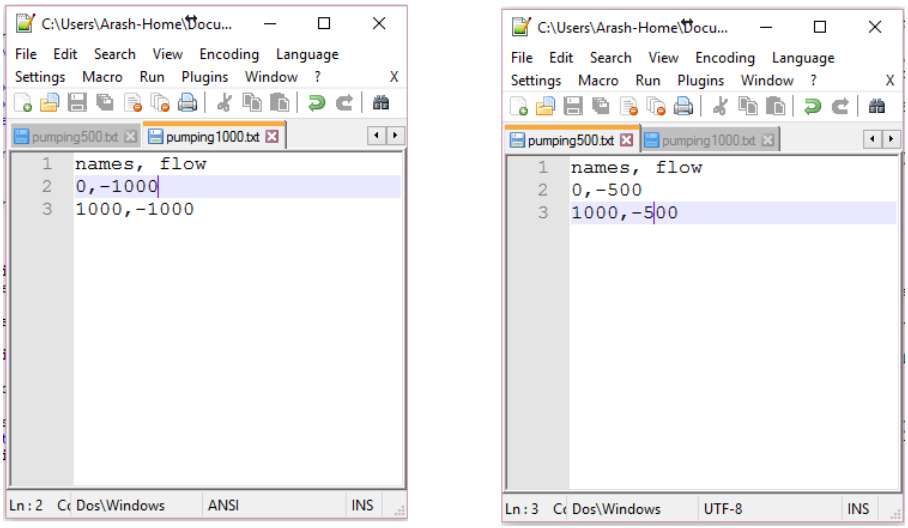


Figure 2.3: Pumping time-series files

intervals equal to the initial time step size. So having the initial time step at 0.01 day (default value) while the simulation time is 1000 days will make the size of the results to be stored in the memory for post-processing too large. From the **Settings→Solver Settings** choose **Initial time step size** and change the value to 1 day.

- Save the project.
- **Running the model:** The model is now ready for running. From the left hand ribbon click on the run button and wait until the simulation ends.
- **Inspecting the results:**
  - Right-click on a block of your choice and select **Plot Hydraulic Results→Plot Storage** from the drop-down menu that appears. You may copy and paste the results on one graph to another one for comparison. For example figure 2.4 shows the storage in blocks *Darcy (53)* to *Darcy (57)*. As it can be seen the drop in the hydraulic head at the wells are quite significant. This is due to the high pumping rates relative to the hydraulic conductivities of the aquifer.

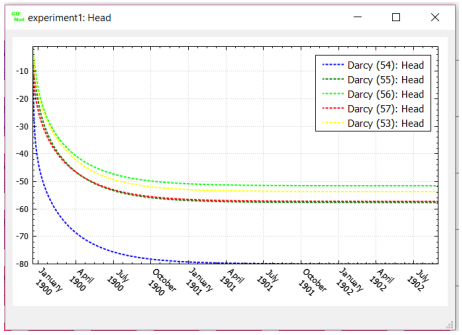


Figure 2.4: Hydraulic head in select blocks

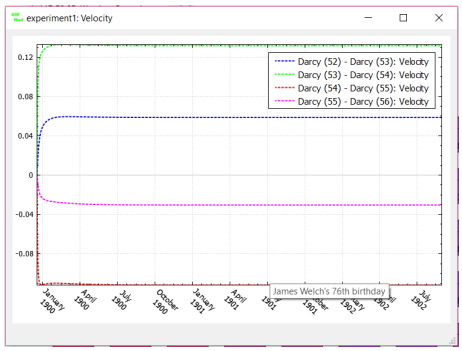


Figure 2.5: Darcy flux in select blocks

  - Right-click on connectors of your choice and select **Velocity** from the drop-down menu. Figure 2.5 shows the flow rate in connectors connecting *Storage(54)* to *Darcy (57)*. This shows the Darcy flux in the connectors.

- **Examining the spatio-temporal variation of state variables:** From the top menu bar click on post-processing and then select **Blocks**→**Head**. Using the scroll bar in the legend box that will appear, change the time at which you would like to see the spatial distribution of hydraulic head over the domain (Figure 2.6).

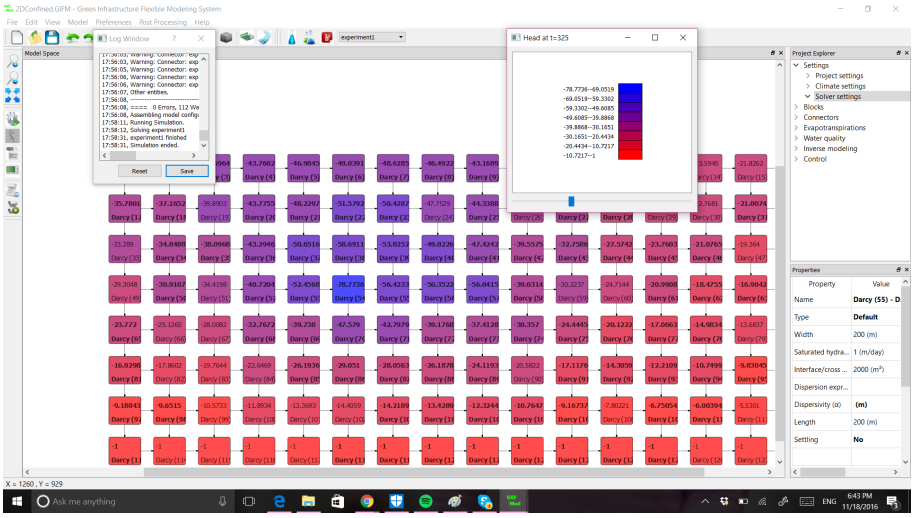


Figure 2.6: Spatial distribution of hydraulic head at t=325

2.1 Revising the example: recovery as a result of reduced pumping after 200 days

Here we are going to modify the previous example by reducing the pumping rate by a factor of five after 200days.

- Make a copy of the pumping files and modify them as shown in figure 4.6. Save the newly created pumping files with a new names.
- Select the revised inflow time-series files as **Inflow time series** for blocks *Storage(54)* and *Storage (57)* respectively.
- Rerun the program.
- Select desired blocks and connectors and check the new variation of state variables over time.

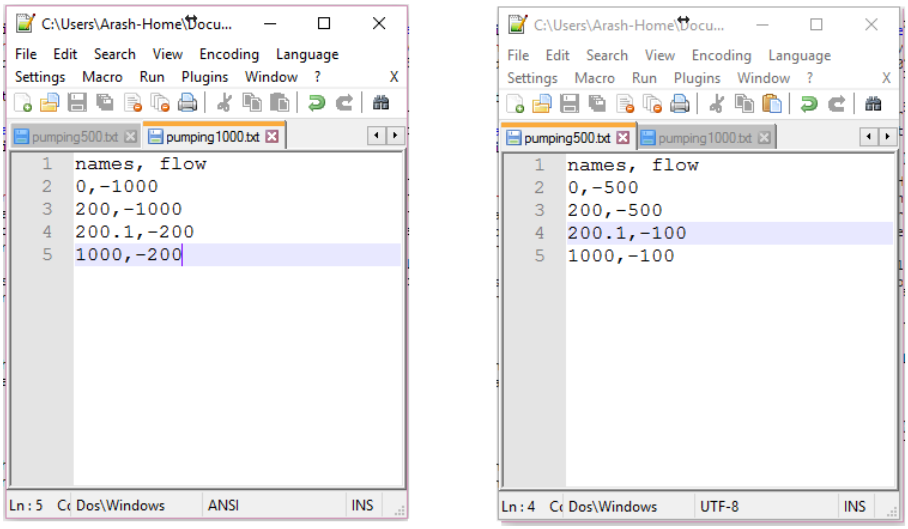


Figure 2.7: Revised pumping time-series files

3

Transport of a conservative pollutant in a two dimensional confined aquifer system

In this example we will add transport of a conservative contaminant to the example done in the previous chapter 2.

The initial location of a pollutant spill is shown in figure 3.2

Below are the steps to introduce transport to the previously built model in chapter 2:

- **Loading the hydraulic model:** Load the input file saved at the end of constructing the 2-D confined aquifer hydraulic model in chapter 2 or load the file named *"2DConfined.GIFM"* from the GIFMod examples folder under the folder *2DConfinedAquifer*.
- **Introducing a new water quality constituent:** Right click on **Project Explorer→Water Quality→Constituents** and select **Add Constituent**. Change the name of the new constituent to PDB. Leave the rest of the properties unchanged. This means that the pollutant will behave without any interactions with the solid matrix and will not be affected by gravity and that the molecular diffusion and dispersion are zero.
- **Setting the initial condition:** Select the block labeled as *Darcy (68)* and from the properties window click on **Initial Constituent**

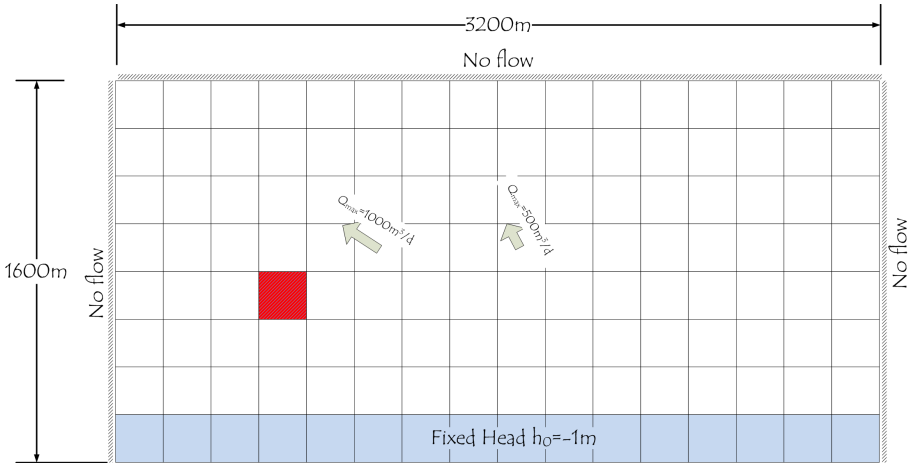


Figure 3.1: The initial location of the spill

Concentration property. In the window that will show up, assign a concentration of 10 to *PCB*.

- **Run the model**
- **Inspecting the results:** From the **Post-processing menu** choose **Water Quality**→*PCB* and use the scroll button to see the evaluation of PCD concentration in the aquifer (Figure **??**).

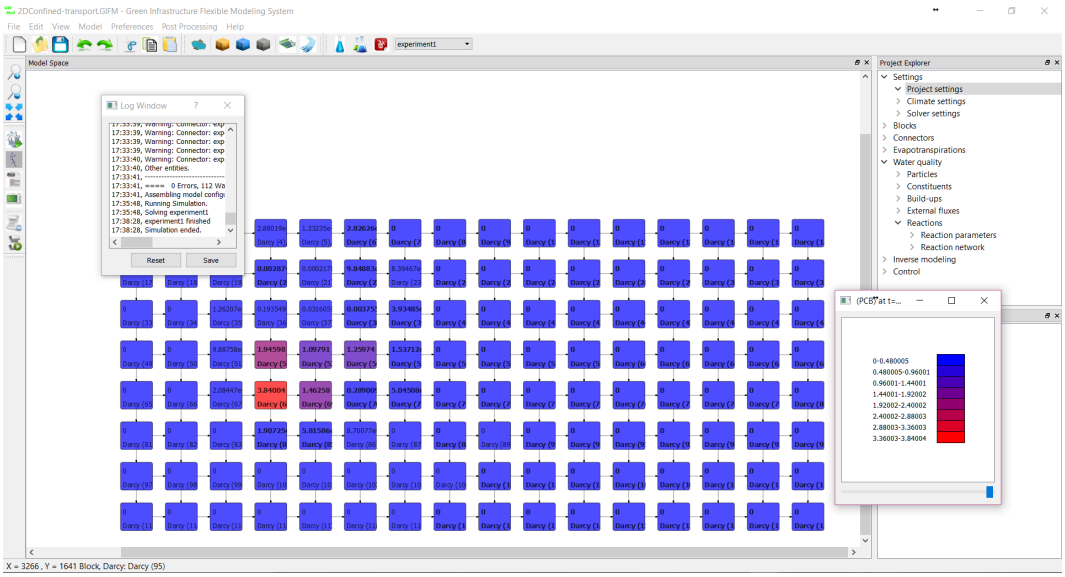


Figure 3.2: The spread of PCB plume after 1000 days

4

Two dimensional flow in an unconfined aquifer

In this example, we will create a model of a two dimensional groundwater flow system in an unconfined aquifer. The groundwater system is composed on three no-flow boundary conditions, one fixed head boundary, and two wells. The aquifer has a depth of 11m, and a hydraulic conductivity of 1m/day, a porosity of 0.35 and a specific yield of $S_y = 0.1$. Figure 4.1 shows a representation of the modeled system.

Storage blocks will be used to create the model because they allow partially saturated elements, consistent with an unconfined aquifer.

4.1 Constant pumping rates

- start GIFMod
- **Create a single Storage block:**
  From the top ribbon click on the Darcy icon  . Set the following properties:
  - Bottom area: *40000m*^{2}.
  - Initial moisture content: *0.1* (results in a specific yield of 0.1)
  - Saturated moisture content: *0.1*
  - Saturated hydraulic conductivity: *1m/day*
  - Precipitation: *Yes* (This allows introducing recharge using the precipitation feature.)

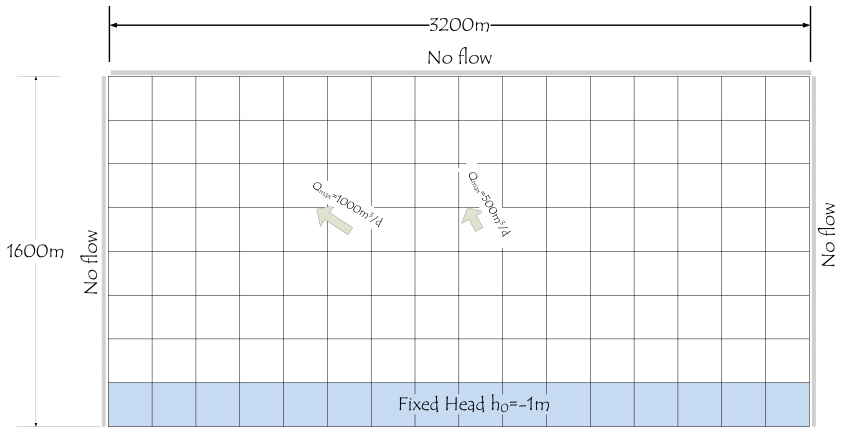


Figure 4.1: The schematic of he 2-D unconfined aquifer system

- Storage coefficient: $0.0001m^{-1}$ (only becomes effective if a block's moisture content exceeds the saturation moisture content)
- Bottom elevation: *-11m* (this sets the datum on ground surface.)
- Initial water depth: *10m*
- Depth: *11m*
- Width: *200m*
- Length: *200m*
- Dispersivity: *0.05m* (This value is not used in hydraulic simulation, but it will be used when a contaminant transport component is added to the model.)

Leave the rest of the properties unchanged. Default values will be used.

- **Create an array of blocks:**
  In this step we create an array of the Darcy block created in the previous step. The array will be composed of 8 rows and 16 columns.
  - Right-click on the Darcy block created in the previous step and choose **Make array of blocks** from the drop-down menu.
  - Choose the **Horizontal 2D array** option and enter the "16" in the text box labeled **Number of columns** and "8" in the text box labeled **Number of rows**.
  - For the **Horizontal distance between cell grids**, enter 200m.

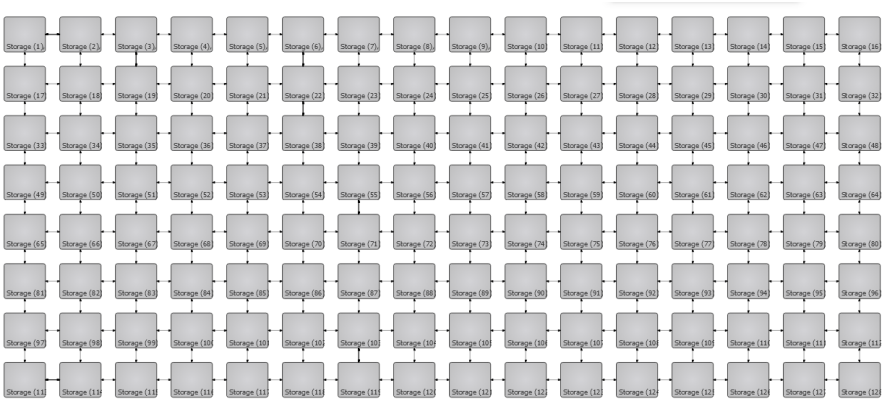


Figure 4.2: 2-D unconfined aquifer model representation in GIFMod

  - For the **Vertical distance between cell grids**, enter 200m.
  - Click on **Ok** button.

  Once you have created the array, your screen should look like Figure 4.2.

- **Imposition the fixed-head boundary condition:** To impose the fixed head boundary condition at $h_0 = -1m$ select the storage blocks on the bottom row.

  - Select the Storage block labeled "Storage(113)" and type "-1" in the property **Head-storage relationship**.
  - Repeat the previous step for all block in the lowest row (Storage(114)-Storage(128)).

- **Introducing the pumping wells:**

  At the time we consider a constant pumping from storage block *Storage(54)* at $1000m^3/day$ and storage block *Storage(57)* at $500m^3/day$ over a 1000days period. The inflow time-series files should look like Figure 4.3. Create the files and save them respectively as "pumping1000.txt" and "pumping500.txt". Select the block labeled *Storage(54)* and from the properties window find the property called **Inflow time series** and choose *pumping1000.txt*. Repeat the previous task for *Storage(57)* block and select *pumping500.txt*.

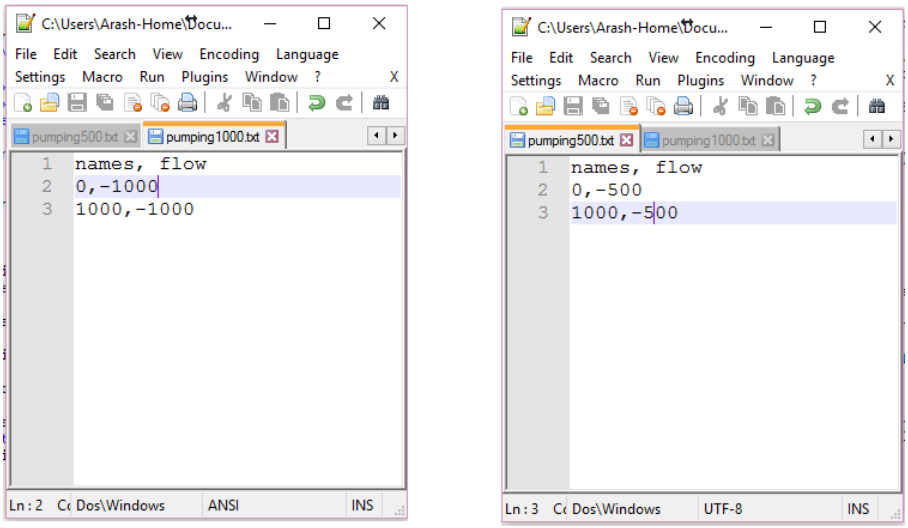


Figure 4.3: Pumping time-series files

- **Setting the duration of the simulation:**
  The duration of the simulation is from day zero to day 1000. From the **Project Explorer** select **Setting→Project settings**. From the property window fine right-click in the label **Simulation end time** and click on **Input Number**. Enter 1000 in the input box that appear.

- Save the project.

- **Running the model:** The model is now ready for running. From the left hand ribbon click on the run button  and wait until the simulation ends.

- **Inspecting the results:**

  – Right-click on a block of your choice and select **Plot Hydraulic Results→Plot Storage** from the drop-down menu that appears. You may copy and paste the results on one graph to another one for comparison. For example figure 4.4 shows the storage in blocks *Storage(54)* to *Storage(57)*. As it can be seen the pumping rate leads to a near depletion of water in the block where pumping takes place.

  – Right-click on connectors of your choice and select **Velocity** from the drop-down menu. Figure 4.5 shows the flow rate in connectors

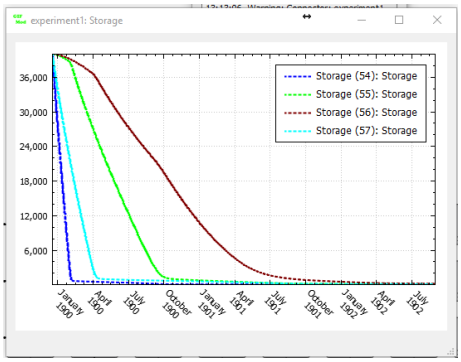


Figure 4.4: Storage variation in select blocks

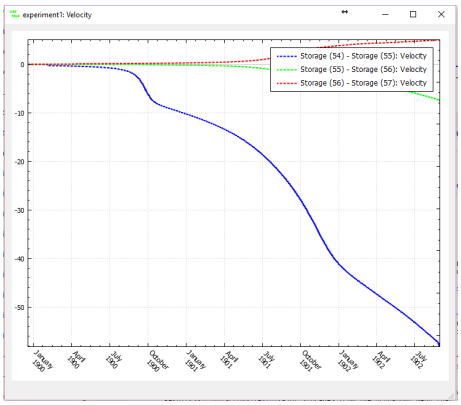


Figure 4.5: Darcy flux in select blocks

connecting *Storage(54)* to *Storage(57)*. This shows the Darcy flux in the connectors.

4.2 Revising the example: recovery as a result of reduced pumping after 200 days

Here we are going to modify the previous example by reducing the pumping rate by a factor of five after 200days.

- Make a copy of the pumping files and modify them as shown in figure 4.6. Save the newly created pumping files with a new names.

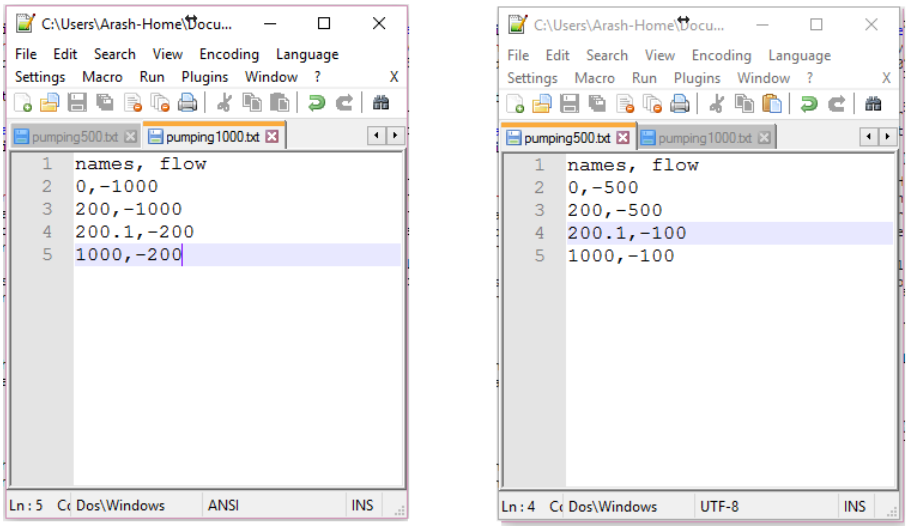


Figure 4.6: Revised pumping time-series files

- Select the revised inflow time-series files as **Inflow time series** for blocks *Storage(54)* and *Storage (57)* respectively.
- Rerun the program.
- Select desired blocks and connectors and check the new variation of state variables over time.

5

PID Control

This example shows how to use a PID control in order to control aeration rate with the purpose of maintaining the DO concentration in a pond constant. The PID controller is assumed to control the aeration rate as governed by K_{La} coefficient. A very simple BOD-DO interaction model is assumed while both BOD and DO limitation effects are considered using Monod kinetics. The processes controlling DO uptake are described using the following simple process:

$$BOD + DO \xrightarrow{r_{max}\frac{BOD}{BOD+K_s}\frac{DO}{DO+K_O}} CO_2 + Biomass + OtherStuff \quad (5.1)$$

Here we only model BOD and DO explicitly. In the following the steps to build the model has been described:

- Start GIFMod.
- Add a pond using the top tool ribbon by clicking on the pond 
- Set the following properties for the pond:
  - **Bottom Area:** $1m^2$
  - **Initial water depth:** $1m$
- **Adding constituents:** Add two water quality constituents named "BOD" and "DO" by right-clicking on **Project Explorer→Water Quality→Constituents** and selecting **Add constituent**.

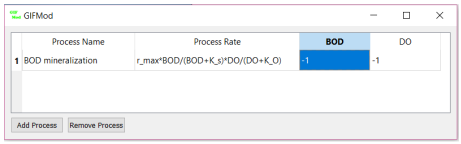


Figure 5.1: Reaction network for the DO control example

- **Adding reaction parameters:** Add the following reaction parameters using **Project Explorer→Water Quality→Reactions→Reaction parameters**.
  - r_{max}, value = 50
  - K_s, value = 10
  - K_O, value = 2
- **Adding the process:** Right-click on **Project Explorer→Water Quality→Reactions→Reaction network** and fill it out as shown in Figure (5.1).
- **Adding a sensor and controller** In order to simulate PID controller we need to first introduce one sensor and one controller.
  - Add a sensor by right-clicking on **Project Explorer→Control→Sensor** and then selecting **Add sensor** from the drop-down menu.
  - Set the following properties for the newly added sensor:
    - **Name:** *DO sensor*
    - **Sub-type:** *Block*, (This indicates that the quantity that will be measured is at a block and not a connector.)
    - **Location:** *Pond(1)* (This indicates the location where the quantity will be measured.)
    - **Quantity:** *DO*, (This indicates that the sensor will measure DO concentration
    - **Error Distribution:** *Normal-Additive*, (This indicates that the sensor measurement error is normal and additive.)
    - **interval** *5 min*, (This indicates that the sensor measures DO concentration with 5 minutes intervals.)
    - **Error Standard Deviation:** *0.1*, (This indicates that the error standard deviation of the sensor measurements is 0.1mg/L).

– Add a controller by right-clicking on **Project Explorer→Control→Controller** and then selecting **Add Controller** from the drop-down menu.

– Set the following properties for the newly added controller:
- **Name:** *Aeration Controller*
- **Type:** *PID-Manual*
- **Sensor:** *DO Sensor* (This indicates that this controller will use the measurements from the DO sensor that was previously introduced.)
- **Setpoint:** *3* (This specify the set-point value for DO, i.e. that the controller's goal is to maintain DO level at 3 mg/L).
- *kp -10* (This is the P gain coefficient for the controller.)
For now we will only use P-controller which means that we will leave the *kd* and *ki* properties empty.
Interval: *5 (min)*, (This indicates the time interval at which the control values are updated).
Initial Value: *10*, (This indicates the initial value of K_{La} that the simulation starts with.)
Minimum value: *0*, (This indicates the minimum value of the actuator physically possible.)
Maximum value: *1000*, (This indicates the maximum value of the actuator physically possible.)

- **Adding Aeration:** Add an "external flux object" by right-clicking on **Project Explorer→Water Quality→External Flux** and then selecting **Add External Flux** from the drop-down menu.

- Attribute the following properties to the added external flux object:
-**Name:** *Aeration*
-**Constituent:** *DO*
-**Model:** *Constant Rate*
Also right-click on the name of the property labeled as **Coefficient** and from the drop-down menu that appears select **Controls→***Aeration Controller* (Figure 5.2).
Saturation: 8.5 , (This specifies a saturation DO concentration of 8.5mg/L)

- To apply the external flux item to the pond. Choose the pond and select "Aeration" for the property labeled as **External flux**.

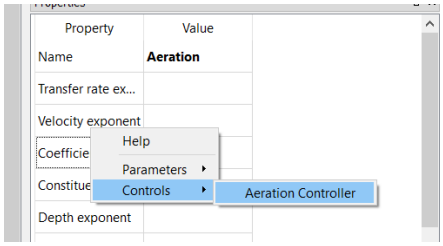


Figure 5.2: Assigning controller to a model property

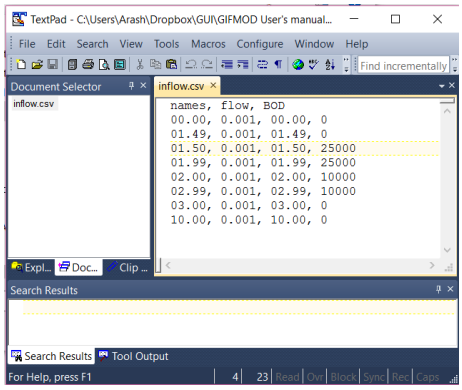


Figure 5.3: Inflow input file for the PID control example

- **Adding BOD loading to the system** Here we add an inflow of BOD to the pond. Create a text file as shown in figure (5.3). The value of the flow is intentionally kept low to minimize the effect of dilution.

- Choose the file that was created as the value for the **Inflow time-series** property of the pond block. To visualize the BOD concentration in the inflow, right click on the file name that was selected and then click on *BOD*. The graph that will appear look like figure 5.4.

- **Changing the simulation period to 10 days** From the **Settings** menu change duration of the simulation by choosing **Input number** for the **Simulation End Time** and entering *10* in the input box that appears.

- **Save the project.**

- **Running the simulation:** Run the simulation by clicking on the

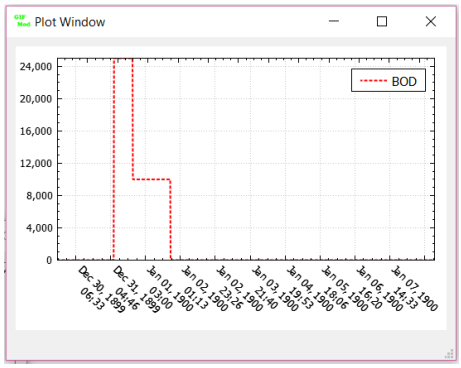


Figure 5.4: BOD concentration variation in the inflow

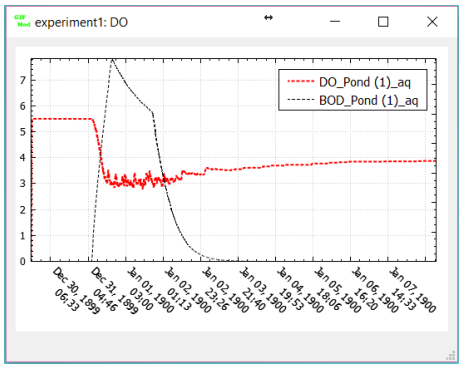


Figure 5.5: Temporal variation of DO and BOD in the DO control example

run button  and wait until the simulation ends.

- **Inspecting the results:** - Right click on the pond block and from the drop-down menu select **Plot Water Quality Results→DO**. This shows the DO concentration variation with time. Do the same thing for BOD and copy and past onto the *DO* plot. The results should look like figure (5.5).

  - Right-click on the *Aeration Controller* object in the **Project Explorer→Control→Controller** and select **Plot Control Data**. This will show a graph representing the variation of K_{La} parameter by the controller during the course of simulation. The result should look like figure (5.6).

  As it can be seen there are oscillations in the actuator value. This is

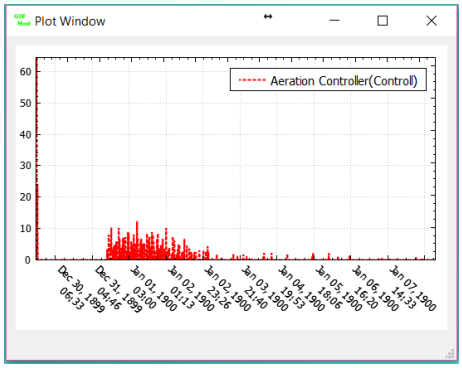


Figure 5.6: Temporal variation of DO and BOD in the DO control example

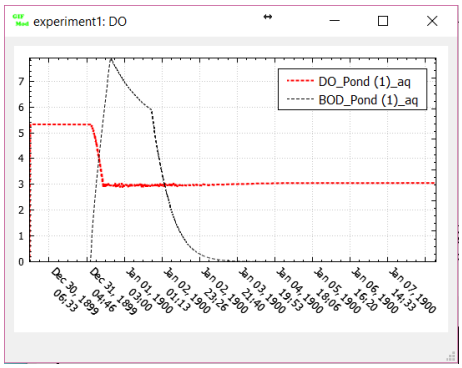
due partly to the noise added to the sensor reading as well as the fact that a simple P controller was used. Let's now reduce the noise and change the control scheme to PID.

- Select the *DO Sensor* from the **Project Explorer→Control→Sensor** and change the value for **Error Standard Deviation** to 0.01.

- Select the *Aeration Controller Object* and type a value of 0.01 for **ki** and 0.001 for **kd**.

- Rerun the program and check DO and BOD concentration and the actuator value. They should look like Figure (5.7).

a)



b)

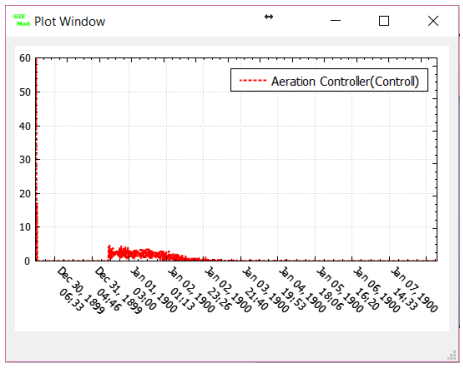


Figure 5.7: Temporal variation of a) DO and BOD in the DO control example and b) actuator value

6

Parameter Estimation of Decay of BOD in an aerated pond

In this example the deterministic and probabilistic parameter estimation capabilities of GIFMod is demonstrated through a simple example consisting of estimating the BOD mineralization and reaeration parameters based on a batch experiment. The experiment is assumed to be done using a $1m^3$ aerated tank with an initial BOD concentration of 25mg/L. For the sake of simplicity, it is assumed that the only process affecting the DO consumption is heterotrophic mineralization of BOD through the following reaction:

$$BOD + DO \xrightarrow{rate=kBOD\frac{DO}{DO+K_o}} CO_2 + H_2O + Biomass \tag{6.1}$$

The effect of increase in biomass concentration is ignored in order to keep the example simple. The reaeration is assumed to be governed by a simple constant-rate exchange of DO between water and the atmosphere with a rate defined expressed as $rate = k_{La}(DO_s - DO)$.
The observed data is provided in the example folder in the file named "DO_observed.txt".

The following steps are needed to construct the model and to set the inverse modeling configurations:

- **Introducing the constituents:** Add the two constituents and name them DO and BOD respectively.

- **Adding External Flux:** Add an external flux and set the following parameters:
  - **Name:** *Aeration*
  - **Constituents:** *DO*
  - **Model:** *Constant Rate*
  - **Saturation:** *8.5*
  - **Coefficient:** *10*
- **Adding the physical batch reactor:** Add a pond and set the following parameters:
  - **Bottom Area:** $1m^2$
  - **Constituent Initial Concentration:**
    - BOD: 25
    - DO: 8.5
  - **External Flux:** *Aeration*
  - **Initial Water Depth:** *1m*
- **Reaction Parameters:** Add the following **reaction parameters**:
  - k, **Value:** 2.5
  - k_O, **Value:** 1.5
- **Setting the reaction network:** Set the reaction network as shown in figure 6.1.
- **Run the model in forward:** You can now save the model and run it in forward mode and check the predicted DO and BOD concentration variation during the simulation period. The results should look like figure 6.2.
- **Configuring inverse modeling:**
  - **Add a new observation:** Add a new observation by right-clicking on **Inverse Modeling→Observations** and set the following properties:
    - **Name:** *DO*
    - **Block/Connector:** *Block*
    - **Error Distribution:** *Normal*

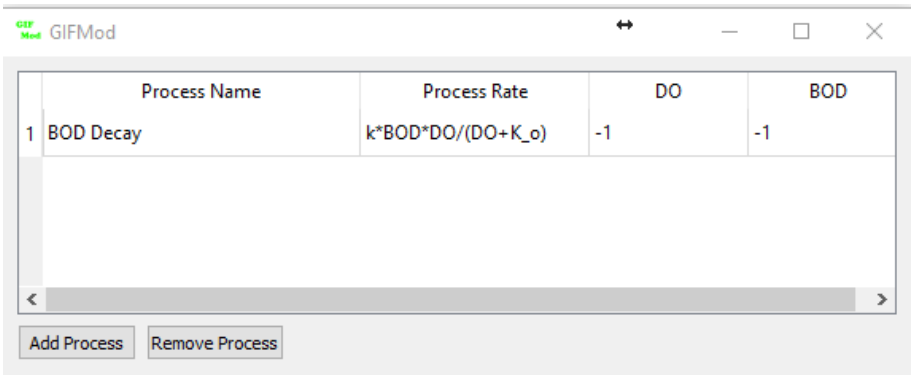


Figure 6.1: Reaction network for the DO uptake inverse modeling example

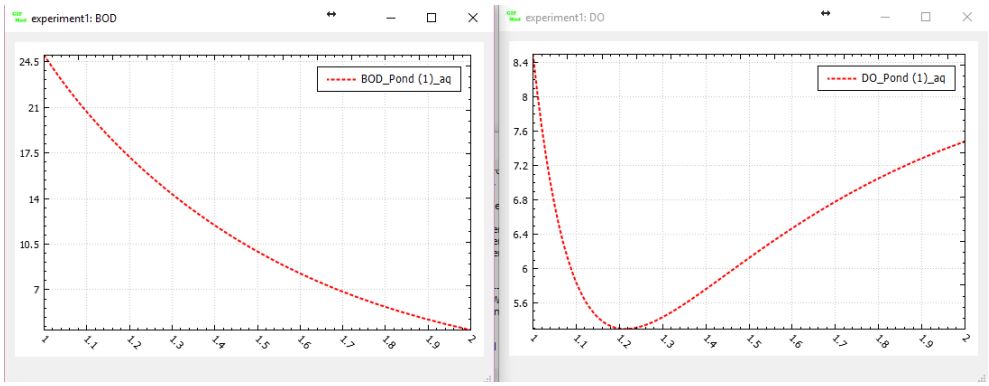


Figure 6.2: Prediction of BOD and DO variation as a result of forward simulation

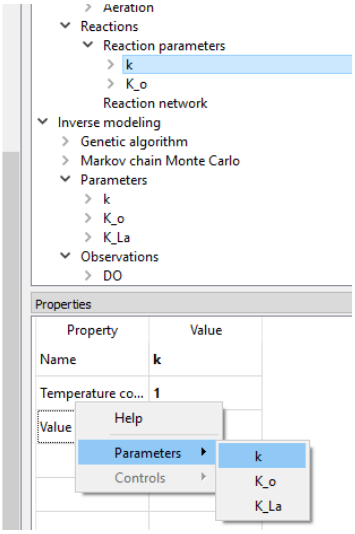


Figure 6.3: Assigning a parameter to a property

  - **Location:** *Pond (1)*
  - **Experiment:** *experiment 1*
  - **Observed data:** *Selected the file "Do_observed.txt" using the file browser*
  - **Quantity:** *Select "DO:Aqueous"*

- **Adding parameters with unknown values:** Add the three parameters to be estimated by right-clicking on **Inverse Modeling→Parameters**:
  - *k*, **Maximum value:** *5*, **Minimum value:** *1*
  - *K_o*, **Maximum value:** *5*, **Minimum value:** *0.5*
  - *K_La*, **Maximum value:** *20*, **Minimum value:** *4*
- **Assigning the unknown parameters:** In the reaction parameters right click on the label of the **value** property of the parameter *k* and select **Parameters→***k*. Do the same thing for the parameter *K_o* and select *K_o*.
- **Assigning the unknown parameter for the aeration rate:** Select **External Flux→***Aeration* from the **Project Explorer** and then right click on the **Coefficient** property and assign the parameter *K_La* to it similar to the other parameters.

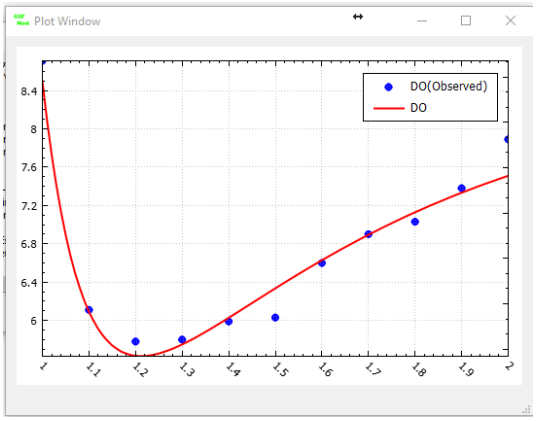


Figure 6.4: Modeled vs. observed plot

- **Genetic Algorithm Settings:** Set the following properties for the **Genetic Algorithm**:
  - **Number of Generations:** *100*
  - **Population:** *50*
- **Turning off the MCMC probabilistic parameter estimation:** At this stage we only do deterministic parameter estimation using Genetic Algorithm. Select **Marcov chain Monte Carlo** from the **Project Explorer** and the value of **Perform MCMC simulation** to *No*
- Save the model
- Click on inverse run icon  and wait for the analysis to finish.
- **Modeled vs. Observed comparison:** In the **Project Explorer**, right-click on **Inverse Modeling**→**Observations**→*DO* and then click on **Plot Modeled Data**. The modeled vs. observed graph (Figure 6.4) should appear.
- **Agreement plot:** In the **Project Explorer**, right-click on **Inverse Modeling**→**Observations**→*DO* and then click on **Agreement plot**. The model-observed agreement graph (Figure 6.5) will appear.

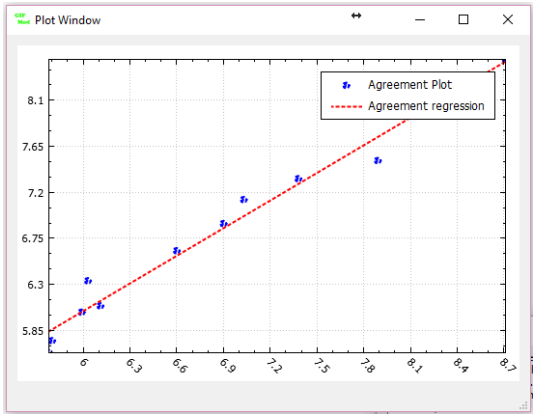


Figure 6.5: Agreement plot

- **Estimated values of the parameters:** The estimated values of the parameters can be seen as the value of the **Value** property for each parameter in the **Inverse Modeling→Parameters**.

- **Probabilistic parameter estimation:** Now turn on the MCMC simulation by changing the value of **Perform MCMC simulation** in **Markov chain Monte Carlo** to *Yes*. Also change the **Number of MCMC samples** to 60000 and change **MCMC Burn-in number** to 20000.

- Change acceptance rate to 0.3. This will adjust the MCMC perturbation factor such that approximately 30% of the samples are accepted.

- Click on inverse run icon  and wait for the analysis to finish.

- **Checking the posterior distribution of the parameters:** Go to **Inverse Modeling→Parameters**, right-click on a parameter and then choose **Plot Posterior distribution histogram**. To see the posterior percentiles of the DO prediction right click on **Inverse Modeling→Observations→***DO* and select **Plot prediction 95 percentiles** (Figure 6.6)

- Right-click Right click on **Inverse Modeling→Parameters** and then select **Plot Percentiles** to see the 95 percentile range of the parameters (Figure 6.7).

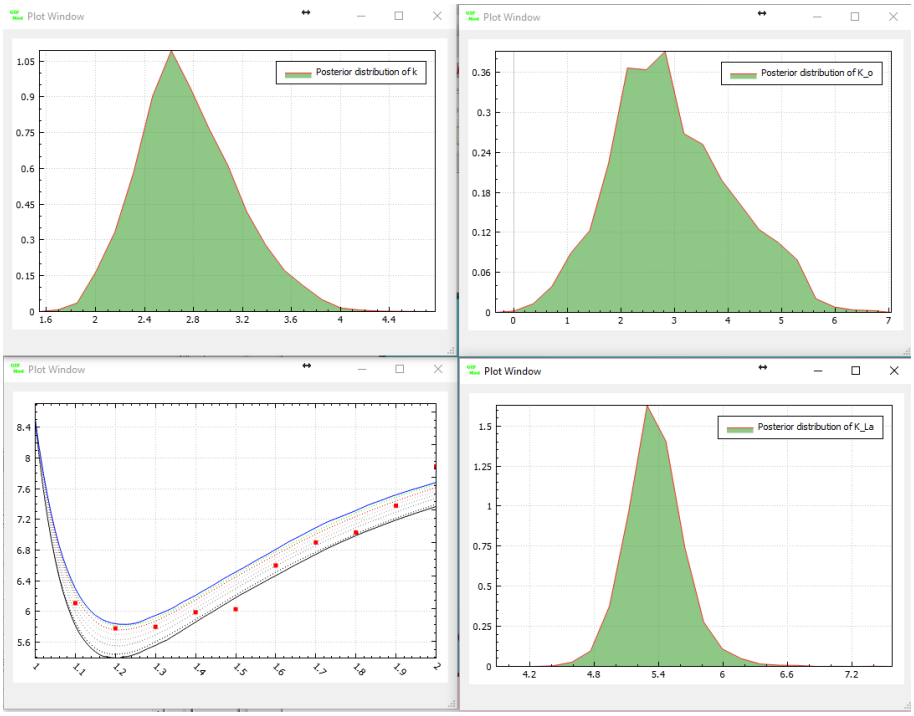


Figure 6.6: Posterior parameter distribution and posterior DO prediction

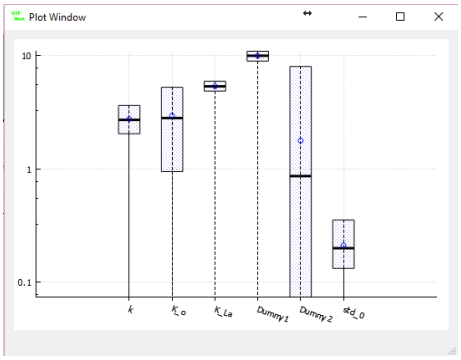


Figure 6.7: Parameter posterior 95 percentiles

- **Log-normal error structure:** In the previous probabilistic parameter estimation simulation, it was assumed that the prior distribution of the model parameters and also the error structure are normally distributed and additive. Now let's see how changing the error structure into a log-normal distribution will change the results. Select **Inverse Modeling**→**Observations**→*DO* and in the **Properties** window, change the **Error Distribution** to *Log-Normal*. Run the inverse simulation again and check the new posterior distributions.

Bibliography