



Education evenings 2018

*Practical introduction
to groundwater modelling*

Computer exercises
02 02 Calibrating the more complex model

1

Purpose

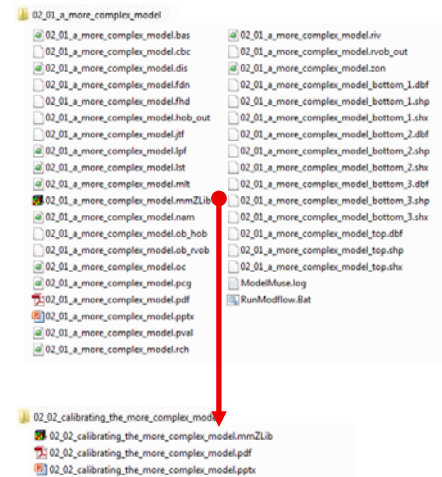
In this exercise, we will use ModelMate to perform

- ✓ 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

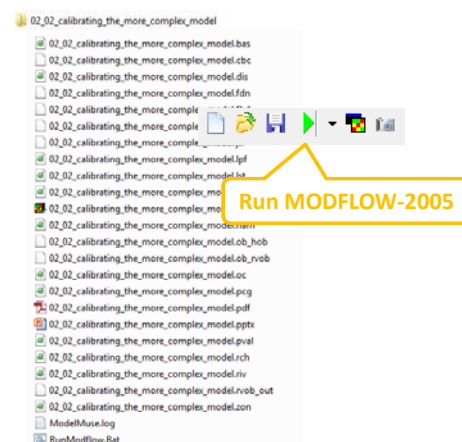
- ✓ Copy file “/02-01_a-more-complex-model/02-01_a-more-complex-model.mmZLib” to folder “/02-02_calibrating-the-more-complex-model/”
- ✓ Change the file name to “02-02_calibrating-the-more-complex-model.mmZLib”



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

Name	Package	Type	Value	Multiplier Array	Zone Array
HK_Par1	LPF	HK	1000	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
HK_Par2	LPF	HK	2000	<input type="checkbox"/>	<input checked="" type="checkbox"/>
HK_Par3	LPF	HK	4000	<input type="checkbox"/>	<input checked="" type="checkbox"/>
RCH_Par1	RCH	RCH	1	<input type="checkbox"/>	<input type="checkbox"/>

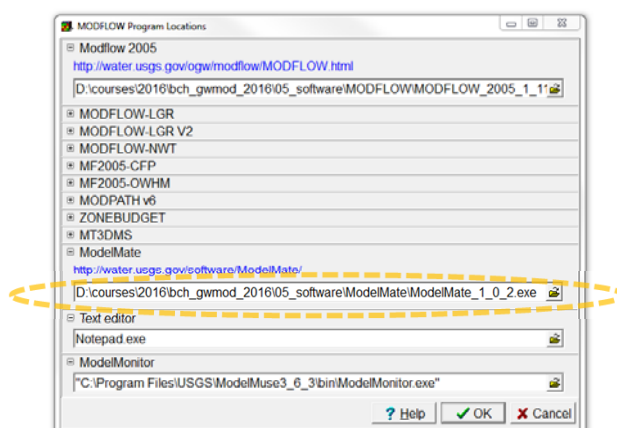
4 Number of parameters ✕ Delete

Import Pval file ? Help ✓ OK ✕ Cancel

5

Set ModelMate executable location

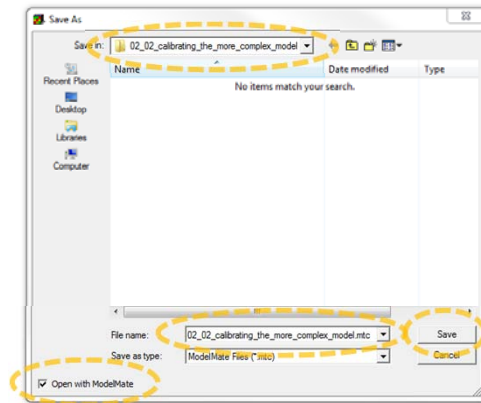
- ✓ Choose **Model | MODFLOW Program locations,**
- ✓ fill in the ModelMate executable location
 ".../bch_gwmod-2018/05_software/modelmate/modelmate-1.0.3.exe", and
- ✓ click **OK**.



6

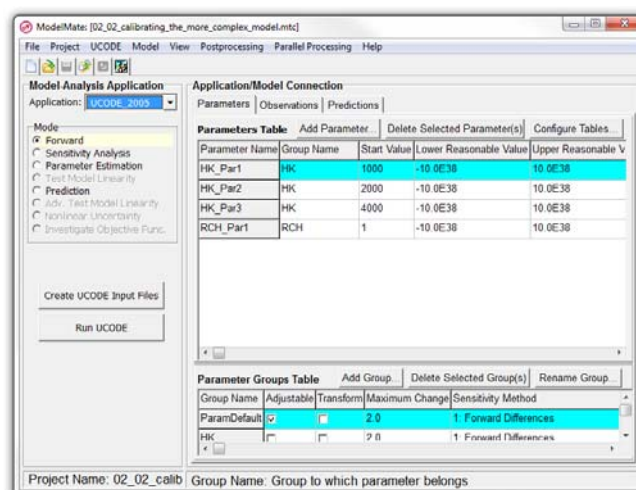
Export ModelMate file

- ✓ 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**.



7

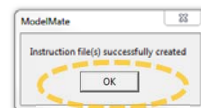
This is what you should get



8

Create instruction files

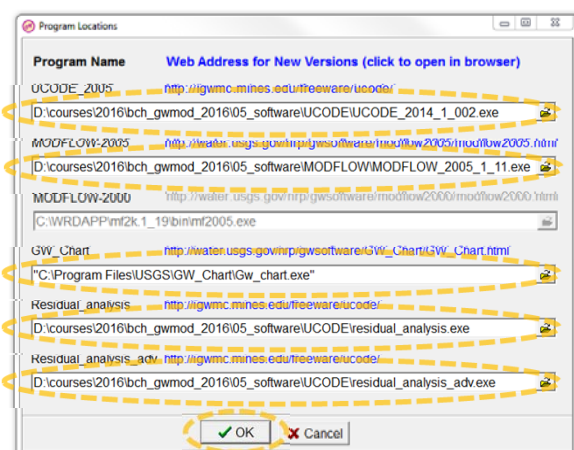
- ✓ Note that ModelMuse did not automatically create instruction files allowing UCODE to adjust the parameters and read the simulated equivalents of our observations.
- ✓ Select **Model | Create Instruction Files For Observations Defined In ModelMuse** in ModelMate,
- ✓ and press **OK**.



9

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 (x86)/USGS/** folder), and select the **GW_Chart.exe** executable.
- ✓ Then press **OK**.



10

Adjust Parameter Groups Table

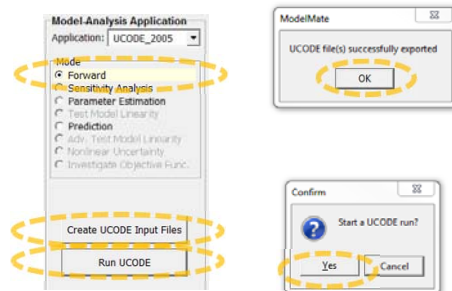
- ✓ In the **Parameter Groups Table**, deselect **Adjustable** for **ParamDefault**, and
- ✓ select it for **HK** and **RCH**. In this way, our hydraulic conductivity and recharge parameters are included in the sensitivity analysis and parameter estimation modes.
- ✓ Set **Maximum Change** to 0.01 for 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"/>	1	2.0	1: Forward Differences
HK	<input checked="" type="checkbox"/>	1	0.01	1: Forward Differences
RCH	<input checked="" type="checkbox"/>	1	0.01	1: Forward Differences

11

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.



12

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 Line step: 86 Ground-Water Flow Eqn.
Solving: Stress period: 5 Line step: 87 Ground-Water Flow Eqn.
Solving: Stress period: 5 Line step: 88 Ground-Water Flow Eqn.
Solving: Stress period: 5 Line step: 89 Ground-Water Flow Eqn.
Solving: Stress period: 5 Line step: 90 Ground-Water Flow Eqn.
Solving: Stress period: 5 Line step: 91 Ground-Water Flow Eqn.
Solving: Stress period: 5 Line 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: 2.285 Seconds

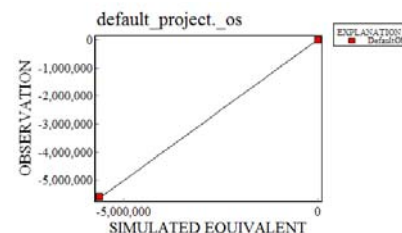
Normal termination of simulation
SUM OF SQUARED, WEIGHTED RESIDUALS: 215.2499
NUMBER OF INCLUDED OBSERVATIONS = 7 OF 7

=====
Job of current iteration of Control Loop is: STOP
=====
Normal termination of UCODE_2814, 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:\coursess\2016\hch_gwmod_2016\02_second_session\02_02_calibrating_the_more_comp
lex_model\pause
Press any key to continue . . .
  
```

13

Plot observations vs simulated equivalents (1/2)

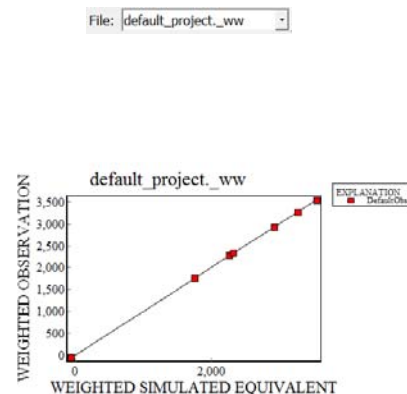
- ✓ Select **Postprocessing | GW_Chart**, or use the corresponding button to bring up the observed compared to simulated values graph.
- ✓ Note this plot is not very useful because of the differences in magnitude between the head and river observations.



14

Plot observations vs simulated equivalents (2/2)

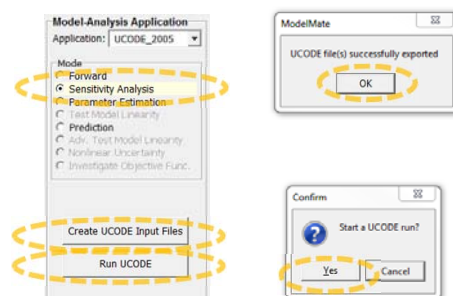
- ✓ Therefore, select **Model Fit** | **default_project._ww** in the **File:** drop-down list.
- ✓ This displays the weighted observed compared to the weighted simulated values, which is more informative in this case.



15

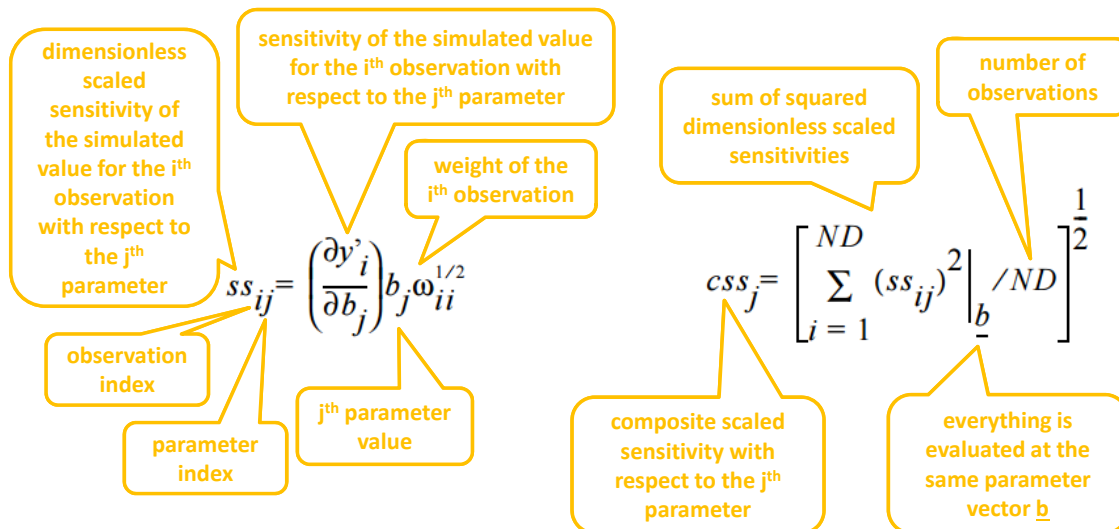
Perform sensitivity analysis

- ✓ 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.



16

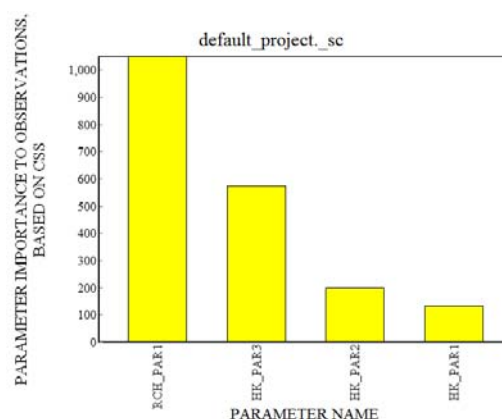
Statistics for sensitivity analysis



17

Visualize composite scaled sensitivities

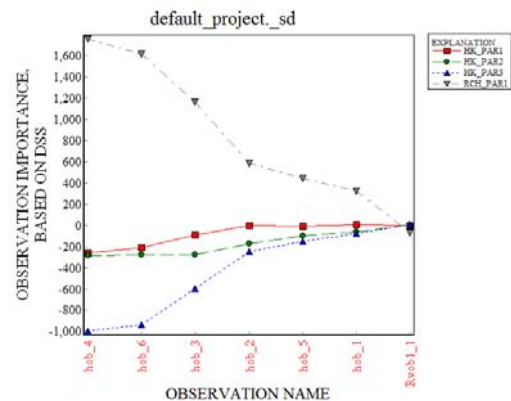
- ✓ Close the command line window after it has finished,
- ✓ and launch GW_Chart again.
- ✓ Now select **O-Par Sens Analysis | default_project._sc** in the **File:** drop-down list.
- ✓ This displays the bar chart of composite scaled sensitivities (indicating parameter importance to all observations).



18

Visualize dimensionless scaled sensitivities

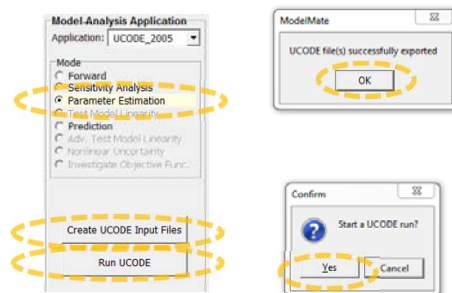
- ✓ Now select **O-Par Sens Analysis** | **default_project._sd** in the **File:** drop-down list.
- ✓ This displays the dimensionless scaled sensitivity for each observation by parameter (indicating the effect of each parameter on each observation).



19

Perform parameter estimation

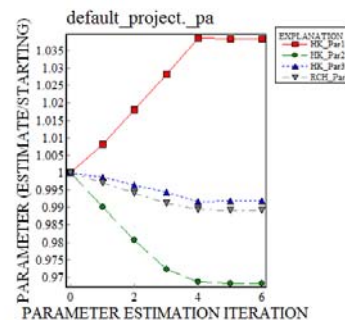
- ✓ Now select the **Parameter Estimation** mode,
- ✓ press **Create UCODE Input Files**,
- ✓ and click **OK**.
- ✓ Then click on the **Run UCODE** button,
- ✓ and click **Yes** to start the UCODE run.



20

Visualize parameter evolution (1/2)

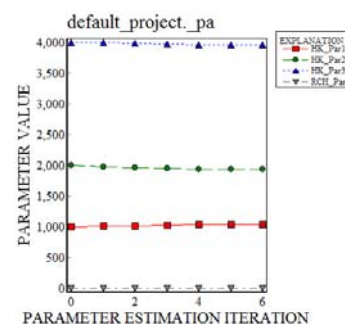
- ✓ Close the command line window after it has finished,
- ✓ and launch GW_Chart again.
- ✓ Now select **Parameter Values | default_project._pa** in the **File:** drop-down list.
- ✓ This displays the evolution of the different parameters with respect to their initial values.



21

Visualize parameter evolution (2/2)

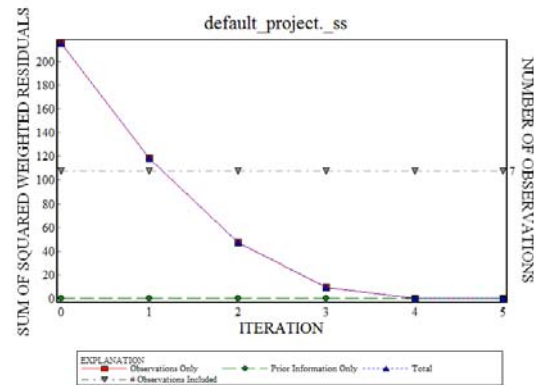
- ✓ Deselect the **Divide parameter values by their initial values** to display the actual evolution of the different parameters.



22

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.



23

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.

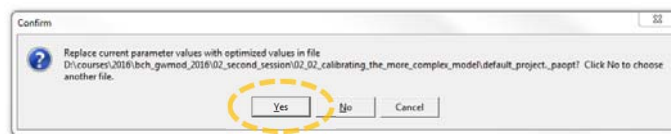
ITER.	OBSERVATIONS	PRIOR INFO.	TOTAL	# INCLUDED OBS
0	215.25	0.0000	215.25	7 OF 7
1	118.52	0.0000	118.52	7 OF 7
2	47.300	0.0000	47.300	7 OF 7
3	9.0819	0.0000	9.0819	7 OF 7
4	0.31305	0.0000	0.31305	7 OF 7
5	0.28164	0.0000	0.28164	7 OF 7
LOWEST	0.28164	0.0000	0.28164	7 OF 7

ITERATION WITH LOWEST SUM OF SQUARED WEIGHTED RESIDUALS: 5

24

Import calibrated parameters in ModelMate

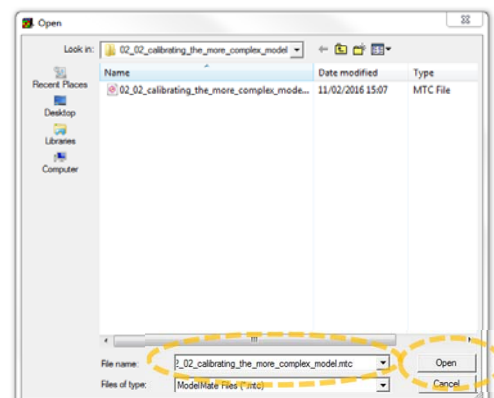
- ✓ Select **File | Import | Optimized Parameters (_paopt file)...**,
- ✓ confirm replacing the current parameter values by clicking **Yes**,
- ✓ and select **File | Save Project**, or use the corresponding button.



25

Import calibrated parameters in ModelMuse

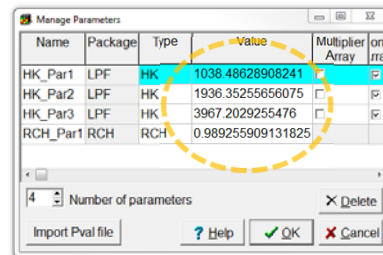
- ✓ Return to the ModelMuse window,
- ✓ and select **File | Import | ModelMate Values**.
- ✓ Choose **"02-02_calibrating-the-more-complex-model.mtc"**,
- ✓ and press **Open**.



26

Check if parameters have changed

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

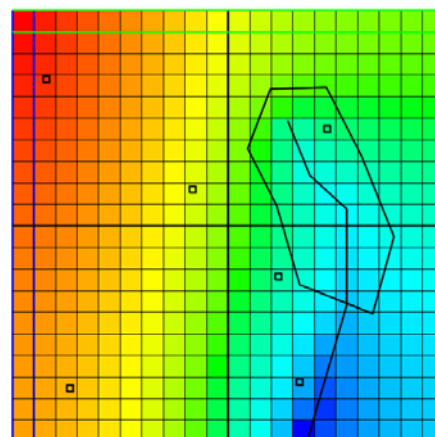


27

Run model and visualize calibrated results

02_02_calibrating_the_more_complex_model.list - Notepad

HEAD AND DRAWDOWN OBSERVATIONS			
OBSERVATION NAME	OBSERVED VALUE	SIMULATED VALUE	DIFFERENCE
hob_1	17.590000153	17.592674255	-2.67410278320e-03
hob_2	22.680000305	22.677005768	2.99453755352e-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			
OBSERVATION NAME	OBSERVED VALUE	SIMULATED VALUE	DIFFERENCE
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			



28



Education evenings 2018

*Practical introduction
to groundwater modelling*

Computer exercises
02 02 Calibrating the more complex model

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

29