Example: Contaminant Transport and Reactions

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In this example, we will show you how to model chemical reaction and transport in *OpenHydroQual*. We will consider two imaginary reactants **A**, and **B** reacting with each other resulting in a product **C**:

$$A + B \rightarrow C \tag{1}$$

according to a Dual-Monod reaction rate expression defined as:

$$r = r_{max} \frac{A}{A + K_A} \frac{B}{B + K_B} \tag{2}$$

where r_{max} is the maximum reaction rate, and K_A and K_B are respectively the half-saturation constants for solutes **A** and **B**.

We will initially apply this reaction to a single *Pond* component that act as a simple batch reactor and then in the next step will add another *Pond* to show the combined impact of reaction and transport. Of course the techniques described in this manual can be used in more complex systems involving other components such as soil, channel, pipe, groundwater, etc.

1 Step 1: Batch reactor

Follow the steps below:

1. **Start OpenHydroQual**

2. **Add the *Pond* plugin to your modeling environment** From **File→Preferences→Add Plugin**, choose the *Pond* plugin. This will add a stormwater pond with its storage-depth relationship being determined by a power equation and a V-notch weir to your components toolbar. We will use the *stormwater pond* component as our batch reactor. Please note that we could use a variety of other components as our batch reactor and the choice would not make any difference on the result of our first step which involves modeling reaction in a batch system because the choice of the component only determine the hydraulic behaviour of our system.

3. **Add a *Stormwater Pond* to your model:** Click on the stormwater pond button on your components toolbar to add a one to your model. Now we need to specify a few of the properties of the pond. For the "coefficient (alpha) in the rating curve S=alpha*d^beta" enter a value of 100. Also enter a value of 100 [m^3] as initial storage. This will indicate that initially there is $100m^3$ of water in the pond.

4. **Adding the three chemicals A, B, and C:** Click three times on the *Constituent* button  on the components toolbar at the top to add three constituents. From the *Object Browser* panel, choose each of the constituents and change their names respectively to **A**, **B**, and **C** through the *Properties* panel. Your GUI window should now look like figure 1.

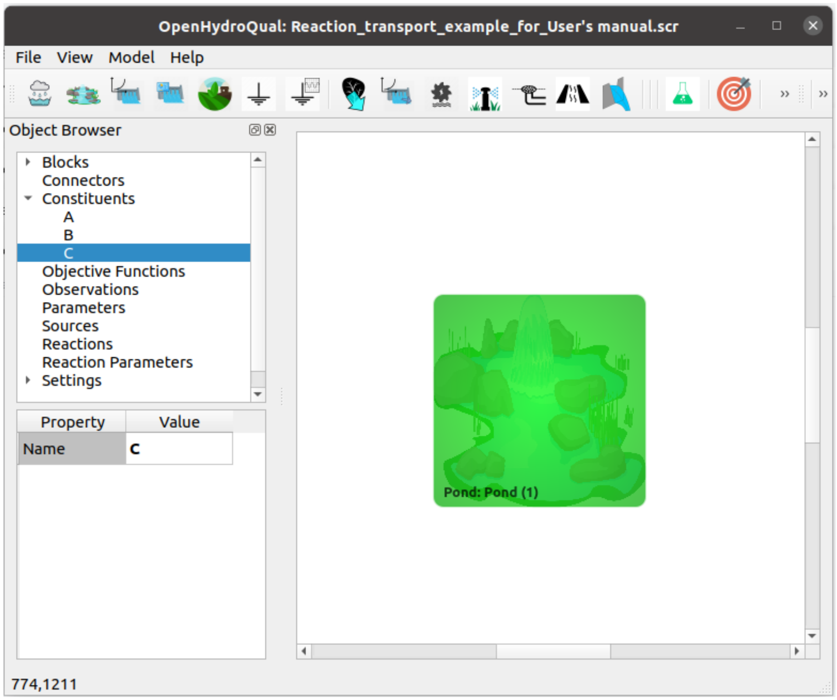
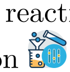


Figure 1: Screenshot of the GUI after adding the stormwater pond and the three chemical constituents

5. **Adding reaction parameters:** Now we need to add the reaction (1) with the reaction rate expression in eq. (2) and the proper stoichiomery. For this purpose we will first define the three reaction parameters r_{max}, K_A, and K_B and will assign their values so we can use them when entering the reaction rate expression. Click on the **Reaction Parameter** button  three times to add three reaction parameters. They will be assigned default names and you should change them to suitable names. Choose the reaction parameters that was just added through the Object Browser panel and change their

name and value through the property panel as follows:

Name	Value
r_max	10 $[mgL^{-1}day^{-1}]$
K_A	1 $[mgL^{-1}]$
K_B	1 $[mgL^{-1}]$

Here we are assigning a value of 10 $[mgL^{-1}day^{-1}]$ to r_{max} and a value of 1 mg/L to K_A and K_B. After this, your GUI should look like figure 2.

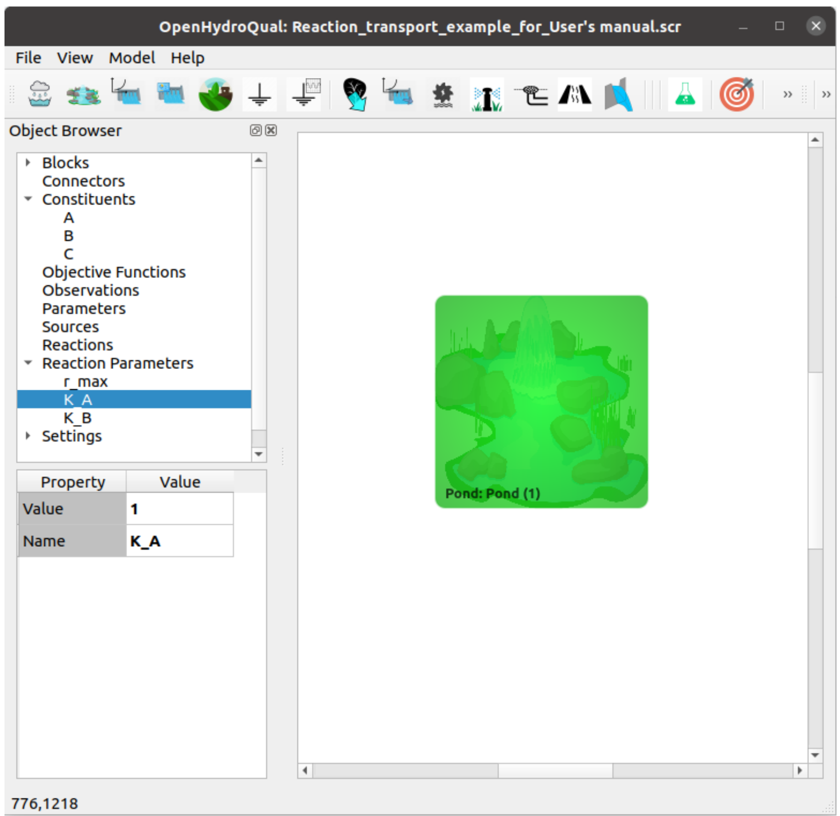


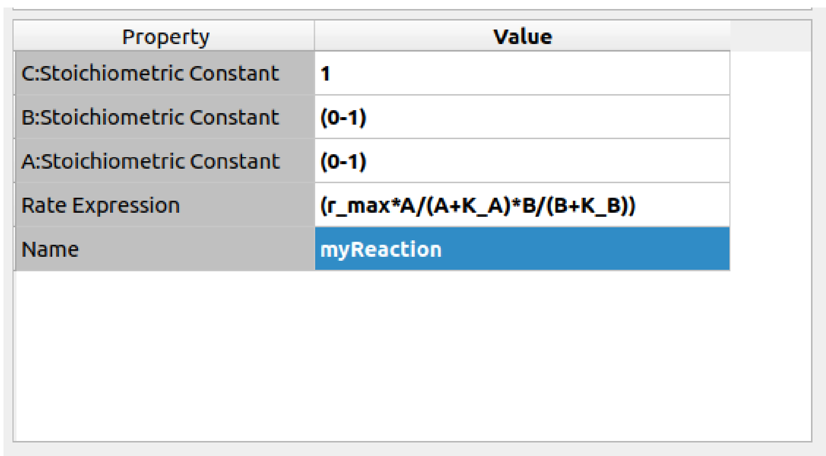
Figure 2: Screenshot of the GUI after adding the reaction parameters

6. **Adding the reaction:** Now, we can add the reaction. Click on the *Reaction* button  on the components toolbar to add a reaction. Choose the reaction from the object browser panel and assign the following properties from the property panel:

   - *C:Stoichiometric Constant:* 1

- *A:Stoichiometric Constant:* -1
- *B:Stoichiometric Constant:* -1
- *Rate Expression:* r_max*A/(A+K_A)*B/(B+K_B)

You can also change the name of the reaction to whatever name you want. Please note that assigning values of -1 to the stoichiomeric constants for **A** and **B** constituents indicates that they are being consumed. Also the stoichiometric constants of 1 indicate that one unit of the constituents are produced as a result of one unit progress of the reaction. After assigning the properties of the reaction your property window for the reaction should look like figure 3.



Property	Value
C:Stoichiometric Constant	1
B:Stoichiometric Constant	(0-1)
A:Stoichiometric Constant	(0-1)
Rate Expression	(r_max*A/(A+K_A)*B/(B+K_B))
Name	myReaction

Figure 3: Screenshot of the properties of the reaction

7. **Set the initial condition:** We have to specify the initial concentrations of constituents **A**, **B**, and **C** in the pond. We will assume that at time $t = 0$, the concentrations of **A**, **B**, and **C** are respectively $5mg/L$, $2mg/L$, and $0mg/L$. Select the pond from either the graphic screen or object browser and enter a value of 5 for *A:Concentration* property and a value of 2 for *B:Concentration* property in the properties window.

8. **Run the simulation:** Save your model and run the model .

9. **Check the results:** Right-click on the stormwater pond icon in your graphics window and select **Results→A:Concentration** and then **B:Concentration**, and **C:Concentration**. You may copy and paste

graphs on the same graph to compare the results. You may also format each curve using a distinct color, line-type or symbol. The results should look something like in figure 4.

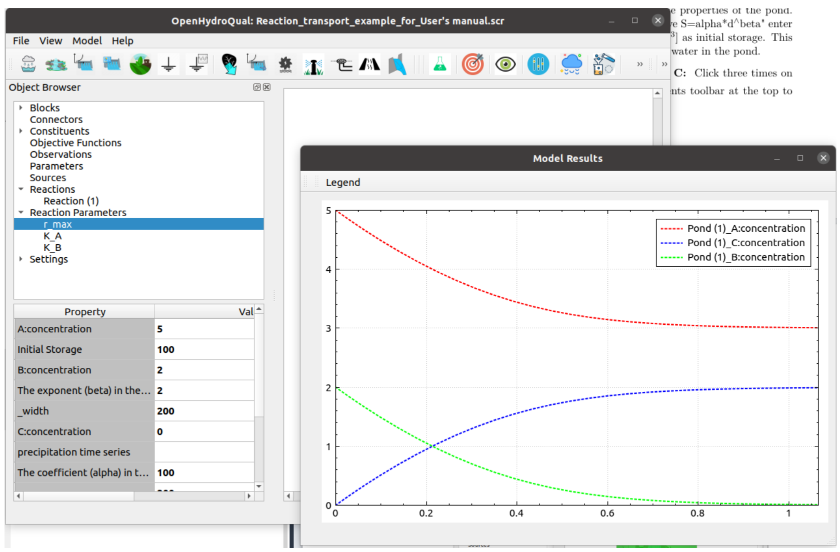


Figure 4: Time variation of **A**, **B**, and **C** in the batch reactor

2 Step 2: Adding transport

In this step, we will add another pond and we will allow water to flow from the first pond to the second pond through a weir while reactions are occurring.

Do the following steps:

1. **Add another stormwater pond:** Add another stormwater pond by  button on your components toolbar. We are going to assign the same hydraulic properties to this pond as the first pond with the exception that we will assume that it contains only $20m^3$ water in it initially. So assign a value of 100 to the parameter "coefficient (alpha) in the rating curve S=alpha*d^beta" and a value of 20 $[m^3]$ to "Initial Storage". Leave the concentrations of **A**, **B**, and **C** at zero.

2. **Connect the two ponds through a weir:** Click on the *V-Notch Weir* connector button  from the components toolbar and then

connect *Pond (1)* to *Pond (2)*. Your GUI screen should look like figure 5.

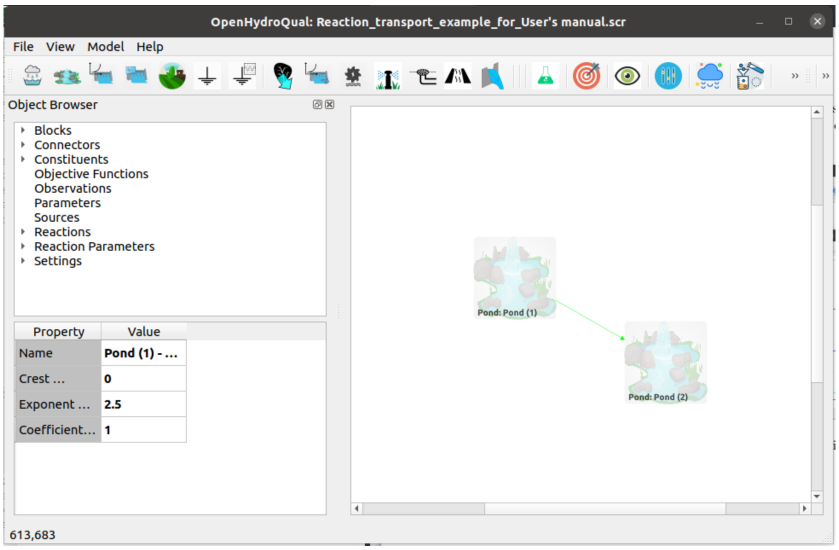


Figure 5: Screenshot of the GUI with two connected reactors

The V-Notch weir controls the flow from a pond to another pond according to a power equation expressed as:

$$Q = \alpha(h - h_0)^{\beta} \tag{3}$$

where α is a coefficient and β is an exponent and h_0 is the minimum depth of water in the upstream pond for the flow to occur. We are going to set α to 20, β to 2, and we will leave h_0 at zero. Select the link from *Pond (1)* to *Pond (2)* as assign the following properties to it through the properties panel:

Name	Value
Exponent beta in ...	2
Coefficient alpha in ...	20

3. **Run the model:** Run the simulation and check the results. You can look at the variation of storage in *Pond (1)* and *Pond (2)*, and the concentrations and masses of constituents **A**, **B**, and **C** in ponds (1) and (2) and the flow rate from *Pond (1)* to *Pond (2)* and also mass transfer rates of the constituents from *Pond (1)* to *Pond (2)*.

4. **Increase the duration of simulation and rerun the model:** If you want to see the simulation results over a longer period, change the simulation end time through **Settings→General Settings** and changing the simulation end time to a larger value (for example 10 days) and check the results again (figure 6).

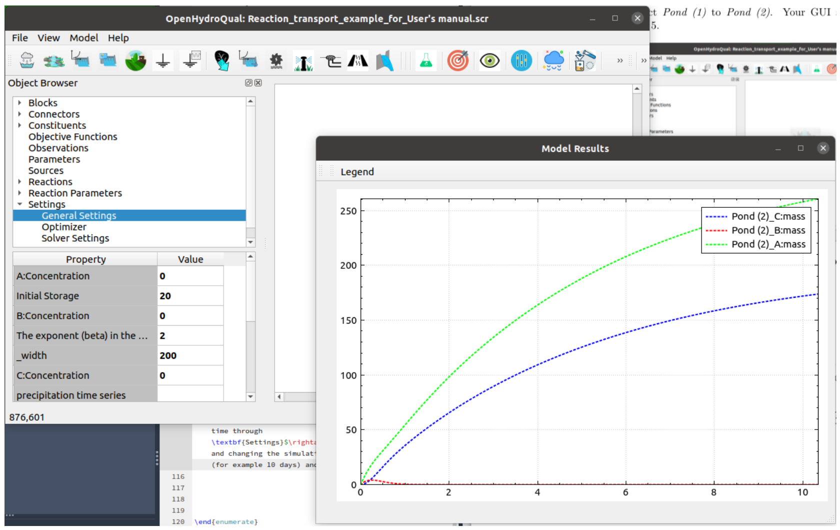


Figure 6: The results for the two-pond scenario over a 10 days period