# Parameter Estimation of BOD removal processes in an aerated pond

December 31, 2016

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:

$$BOD + DO \xrightarrow{rate=kBOD\frac{DO}{DO+K_o}} CO_2 + H_2O + Biomass \qquad (1)$$
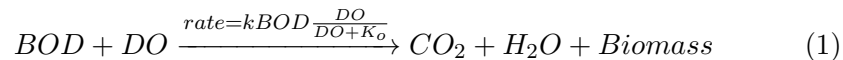
The effect of increase in biomass concentration is ignored in order to keep the example simple. The reaeration is assumed to be governed by a simple constant-rate exchange of DO between water and the atmosphere with a rate defined expressed as $rate = k_{La}(DO_s - DO)$.

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*

Figure 1: Reaction network for the DO uptake inverse modeling example

- **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 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 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*
        * **Location:**   *Pond (1)*
        * **Experiment:**   *experiment 1*
        * **Observed data:**   *Selected the file "Do_observed.txt" using the file browser*
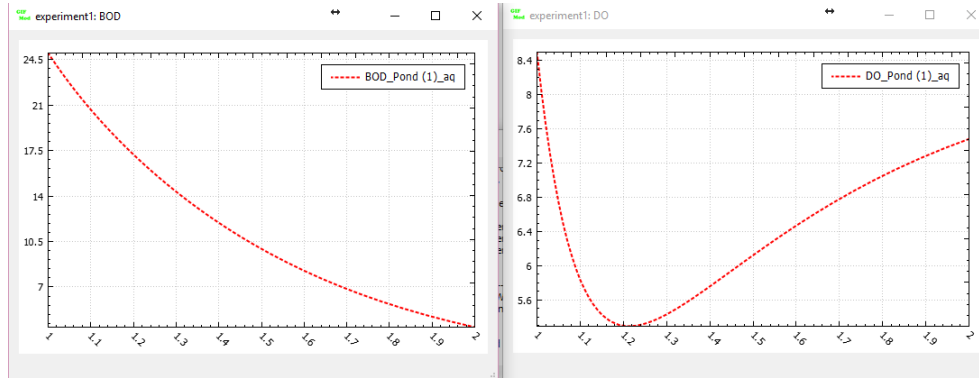
Figure 2: Prediction of BOD and DO variation as a result of forward simulation

            ∗ **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.

- **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
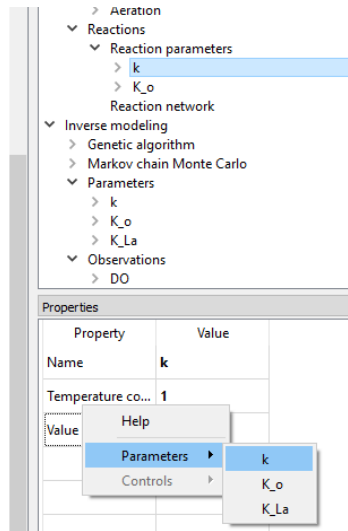
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Figure 3: Assigning a parameter to a property

Project Explorer and the value of **Perform MCMC simulation** to *No*

- Save the model

- Click on inverse run icon ![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 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 5) will appear.

- **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**
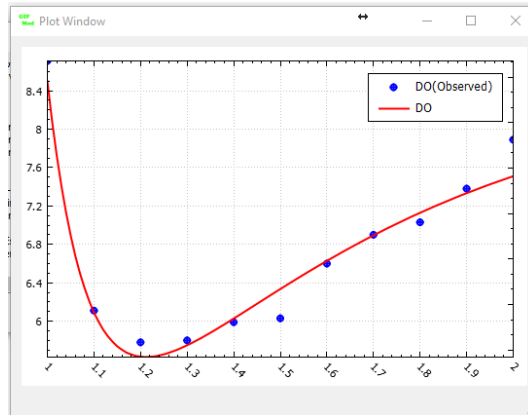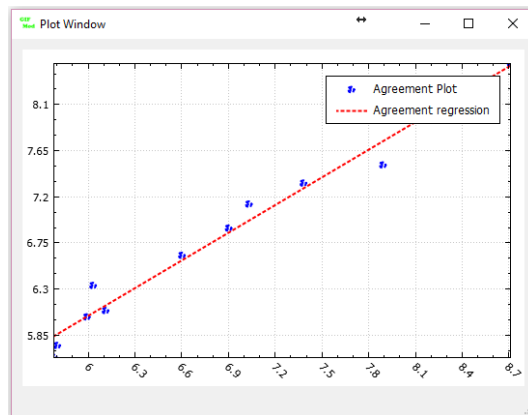
Figure 4: Modeled vs. observed plot

Figure 5: Agreement plot

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      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)

- Right-click Right click on **Inverse Modeling→Parameters** and then select **Plot Percentiles** to see the 95 percentile range of the parameters (Figure 7).

- **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.
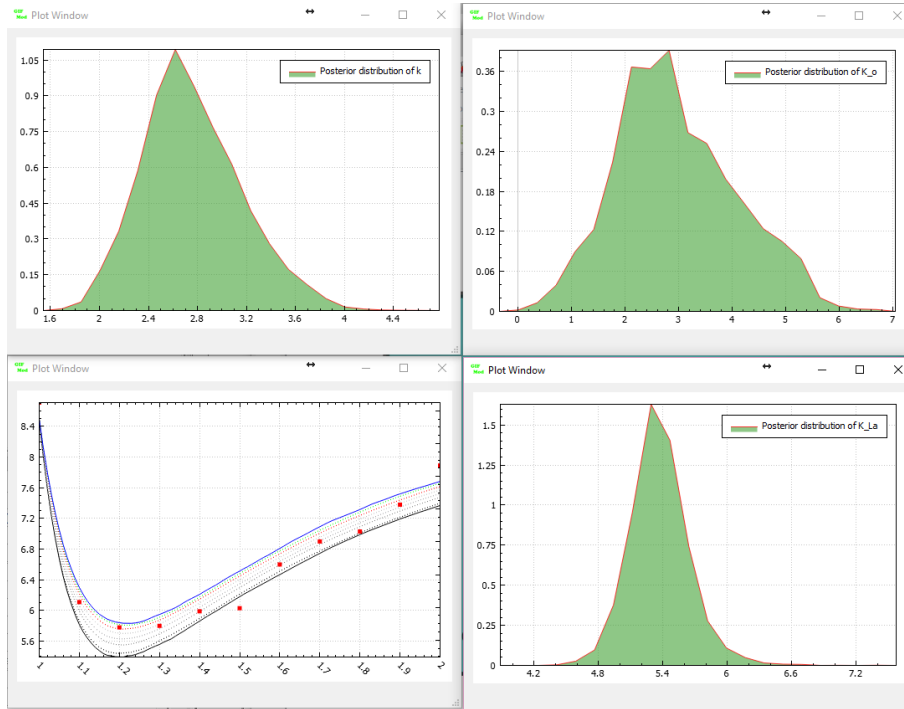
Figure 6: Posterior parameter distribution and posterior DO prediction

Figure 7: Parameter posterior 95 percentiles