Education evenings 2016

Practical introduction to groundwater modelling

Computer exercises
02 02 Calibrating the more complex model

1

Purpose

In this exercise, we will use ModelMate to perform

- ✓ local sensitivity analysis and
- ✓ local optimization or calibration

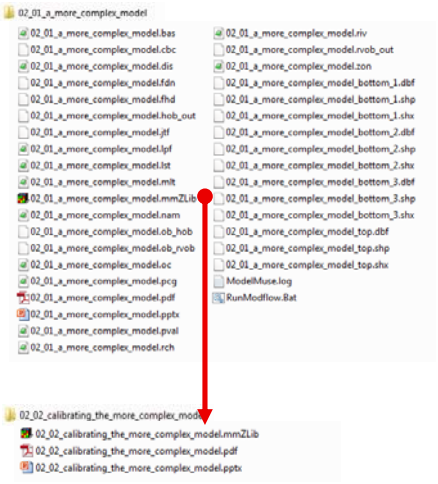
of the parameters we defined in our more complex model, and

- ✓ import the results back to ModelMuse.

2

Copy file previous exercise

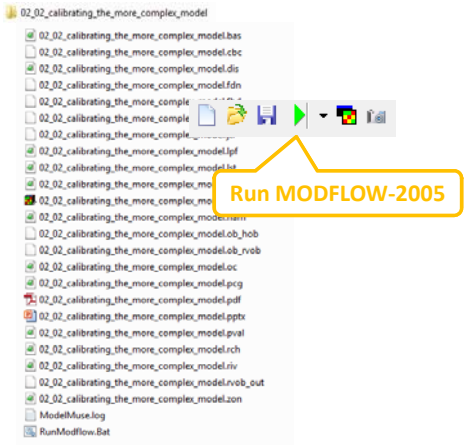
- ✓ Copy file "/02_01_a_more_complex_model/02_01_a_more_complex_model.mmZLib" to folder "/02_02_calibrating_the_more_complex_model/"
- ✓ Change the file name to "02_02_calibrating_the_more_complex_model.mmZLib"



3

Run MODFLOW again

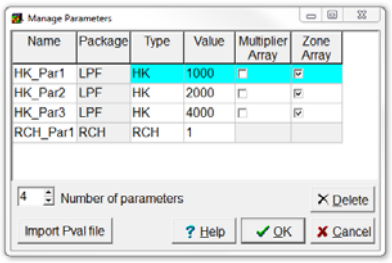
- ✓ Open ModelMuse file "02_02_calibrating_the_more_complex_model.mmZLib"
- ✓ Press the **Run MODFLOW-2005** button, save the name file and execute the model.
- ✓ Close ModelMonitor, the listing file and the command line window. All necessary files are now available for ModelMate.



4

Check model parameters

- ✓ Select **Model|Manage Parameters…**
- ✓ Note that we defined four parameters during the previous exercise:
  - ✓ **HK_Par1** defines horizontal hydraulic conductivity in the left half of our first layer
  - ✓ **HK_Par2** defines horizontal hydraulic conductivity in the right half of our first layer
  - ✓ **HK_Par3** defines horizontal hydraulic conductivity in our third layer, and the vertical hydraulic conductivity of the non-simulated second layer also depends on it
  - ✓ **RCH_Par1** is multiplied with the recharge multipliers to obtain the recharge value



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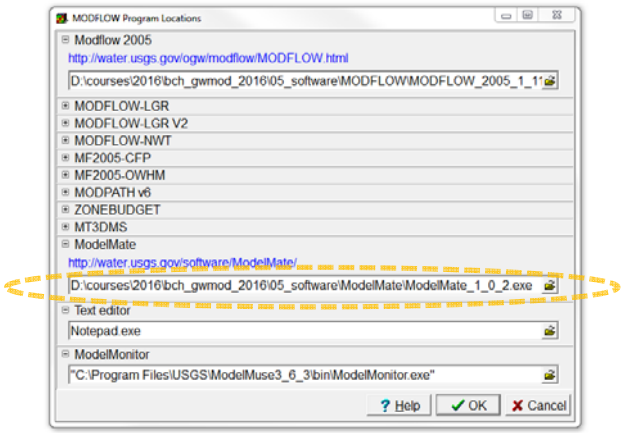
Set ModelMate executable location

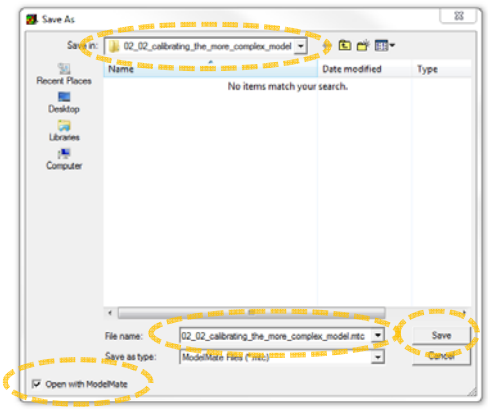
- ✓ Choose **Model|MODFLOW Program locations,**
- ✓ fill in the ModelMate executable location "…/bch_gwmod_2016/05_software/ModelMate/ModelMate_1_0_2.exe", and
- ✓ click **OK**.



6

Export ModelMate file

- ✓ Select **File|Export|Export or Update ModelMate File**,
- ✓ use file name "02_02_calibrating_the_more_complex_model.mtc",
- ✓ make sure the **Open with ModelMate** checkbox is checked,
- ✓ and press **Save**.



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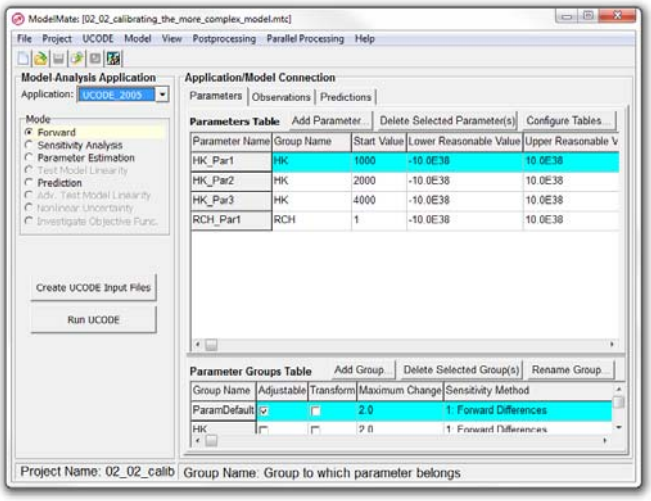
This is what you should get



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Create instruction files

- ✓ Note that ModelMuse did not automatically create instruction files allowing UCODE to adjust the parameters and read the simulated equivalents of our observations.
- ✓ Select **Model|Create Instruction Files For Observations Defined In ModelMuse** in ModelMate,
- ✓ and press **OK**.

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Set program locations

- ✓ Select **Project|Program locations**,
- ✓ and fill in the **UCODE_2005**, **MODFLOW-2005**, **Residual_analysis**, and **Residual_analysis_adv** program names with the corresponding executables in the /05_software/ folder (as in the image on the right).
- ✓ For **GW_Chart**, locate the installation folder of GW_Chart (typically in the C:/Program Files/USGS/ folder), and select the GW_Chart.exe executable.
- ✓ Then press **OK**.

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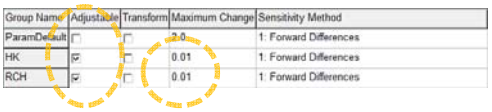
Adjust Parameter Groups Table

- ✓ In the **Parameter Groups Table**, deselect **Adjustable** for **ParamDefault**, and
- ✓ select it for **HK** and **RCH**. In this way, our hydraulic conductivity and recharge parameters are included in the sensitivity analysis and parameter estimation modes.
- ✓ Set **Maximum Change** to 0.01 for both **HK** and **RCH**, to limit the size of parameter changes in one parameter-estimation iteration.



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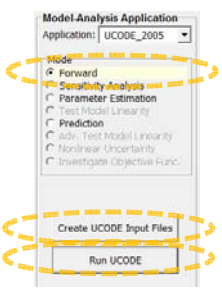
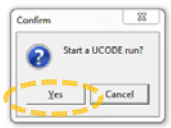
Perform forward simulation

- ✓ Check if the **Forward** UCODE mode is selected,
- ✓ press **Create UCODE Input Files**,
- ✓ and click **OK**.
- ✓ Then click on the **Run UCODE** button,
- ✓ and click **Yes** to start the UCODE run.





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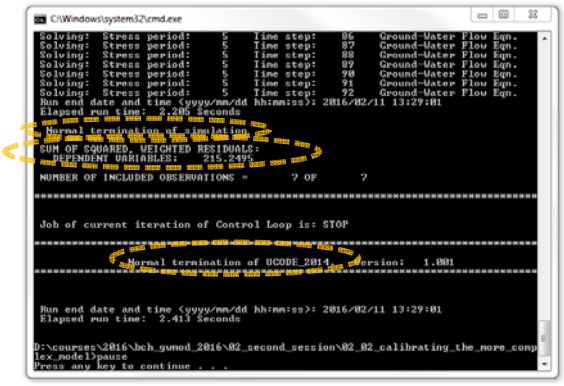
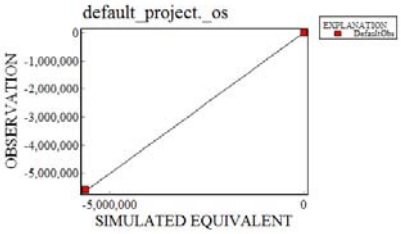
Check normal terminations of codes

- ✓ In the command line window, check for normal terminations of MODFLOW and UCODE.
- ✓ Also note the **SUM OF SQUARED, WEIGHTED RESIDUALS**, which is about 215 with our initial parameter values.
- ✓ Close the command line window.



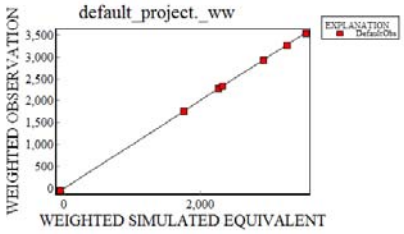
Plot observations vs simulated equivalents (1/2)

- ✓ Select **Postprocessing|GW_Chart**, or use the corresponding button to bring up the observed compared to simulated values graph.
- ✓ Note this plot is not very useful because of the differences in magnitude between the head and river observations.



Plot observations vs simulated equivalents (2/2)

- ✓ Therefore, select **Model Fit| default_project._ww** in the **File:** drop-down list.
- ✓ This displays the weighted observed compared to the weighted simulated values, which is more informative in this case.



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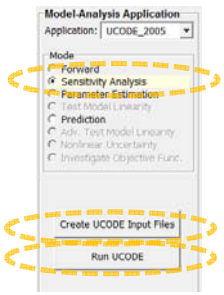
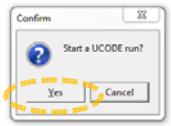
Perform sensitivity analysis

- ✓ Now select the **Sensitivity Analysis** mode,
- ✓ press **Create UCODE Input Files**,
- ✓ and click **OK**.
- ✓ Then click on the **Run UCODE** button,
- ✓ and click **Yes** to start the UCODE run.





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Statistics for sensitivity analysis

$$ss_{ij} = \left(\frac{\partial y'_i}{\partial b_j}\right) b_j \omega_{ii}^{1/2}$$

- ss_{ij}: dimensionless scaled sensitivity of the simulated value for the i^{th} observation with respect to the j^{th} parameter
- $\frac{\partial y'_i}{\partial b_j}$: sensitivity of the simulated value for the i^{th} observation with respect to the j^{th} parameter
- $\omega_{ii}^{1/2}$: weight of the i^{th} observation
- i: observation index
- j: parameter index
- b_j: j^{th} parameter value

$$css_j = \left[\sum_{i=1}^{ND} (ss_{ij})^2 \Big|_{\underline{b}} / ND\right]^{\frac{1}{2}}$$

- css_j: composite scaled sensitivity with respect to the j^{th} parameter
- $\sum_{i=1}^{ND} (ss_{ij})^2$: sum of squared dimensionless scaled sensitivities
- ND: number of observations
- $\underline{b}$: everything is evaluated at the same parameter vector $\underline{b}$

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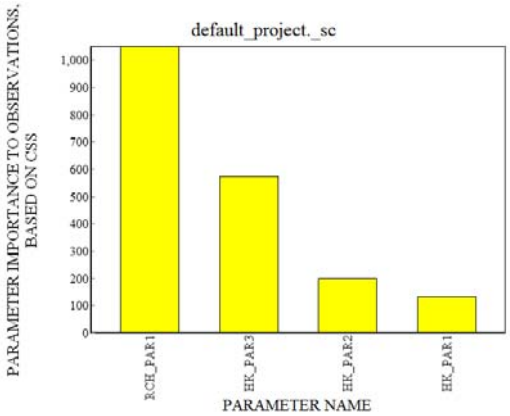
Visualize composite scaled sensitivities

- ✓ Close the command line window after it has finished,
- ✓ and launch GW_Chart again.
- ✓ Now select **O-Par Sens Analysis| default_project._sc** in the **File:** drop-down list.
- ✓ This displays the bar chart of composite scaled sensitivities (indicating parameter importance to all observations).



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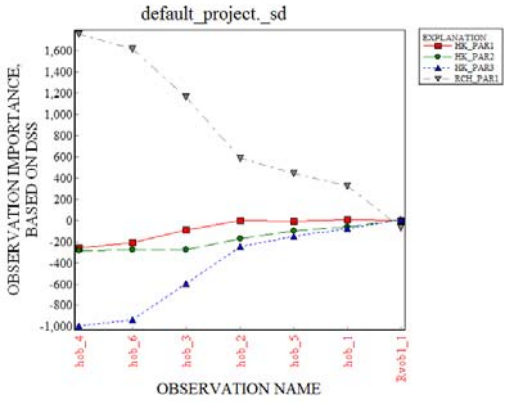
Visualize dimensionless scaled sensitivities

- ✓ Now select **O-Par Sens Analysis| default_project._sc** in the **File:** drop-down list.
- ✓ This displays the dimensionless scaled sensitivity for each observation by parameter (indicating the effect of each parameter on each observation).



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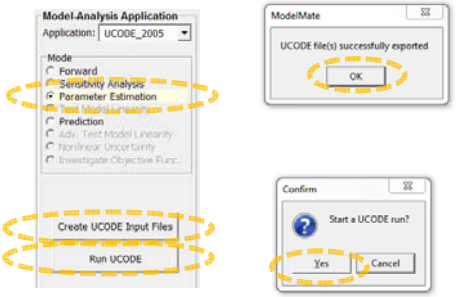
Perform parameter estimation

- ✓ Now select the **Parameter Estimation** mode,
- ✓ press **Create UCODE Input Files**,
- ✓ and click **OK**.
- ✓ Then click on the **Run UCODE** button,
- ✓ and click **Yes** to start the UCODE run.



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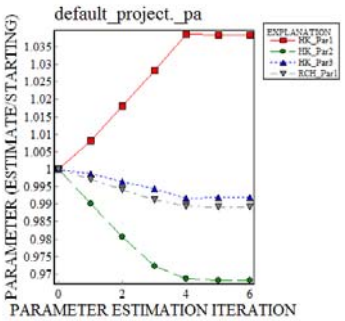
Visualize parameter evolution (1/2)

- ✓ Close the command line window after it has finished,
- ✓ and launch GW_Chart again.
- ✓ Now select **Parameter Values| default_project._pa** in the **File:** drop-down list.
- ✓ This displays the evolution of the different parameters with respect to their initial values.



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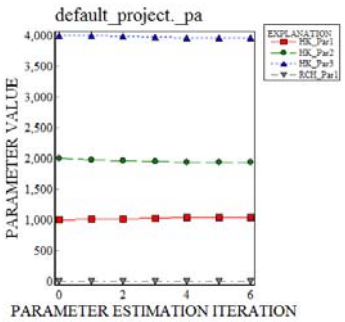
Visualize parameter evolution (2/2)

- ✓ Deselect the **Divide parameter values by their initial values** to display the actual evolution of the different parameters.



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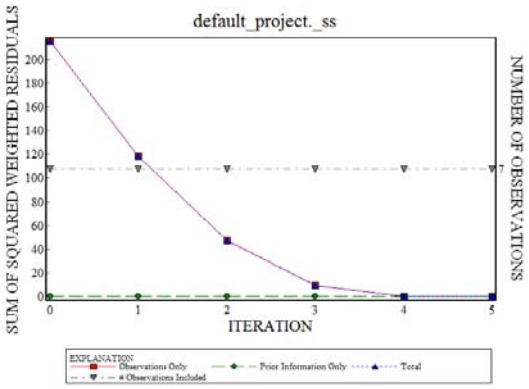
Visualize model performance evolution

- ✓ Now select **Model Fit|default_project._ss** in the **File:** drop-down list.
- ✓ This displays the sum of squared, weighted residuals for each parameter-estimation iteration.



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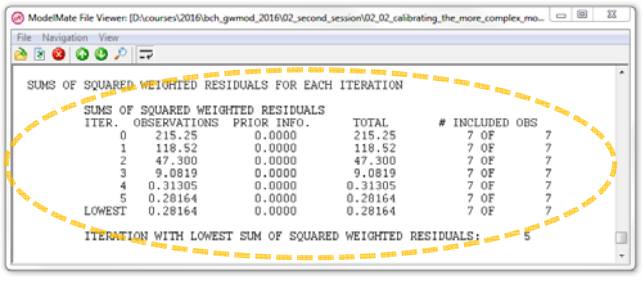
View the UCODE main output file

- ✓ Select **View|UCODE Main Output File**,
- ✓ and scroll down to the bottom of the viewer window.
- ✓ Just before the end of the file, you should find the table on the right, which also provides the sum of squared weighted residuals for each parameter-estimation iteration.



SUMS OF SQUARED WEIGHTED RESIDUALS FOR EACH ITERATION

SUMS OF SQUARED WEIGHTED RESIDUALS

ITER.	OBSERVATIONS	PRIOR INFO.	TOTAL	# INCLUDED OBS
0	215.25	0.0000	215.25	7 OF 7
1	118.52	0.0000	118.52	7 OF 7
2	47.300	0.0000	47.300	7 OF 7
3	9.0819	0.0000	9.0819	7 OF 7
4	0.31305	0.0000	0.31305	7 OF 7
5	0.28164	0.0000	0.28164	7 OF 7
LOWEST	0.28164	0.0000	0.28164	7 OF 7

ITERATION WITH LOWEST SUM OF SQUARED WEIGHTED RESIDUALS: 5

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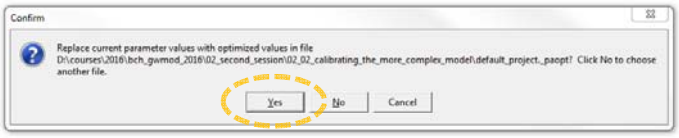
Import calibrated parameters in ModelMate

- ✓ Select **File|Import|Optimized Parameters (_paopt file)…**,
- ✓ confirm replacing the current parameter values by clicking **Yes**,
- ✓ and select **File|Save Project**, or use the corresponding button.



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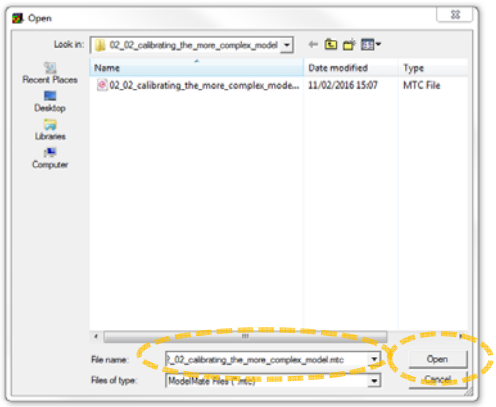
Import calibrated parameters in ModelMuse

- ✓ Return to the ModelMuse window,
- ✓ and select **File|Import|ModelMate Values**.
- ✓ Choose "02_02_calibrating_the_more_complex_model.mtc",
- ✓ and press **Open**.



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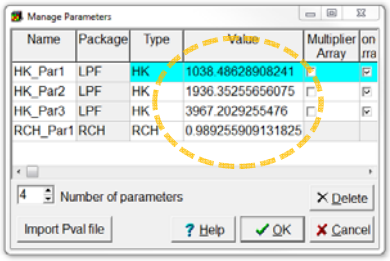
Check if parameters have changed

- ✓ Select **Model|Manage Parameters…** to see if the parameter values in ModelMuse have actually been modified.



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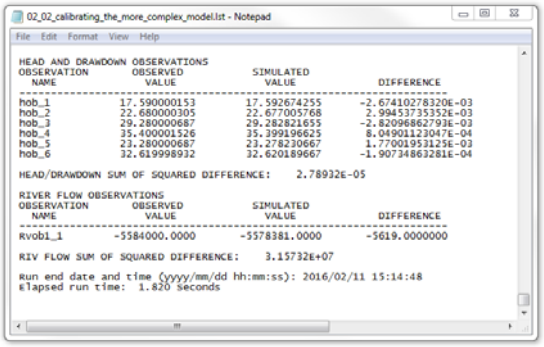
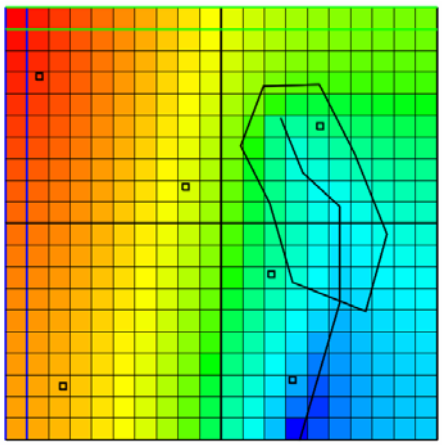
Run model and visualize calibrated results





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Questions? Found an error?
Please contact B. Rogiers at brogiers@sckcen.be.

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