

# Education evenings 2016

*Practical introduction  
to groundwater modelling*

Computer exercises  
02 02 Calibrating the more complex model

# Purpose

In this exercise, we will use ModelMate to perform

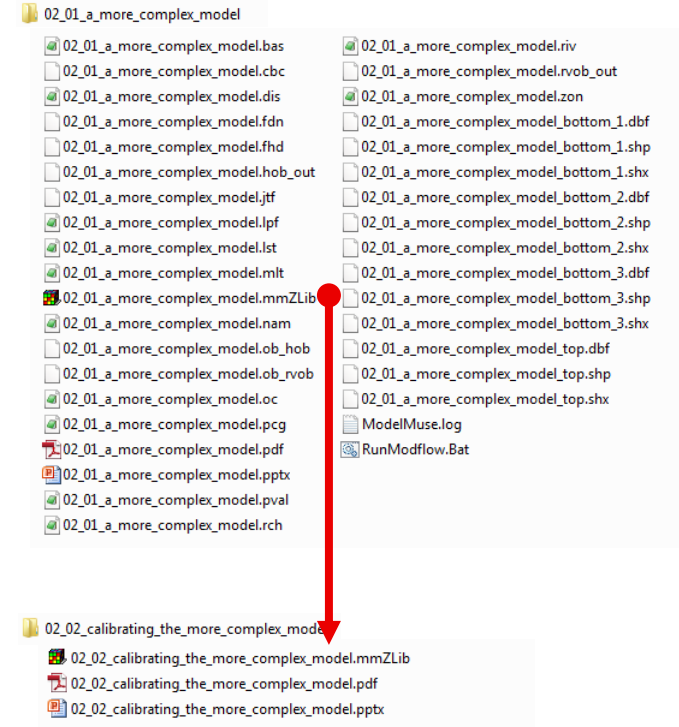
- ✓ local sensitivity analysis and
- ✓ local optimization or calibration

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

- ✓ import the results back to ModelMuse.

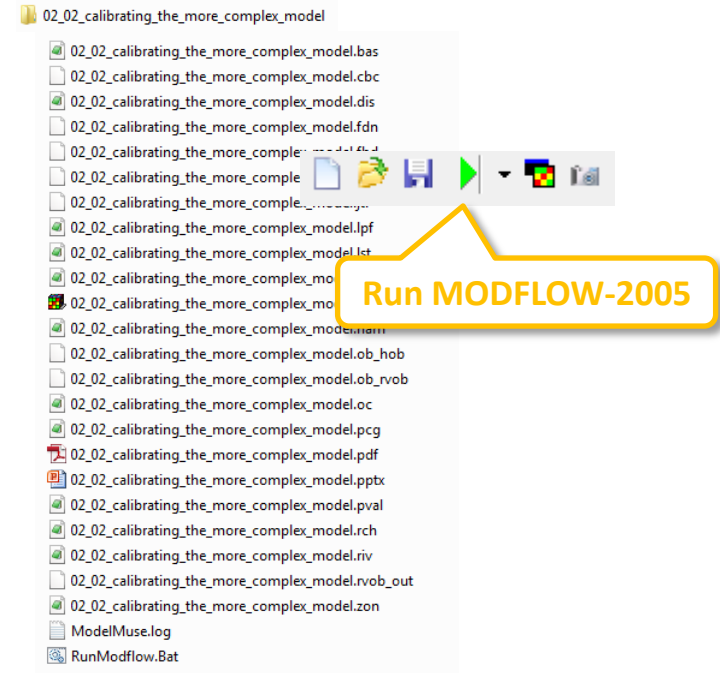
# Copy file previous exercise

- ✓ Copy file  
“/02\_01\_a\_more\_complex\_model/  
02\_01\_a\_more\_complex\_model.m  
mmZLib”  
to folder  
“/02\_02\_calibrating\_the\_more\_  
complex\_model/”
- ✓ Change the file name to  
“02\_02\_calibrating\_the\_more\_  
complex\_model.mmZLib”



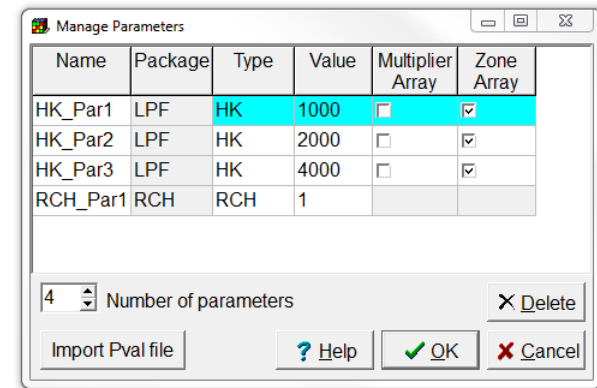
# Run MODFLOW again

- ✓ 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.



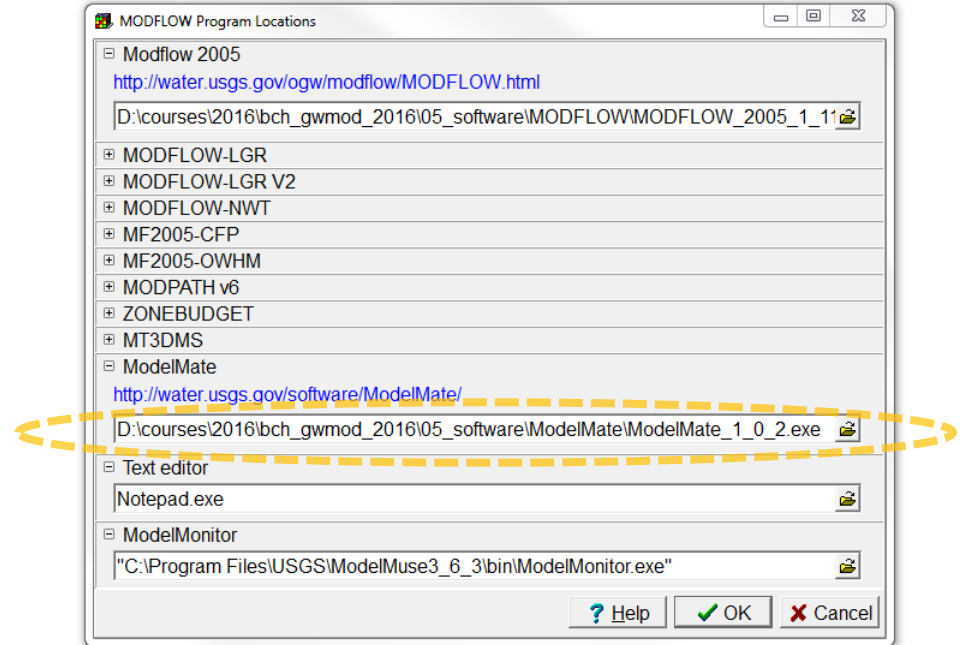
# Check model parameters

- ✓ 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



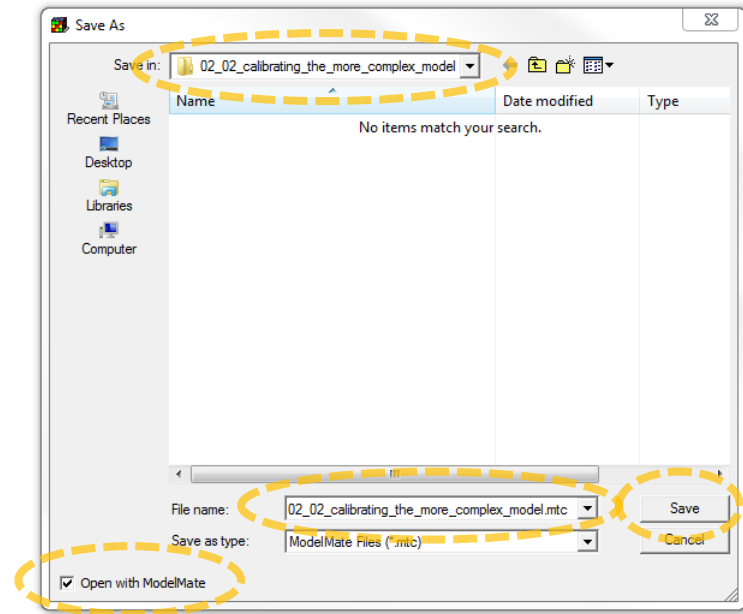
# Set ModelMate executable location

- ✓ 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.**

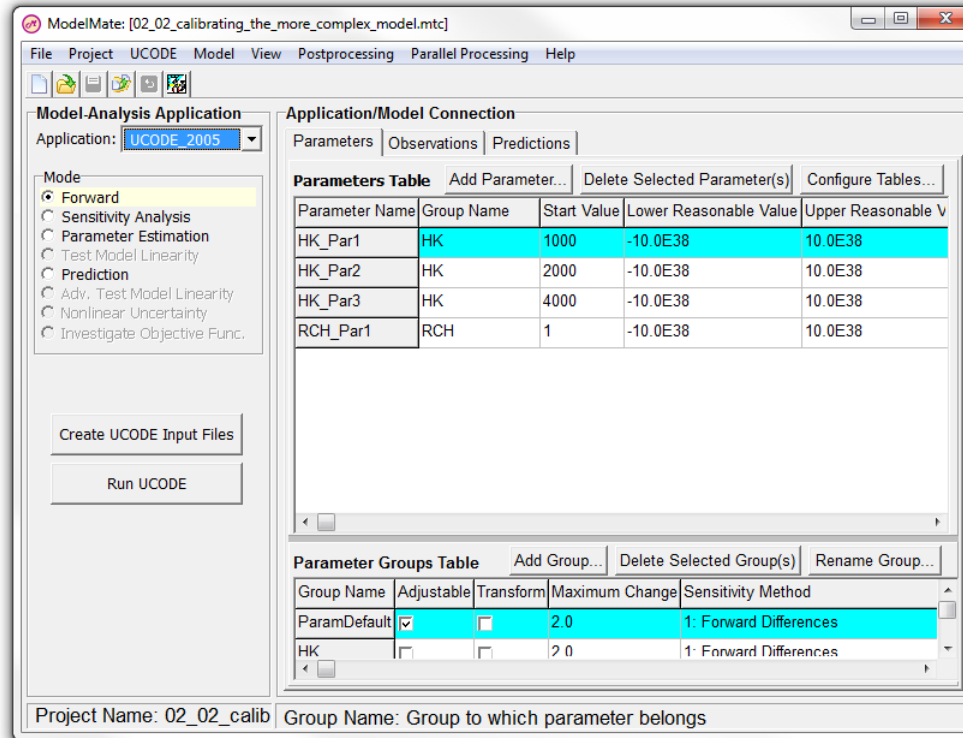


# Export ModelMate file

- ✓ 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**.



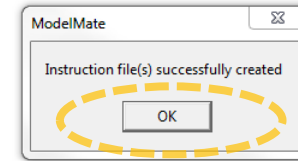
# This is what you should get





# 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**.



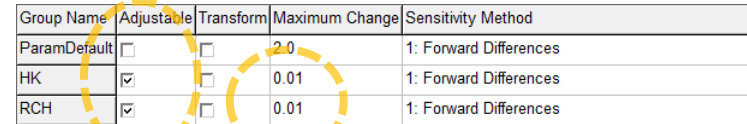
# Set program locations

- ✓ 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**.



# Adjust Parameter Groups Table

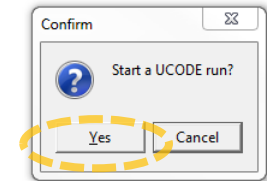
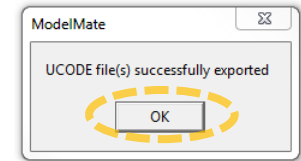
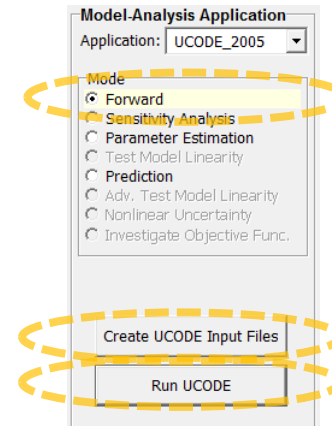
- ✓ In the **Parameter Groups Table**, deselect **Adjustable** for **ParamDefault**, and
- ✓ select it for **HK** and **RCH**. In this way, our hydraulic conductivity and recharge parameters are included in the sensitivity analysis and parameter estimation modes.
- ✓ Set **Maximum Change** to 0.01 for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



Group Name	Adjustable	Transform	Maximum Change	Sensitivity Method
ParamDefault	<input type="checkbox"/>	<input type="checkbox"/>	2.0	1: Forward Differences
HK	<input checked="" type="checkbox"/>	<input type="checkbox"/>	0.01	1: Forward Differences
RCH	<input checked="" type="checkbox"/>	<input type="checkbox"/>	0.01	1: Forward Differences

# 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.



# 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.

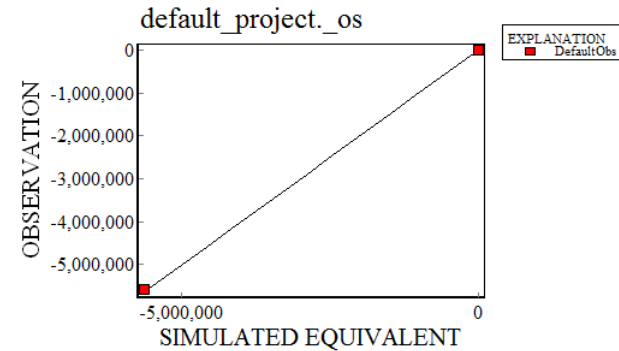
```
C:\Windows\system32\cmd.exe
Solving: Stress period: 5 Time step: 86 Ground-Water Flow Eqn.
Solving: Stress period: 5 Time step: 87 Ground-Water Flow Eqn.
Solving: Stress period: 5 Time step: 88 Ground-Water Flow Eqn.
Solving: Stress period: 5 Time step: 89 Ground-Water Flow Eqn.
Solving: Stress period: 5 Time step: 90 Ground-Water Flow Eqn.
Solving: Stress period: 5 Time step: 91 Ground-Water Flow Eqn.
Solving: Stress period: 5 Time step: 92 Ground-Water Flow Eqn.
Run end date and time (yyyy/mm/dd hh:mm:ss): 2016/02/11 13:29:01
Elapsed run time: 2.205 Seconds
Normal termination of simulation
SUM OF SQUARED, WEIGHTED RESIDUALS:
DEPENDENT VARIABLES: 215.2495
NUMBER OF INCLUDED OBSERVATIONS = 7 OF 7
*****
Job of current iteration of Control Loop is: STOP
*****
Normal termination of UCODE_2014. Version: 1.001
*****
Run end date and time (yyyy/mm/dd hh:mm:ss): 2016/02/11 13:29:01
Elapsed run time: 2.413 Seconds
D:\courses\2016\bch_gwmod_2016\02_second_session\02_02_calibrating_the_more_complex_model>pause
Press any key to continue . . .
```

# 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.



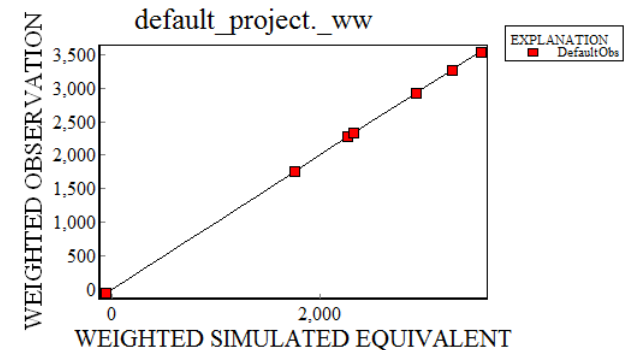
Start  
GW\_Chart



# Plot observations vs simulated equivalents (2/2)

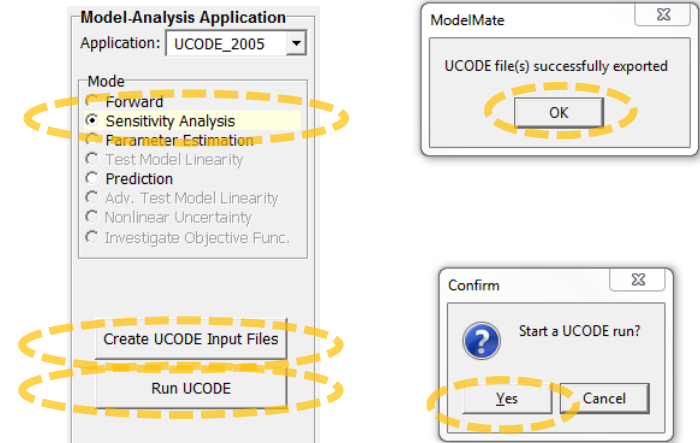
- ✓ Therefore, select **Model Fit | default\_project.\_ww** in the **File:** drop-down list.
- ✓ This displays the weighted observed compared to the weighted simulated values, which is more informative in this case.

File: default\_project.\_ww



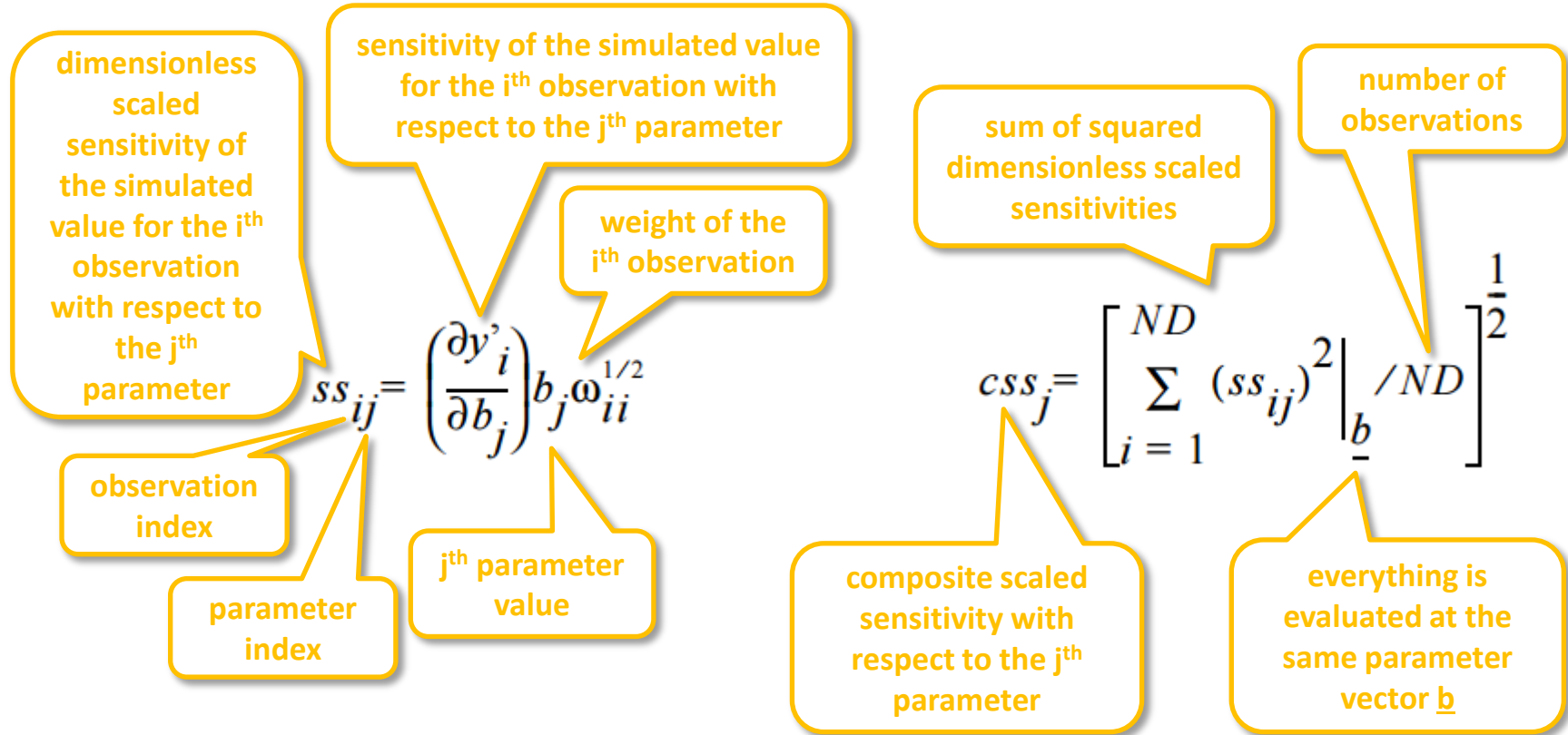
# Perform sensitivity analysis

- ✓ 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.



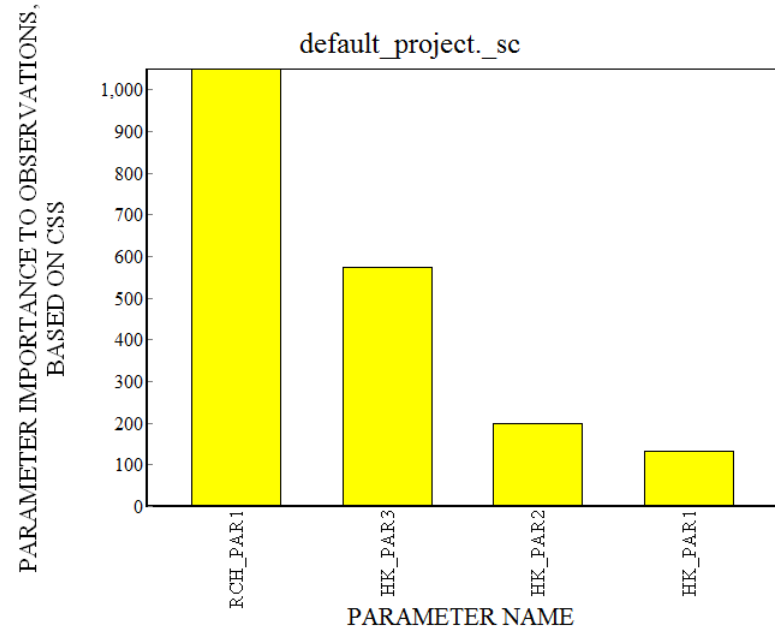


# Statistics for sensitivity analysis



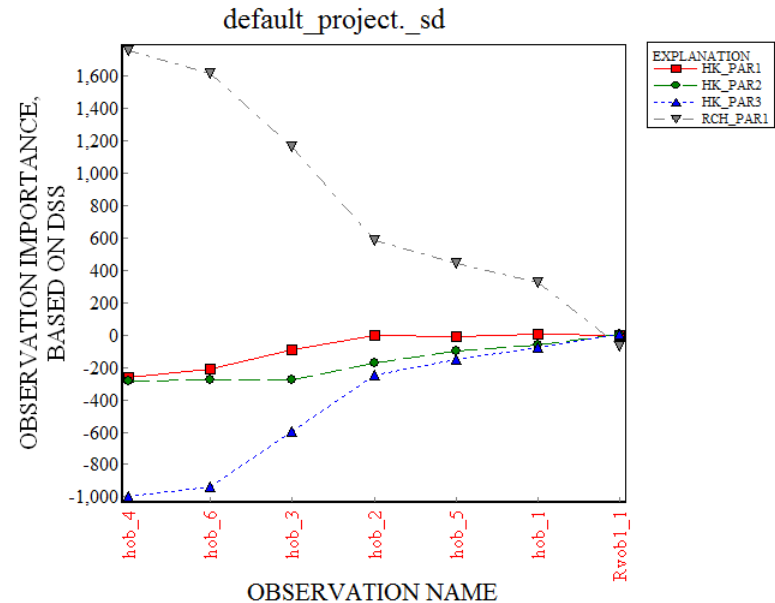
# Visualize composite scaled sensitivities

- ✓ 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).



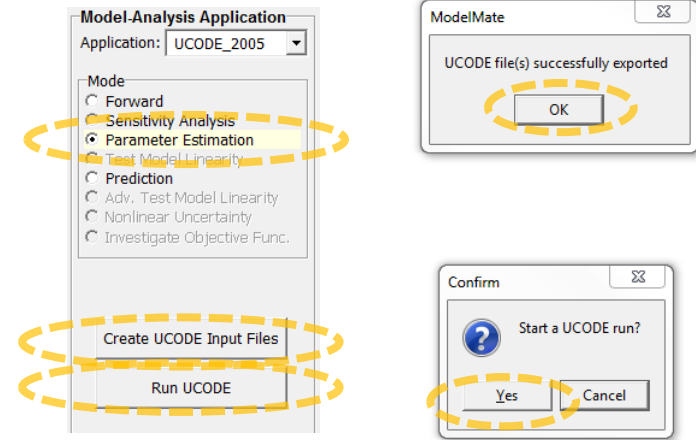
# Visualize dimensionless scaled sensitivities

- ✓ 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).



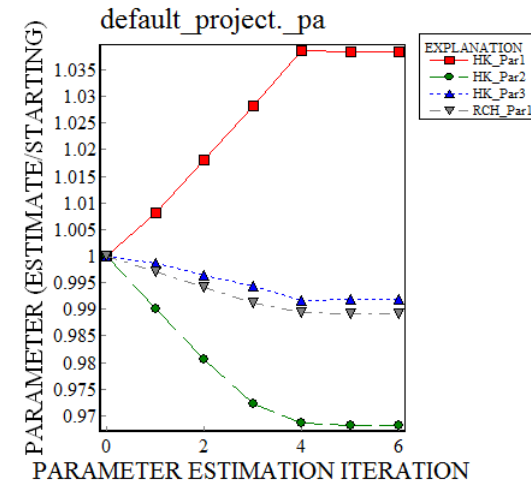
# Perform parameter estimation

- ✓ 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.



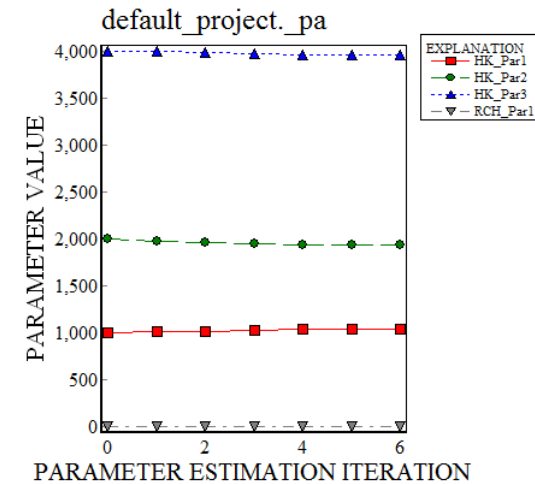
# Visualize parameter evolution (1/2)

- ✓ 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.



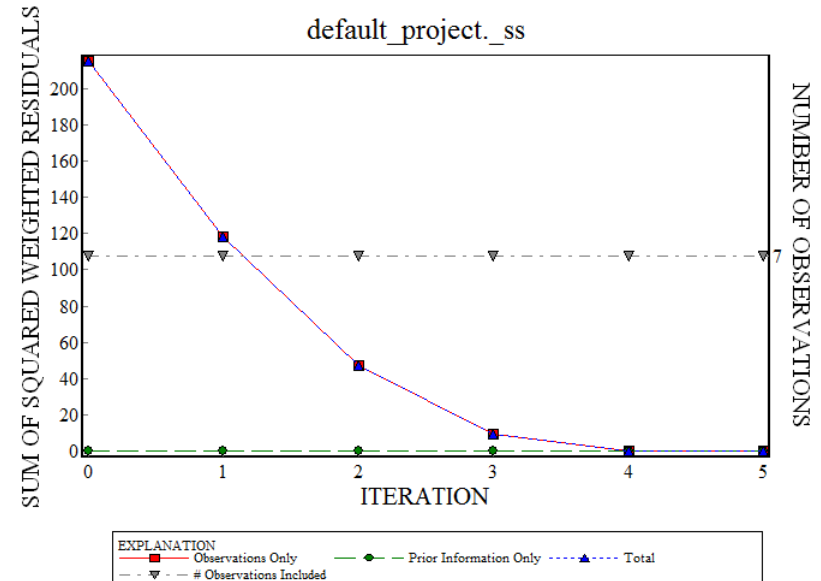
# Visualize parameter evolution (2/2)

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



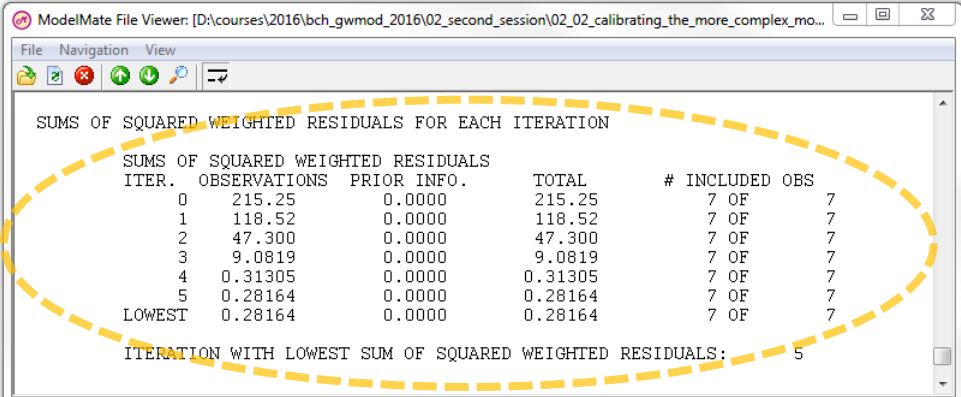
# Visualize model performance evolution

- ✓ 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.



# 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.



ModelMate File Viewer: [D:\courses\2016\bch\_gwmod\_2016\02\_second\_session\02\_02\_calibrating\_the\_more\_complex\_mo...

File Navigation View

SUMS OF SQUARED WEIGHTED RESIDUALS FOR EACH ITERATION

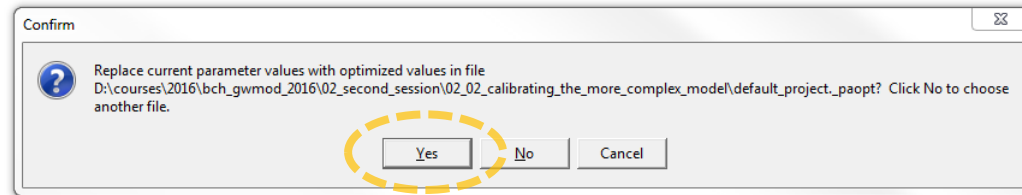
ITER.	OBSERVATIONS	PRIOR INFO.	TOTAL	# INCLUDED	OBS
0	215.25	0.0000	215.25	7 OF	7
1	118.52	0.0000	118.52	7 OF	7
2	47.300	0.0000	47.300	7 OF	7
3	9.0819	0.0000	9.0819	7 OF	7
4	0.31305	0.0000	0.31305	7 OF	7
5	0.28164	0.0000	0.28164	7 OF	7
LOWEST	0.28164	0.0000	0.28164	7 OF	7

ITERATION WITH LOWEST SUM OF SQUARED WEIGHTED RESIDUALS: 5



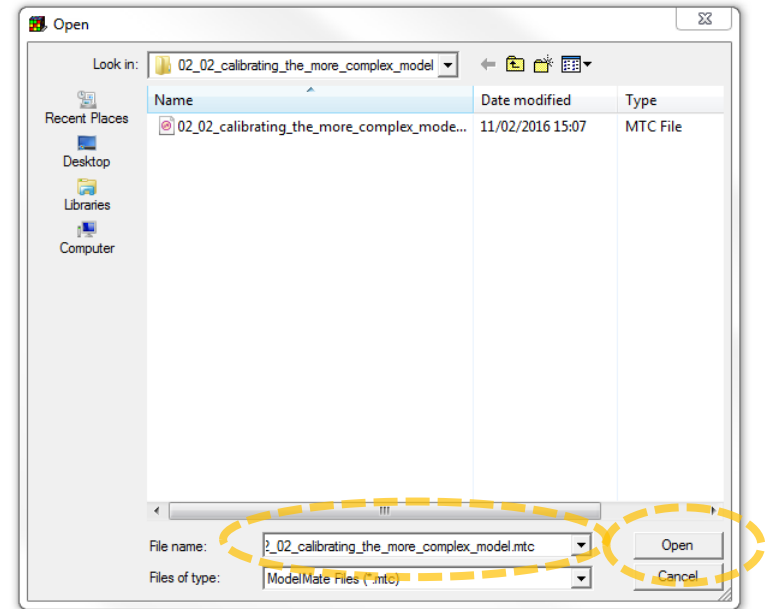
# Import calibrated parameters in ModelMate

- ✓ 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.



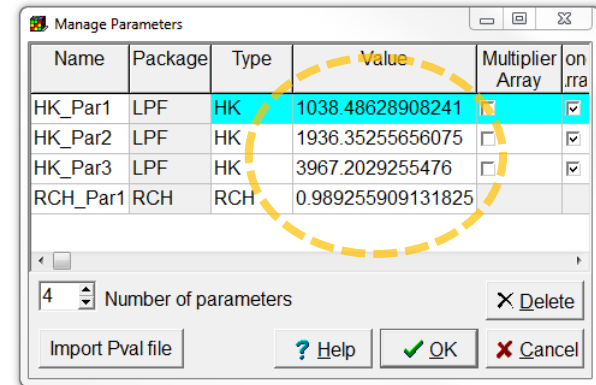
# Import calibrated parameters in ModelMuse

- ✓ Return to the ModelMuse window,
- ✓ and select **File | Import | ModelMate Values.**
- ✓ Choose “02\_02\_calibrating\_the\_more\_complex\_model.mtc”,
- ✓ and press **Open.**



# Check if parameters have changed

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



# Run model and visualize calibrated results

02\_02\_calibrating\_the\_more\_complex\_model.lst - Notepad

File Edit Format View Help

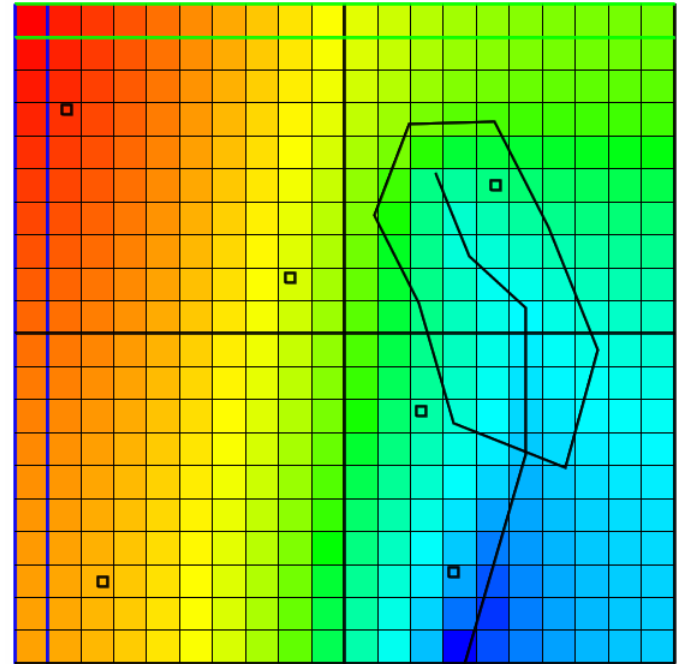
HEAD AND DRAWDOWN OBSERVATIONS	OBSERVED	SIMULATED	DIFFERENCE
OBSERVATION NAME	VALUE	VALUE	
hob_1	17.590000153	17.592674255	-2.67410278320E-03
hob_2	22.680000305	22.677005768	2.99453735352E-03
hob_3	29.280000687	29.282821655	-2.82096862793E-03
hob_4	35.400001526	35.399196625	8.04901123047E-04
hob_5	23.280000687	23.278230667	1.77001953125E-03
hob_6	32.619998932	32.620189667	-1.90734863281E-04

HEAD/DRAWDOWN SUM OF SQUARED DIFFERENCE: 2.78932E-05

RIVER FLOW OBSERVATIONS	OBSERVED	SIMULATED	DIFFERENCE
OBSERVATION NAME	VALUE	VALUE	
Rvob1_1	-5584000.0000	-5578381.0000	-5619.0000000

RIV FLOW SUM OF SQUARED DIFFERENCE: 3.15732E+07

Run end date and time (yyyy/mm/dd hh:mm:ss): 2016/02/11 15:14:48  
Elapsed run time: 1.820 Seconds



# Education evenings 2016

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02 02 Calibrating the more complex model

*Questions? Found an error?  
Please contact B. Rogiers at [brogiers@sckcen.be](mailto:brogiers@sckcen.be).*