Assignment # 6 Steady State Model Calibration: Calibrate your model. If you want to conduct a transient calibration, talk with me first. Perform calibration using UCODE. Be sure your report addresses global, graphical, and spatial measures of error as well as common sense. Consider more than one conceptual model and compare the results. Remember to make a prediction with your calibrated models and evaluate confidence in your prediction. Be sure to save your files because you will want to use them later in the semester. Suggested Calibration Report Outline

Title

Introduction

describe the system to be calibrated (use portions of your previous report as appropriate) Observations to be matched in calibration

type of observations

locations of observations

observed values

uncertainty associated with observations

explain specifically what the observation will be matched to in the model

Calibration Procedure

Evaluation of calibration

residuals

parameter values

quality of calibrated model

Calibrated model results

predictions

uncertainty associated with predictions

problems encountered, if any

Comparison with uncalibrated model results

Assessment of future work needed, if appropriate

Summary/Conclusions

Reference

submit the paper as hard copy and include it in your zip file of model input and output submit the model files (input and output for both simulations) in a zip file labeled: ASSGN6_LASTNAME.ZIP

Overview of UCODE & Associated Codes Modes that can be accomplished:

Forward Process Model run with Residuals

Conduct Sensitivity Analysis

Estimate Optimal Parameter values and associated linear uncertainty

Evaluate quality of the model

Estimate values of Predictions and associated linear uncertainty

Evaluate model linearity

Evaluate NonLinear uncertainty associated with

estimates of parameter values and predicted values

Auxiliary: Investigate Objective Function

See UCODE Manual

Chapter 1 for overview and description of manual contents
Chapter 2 for overview and program control

Also Chapter 4 Table 3

Overview of UCODE in Parameter Estimation Mode

- 1) manipulates application model input files and reads simulated values from application model output files
- 2) compares user-provided observations with equivalent simulated values derived from the values read from the application model output files using a weighted least-squares objective function
- 3) uses a modified Gauss-Newton method to adjust the value of user selected input parameters in an iterative procedure to minimize the value of the weighted least-squares objective function
- 4) reports the estimated parameter values
- 5) calculates and prints statistics to be used to
 - * diagnose inadequate data
 - * identify parameters that probably cannot be estimated
 - * evaluate estimated parameter values
 - * evaluate accuracy of model representation of processes
 - * quantify the uncertainty of model simulated values

See UCODE Manual Chapter 2 for Flow Chart

See UCODE Manual Chapter 3 for general issues related to using UCODE for Nonlinear Regression

In parameter estimation mode, UCODE performs inverse modeling, using nonlinear regression. Sensitivities are calculated by perturbation (many significant figures are needed) or read from a process model output file.

Any application/process model or set of models (pre/post processors)

Must have numerical (ASCII text) input and output files, with numbers of sufficient significant digits

Estimated parameter can be a quantity in the input files, or one used in conjunction with functions to calculate that quantity

Observations can be any quantity for which a simulated equivalent value can be read or calculated from values in model output files using additive/multiplicative functions

Prior information on estimated parameters also can be included

KEEP UP-TO-DATE on

New Developments

And

UCODE Software updates

USGS Software Web Site
http://water.usgs.gov/nrp/gwsoftware/
Also on the USGS general software page

BOOKMARK THAT PAGE! DOWNLOAD AND INSTALL THE LATEST version of UCODE

MODFLOW is our process model to be calibrated

MODFLOW-2000/2005 include: GLO Global Process that controls overall program flow GWF Ground-water Flow Process OBS Observation Process

MODFLOW-2000 also includes: SEN Sensitivity Process (slated for MF2005) PES Parameter Estimation Process (being discontinued)

UCODE INPUT

Once we have a working forward model that runs in batch mode

Set up UCODE files and run the forward model through UCODE to be sure everything is functioning properly.

NEVER bypass this step.

Follow input directions in the UCODE MANUAL provided (review Chapters 1-3 for an overview, Chapter 4 for how to execute UCODE, and Chapter 5 for the general block format input that is used throughout the UCODE input file.

OR USE THE NEW USGS code

MODELMATE TO SET UP UCODE FILES

UCODE INPUT

We'll use a beta version of the soon-to-be-released ModelMate and a Tutorial tailored to our class example to generate ucode files from MF2005 files (** first!! download software, tutorial for our example, MFfiles-PreMM today's class web page) It is easier to learn the input after you have a better idea of the process So approach this with the idea of absorbing the gestalt vs the details

UCODE Manual Chapter 5, Table 4, OVERVIEW of INPUT BLOCKS

Follow tutorial and see:

Ucode_main.in

Major items of note General Input Format (note these in main ucode input file on web page link):

- a # in column 1 specifies a comment and the line is not read by the code
- Input is specified in blocks, these are designated with a BEGIN and an END
- Notice the Block Names, their order and whether they are required or optional.
- Begin is followed by the block name and the format option for how the input will be entered (keywords or table, or file format: the default is keywords), and END is followed by the block name
- Blocks have keywords to identify the start of a new group of information
- Some input data are matrices which may be input as Standard or Compressed format (see an example of the compressed format in the Matrix Input Format section)

			Follow	tutorial and	see Ucode_main.in	
	Orig	inal	_	D		Default column
Chapter	Ригроѕе	Blocklabel	Default col- umn order ²	Purpose	Options	order ²
⁴ 6	Define UCODE_2005 operation	Options Merge_Files ³ UCODE_Control_Data ³ Reg_GN_Controls ³ Reg_GN NonLinInt ^{3,4}	No No No No No	Define UCODE_2005 operation	Merge Files UCODE Control Data Reg GN Controls Reg GN NonLinInt Model Command Lines Parameter Groups	No No No No No No
7	Define parameters	Model Command Lines Parameter_Groups Parameter_Data Parameter_Values Derived Parameters	No No No Yes Yes Yes	Define parameters	Parameter Groups For Prediction Parameter Data Parameter Data Parameter Data Parameter Values Derived Parameters Derived Parameters Parameter Values	No Yes Yes Yes Yes Yes
8	Define observations	Observation_Groups Observation_Data Derived_Observations	No Yes Yes	Define observations	Observation Groups Observation Data Derived Observations Prediction Groups	No Yes Yes No
δ	Define predictions	Prediction_Groups Prediction_Data ⁶ Derived Predictions	No Yes Yes	Define predictions Define prior	Prediction Data Derived Predictions Prior Information Groups Prior Information Groups For Prediction	Yes Yes No No
9	Define prior information	Prior_Information_Groups Linear Prior Information	No Yes	information	Linear Prior Information Linear Prior Information For Prediction	Yes Yes
10	Define variance-covariance matrices to weight groups of observations or prior information with correlated errors.	Matrix_Files	No	Define variance- covariance matrices to weight groups of observations or prior information with correlated errors.	Matrix_Files	No
11	Interact with process-model input and output files.	Model_Input_Files Model_Output_Files	Yes Yes	Interact with process- model input and output files.	Model Input Files Model_Output_Files	Yes Yes
12	Run process model(s) using multiple processors	Parallel_Control Parallel_Runners	No Yes	Run process model(s) using multiple processors	Parallel_Control Parallel_Runners	No Yes

	format options.
Blockformat	Prescribed input format
KEYWORDS	Blockbody consists of a series of lines of the form: Keyword=value
	Under some circumstances there are restrictions on how the lines
	are ordered; see the input block instructions.
	If no blockformat is specified, KEYWORDS is assumed, but it is
	advisable to explicitly identify the block format to reduce errors. Comments are allowed. 1.2
TABLE	Blockbody consists of a table of data that may have labels on the
	columns and may be read from the main input file or from another
	input file. See the text for additional information.
	Comments are allowed right after the BEGIN statement but not in
	the rest of the input block. 1
FILES	Blockbody consists of the pathname for one or more files.
	Comments are allowed. ^{1,2}
	To allow the format to be specified, the contents of each of the
	listed files needs to begin with a 'Begin Blocklabel [Blockformat]' line and end with an
	'End Blocklabel' line. The Blocklabel needs to be the same as in
	the 'Begin Blocklabel FILES' block within which the files are
	listed. See the section "Observation Data Input Block" for an
	example.

Follow tutorial and see Ucode_main.in OPTIONS BLOCK Chapter 6 (p52) Default col-umn order² ${\bf Chapter}^{\bf 1}$ Blocklabel Purpose Options No In: Merge_Files³ UCODE_Control_Data³ Define UCODE_2005 No Reg_GN_Controls³ Reg_GN_NonLinInt^{3,4} Model_Command_Lines operation No FILE: ep_Ucode_main.in No No Parameter_Groups Parameter_Data³ Parameter_Values³ BEGIN Options No Yes Verbose=0 Define parameters Yes END Options Derived_Parameters³ Yes Observation_Groups No Observation_Data Define observations Yes Derived_Observations Yes Later, if UCODE is not running as Prediction_Groups Prediction_Data⁰ No Define predictions Yes you expect, use 5 Derived_Predictions Yes Prior_Information_Groups No Define prior information Yes Linear_Prior_Information Define variance-covariance Notice other possible input items matrices to weight groups of observations or prior Matrix_Files No information with correlated errors. Interact with process-model Model_Input_Files Yes Model_Output_Files input and output files. Yes Run process model(s) using Parallel_Control multiple processors Parallel_Runners No 12 Yes

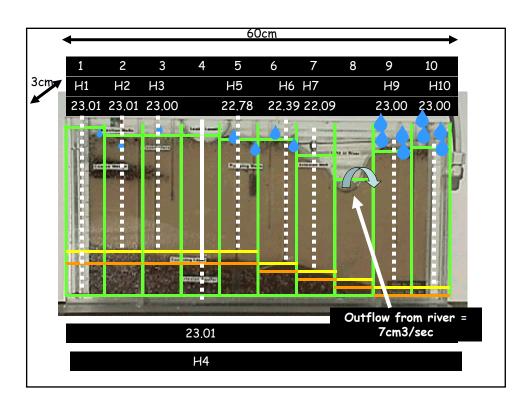
UCODE_CONTROL_DATA BLO	OCK		ow tutorial and Ucode_main.in	
Chapter 6 (p55)	Chapter ¹	Purpose	Blocklabel	Default col- umn order ²
In: ucode1 FILE: ep_Ucode_main.in	46	Define UCODE_2005 operation	Options Merge_Eiles ³ L'CODE_Control_Data ³ Reg_GN_Controls ³ Reg_GN_NonLinInt ^{3,4} Model_Command_Lines	No No No No No
BEGIN UCODE_CONTROL_DATA KEYWORDS ModelName=antfarm ModelLenathUnits=centimeters	7	Define parameters	Parameter_Groups ³ Parameter_Data ³ Parameter_Values ³ Derived_Parameters ³	No Yes Yes Yes
ModelTimeUnits=seconds sensitivities=no optimize=no DataExchange=yes	8	Define observations	Observation_Groups Observation_Data Derived_Observations Prediction_Groups	No Yes Yes No
END UCODE_CONTROL_DATA		Define predictions	Prediction _Data ⁶ Derived _ Predictions Prior Information Groups	Yes Yes No
	9	Define prior information	Linear_Prior_Information	Yes
Later, other options will be of interest, so notice other possible input items	10	Define variance-covariance matrices to weight groups of observations or prior information with correlated errors.	Matrix_Files	No
	11	Interact with process-model input and output files.	Model_Input_Files Model_Output_Files	Yes Yes
	12	Run process model(s) using multiple processors		No Yes

Model Command Lines BLOCK Follow tutorial and see Ucode_main.in Chapter 6 (p65) Default col-Chapter¹ Blocklabel Purpose umn order If a un-required block is skipped, Options the defaults are used Merge_Files³ UCODE_Control_Data³ Nο Define UCODE_2005 No BEGIN MODEL_COMMAND_LINES operation Reg_GN_Controls³ No Reg GN_NonLinInt^{3,4} 'Command=ep.bat' No purpose=forward Model Command Lines Parameter_Groups Parameter_Data³ No CommandId=modflow Yes END MODEL_COMMAND_LINES Define parameters Parameter_Values Yes Derived_Parameters³ The batch file should run all the Observation_Groups Define observations Observation_Data Yes codes you want to run for your Derived Observations Yes calibration Prediction Groups No Prediction Data Define predictions Yes Derived_Predictions Yes ALL SHOULD RUN AND Prior_Information_Groups No Define prior information **CLOSE WITHOUT** Linear_Prior_Information Yes Define variance-covariance HUMAN INTERVENTION matrices to weight groups of observations or prior Matrix_Files No ***** REMOVE PAUSE information with correlated FROM EP.BAT***** Interact with process-model Model Input Files 11 input and output files. Model_Output_Files Yes Run process model(s) using Parallel_Control multiple processors CommandId not used by UCODE at this time

Define UCODE_2005 Options No	Chanton 7 (n68)	Chapter ¹	Purpose	Blocklabel	Default co umn orde
RVCB 1E-5 rch1 0.1 rch1 0.1 rch2 0.05 rch3 0.01 Rriv 1e-3 BEGIN PARAMETER_GROUPS KEYWORDS groupname=Ks transform=yes adjustable=yes groupname=FCH transform=no adjustable=yes groupname=FIXED transform=no adjustable=no END PARAMETER_GROUPS Jse groups to define common characteristics NOTE Log Transforming Parameters: The may help the problem converge more readily Parameter Groups Yes Parameter Groups Poeine parameters Prediction Groups Define observations Prediction Groups Define predictions Prediction Data Yes Prediction Groups Define prior information Proj. Information No Prediction Groups Define prior information No Matrix, Files No Model Input Files Yes Model Output Files Yes Parameter Groups Yes Yes Parameter Groups Yes Parameter S Parameter Groups Yes Parameter S Perior Groups Parameter S Perior Groups Prediction Groups Parameter Groups Yes Parameter Groups Yes Parameter S Parameter S Parameter Groups Yes Parameter S Para	<u>pval</u> package 81 0.01 K2 10.0	46	_	Merge_Files ³ UCODE_Control_Data ³ Reg_GN_Controls ³ Reg_GN_NonLinInr ^{3,4}	No No No No
Kriv 1e-3 BEGIN PARAMETER_GROUPS KEYWORDS groupname=Ks transform=yes adjustable=yes groupname=RCH transform=no adjustable=yes groupname=FIXED transform=no adjustable=no END PARAMETER_GROUPS Jefine predictions Prediction_Data' Yes Derived [Notervations] No Prediction_Data' Yes Derived Predictions Yes Derived Predictions Yes Derived Predictions Proc. Information Groups Linear Prior Information From John Statistics NOTE Log Transforming Parameters: The may help the problem converge more readily Interact with process-model input files World Juput files Yes Model Output Files Yes No Model Output Files Ye	KVCB 1E-5 rch1 0.1 rch2 0.05	7	_	Parameter_Data ³ Parameter_Values ³	Yes Yes
groupname=Ks transform=yes adjustable=yes groupname=RCH transform=no adjustable=yes groupname=FIXED transform=no adjustable=no END PARAMETER_GROUPS Use groups to define common characteristics NOTE Log Transforming Parameters: * may help the problem converge more readily * Prediction Groups Predictions Data Yes Define predictions Predictions On No Define prior information Groups Linear Prior Information Groups Ves Define prior information Groups Linear Prior Information Groups Ves Matrix_Fles No information vitil correlated enters. * Model Input Files Yes included output files Ves model Output Files Yes multiple processors Parallel Runners Yes	Kriv le-3		Define observations	Observation_Data	Yes
## Provided	groupname=Ks transform=yes adjustable=yes	8	Define predictions	Prediction_Groups Prediction_Data ⁰	No Yes
Use groups to define common characteristics 10 10	groupname=FIXED transform=no adjustable=no	9	Define prior information	Prior_Information_Groups	No
NOTE Log Transforming Parameters: * may help the problem converge more readily Transforming Parameters Transforming		10	matrices to weight groups of observations or prior information with correlated	Matrix_Files	No
* may help the problem converge more readily 12 multiple processors Parallel Runners Yes	NOTE Les Transformine Peremeteus:	11			
		12	Run process model(s) using	Parallel_Control	No

FAKA	METER_I	DATA	BLOCK	Chapter	٠ 7	(p69) F	ollow tutori	
BEGIN PAR	AMETER_DATA	TABLE					Ucode_mai	n.ın
nrow=8 n	col=7 colu	mnlabels						
paramname	startvalue	lowerval	lue upperval	ue scalepv	al gı	roupname		
K1	0.01	0.001	0.1	0.00000	1	Ks		
к2	10.0	1.0	100.0	0.0010		Ks		
KVA	1.0	0.1	10.0	1e-4		FIXED		
KVCB	1e-5	1e-6	10.0	1e-1 1e-9				
				-0 2		Ks		
rch1	0.1	0.01	1.0	1e-5		RCH		
rch2	0.05	0.005	0.5	5e-7		RCH		
rch3	0.01	0.001	0.1	1e-7		RCH		
Kriv	1.E-1	1.E-2	1.E-0	1.E-5		Ks		
END PARAM	ETER_DATA				Chapter ¹	Purpose	Blocklabel	Default col umn order
· · · · · · · · · · · · · · · · · · ·								No
affect th	ne regression	1			46	Define UCODE_2005 operation	UCODE Control Data ³ Reg GN Controls ³ Reg GN NonLinInt ^{3,4}	No No No
It is bes	t to NOT im r values, bu	npose limi t this ca	ts on estima n be done in		7		Reg GN Controls ³	No No
It is bes	t to NOT im	npose limi t this ca			7	operation	Reg GN_Controls ² Reg GN_NonLinInt ^{3,4} Model Command Lines Parameter Compata Parameter Data ³ Parameter Values ⁴	No No No No
It is best paramete with the	t to NOT im r values, bu Constrain vo training may	npose limi t this ca ariable yield uni	n be done in reasonable v	UCODE	7 8	Define parameters	Reg. GN. Controls Reg. GN. NonLinlin ¹⁸ Model Command Lines Parameter Data Parameter Data Parameter Data Parameter Values Observation, Groups Observation, Groups Observation Data Derived Observations Prediction, Groups Prediction, Data	No No No No No Vo
It is best paramete with the Not const that are	t to NOT im r values, bu Constrain vo training may	npose limi t this ca ariable yield uni identify	n be done in reasonable vi ing conceptu	UCODE	7 8 9	Define parameters Define observations	Reg. GN. Controls Reg. GN. NonLining Reg. GN. NonLining Model Command Lines Parameter Data? Parameter Data? Parameter Data? Danised Basameter Observation, Groups Observation, Groups Prediction, Groups Prediction, Groups	No No No No No Yes Yes Yes No Yes
It is best paramete with the Not const that are errors, d	t to NOT imer values, bu Constrain values training may valuable for lata errors, constrain if	npose limi t this ca uriable yield un identify or insuff	n be done in reasonable vi ing conceptu	UCODE alues, al model	7	Define parameters Define observations Define predictions	Reg. GN. Controls? Reg. GN. Controls? Reg. GN. Noul. Inflat. Model Command Lines Parameter Data? Parameter Data? Parameter Values? Observation Groups Observation Groups Observation Groups Prediction Groups	No No No No No No Yes Yes No Yes No No
It is best paramete with the Not const that are errors, d Only use that value	t to NOT imer values, bu Constrain values training may valuable for lata errors, constrain if	npose limi t this ca uriable yield uni identify or insuff the mod	n be done in reasonable voing conceptuo icient info el will crash	UCODE alues, al model	7 8 9	Define parameters Define observations Define productions Define productions Define prior information Define verialize-covariance manifest to weight groups of observations or prior information with correlated	Reg. GN. Controls' Reg. GN. Nool, Intel Model Command Lines Parameter Control Research Parameter Data Parameter Data Parameter Data Parameter Data Parameter Data Parameter Data Data Data Demodel Observations Prediction Data Period Observations Prediction Data Derived Prediction Data Derived Prediction Data Derived Prediction Data Derived Prediction Data Linear Prior Information	No N

Follow tutorial/see Ucode main.in **OBSERVATIONS** Chapter 8 Default col-Chapter¹ Purpose Blocklabel We use the simple approach of umn order Options No reading the observation in Merge_Files³ UCODE_Control_Data³ Reg_GN_Controls³ order from the MODFLOW Define UCODE_2005 No No os file Reg_GN_NonLinInt^{3,4} Model_Command_Lines No Parameter_Groups Parameter_Data³ No You can do very complex Yes Define parameters Parameter Values extractions, involving searching Yes Derived Parameters³ Yes for character strings and Define observations One or the other Observation_Data counting lines and sapces such Derived_Observations that values can be extracted Prediction_Groups Define predictions Prediction_Data⁰ Yes from ANY format of text file Derived_Predictions Yes Prior_Information_Groups No Define prior information Linear_Prior_Information Yes Also you can make calculations Define variance-covariance matrices to weight groups from the items you extract to of observations or prior Matrix_Files No obtain simulated equivalents information with correlated Interact with process-model Model_Input_Files Model_Output_Files input and output files. Yes Run process model(s) using Parallel_Control No Parallel_Runners Yes multiple processors



```
Head Observations 95% confidence is 0.1 cm
                                         HEAD
 1 \times 1.5 \text{ y} = 1.5 \text{ multilayer } 23.01 \text{ cm column } 1 \text{ coff}
 2 \times = 7.5 \text{ y} = 1.5 \text{ layer } 1
                                       23.01 cm column 2 coff
 3 \times 13.5 \text{ y} = 1.5 \text{ layer } 1
                                        23.00 cm column 3 coff
                                                                           0
 4 \times 19.5 \text{ y} = 1.5 \text{ layer } 2
                                        23.00 cm column 4 coff
                                                                           0
 5 \times 25.5 \text{ y} = 1.5 \text{ layer } 1
                                        22.78 cm column 5 coff
 6 \times = 33.0 \text{ y} = 1.5 \text{ layer } 1
                                        22.39 cm column 6 coff
                                                                           0.25
 7 \times 37.5 \text{ y=1.75 layer 1}
                                       22.08 cm column 7 coff -0.25
 8 \times 49.5 \text{ y} = 1.5 \text{ layer } 1
                                      22.99 cm column 9 coff
 9 \times = 55.5 \text{ y} = 1.5 \text{ layer } 1
                                        23.01 cm column 10 coff 0
 Flow Observation 95% confidence +/-5%
   Outflow from river = 7.0cm<sup>3</sup>/sec
```

add to name file: data 22 ep._os

hob package

```
1.0
H1 -2 2 1 1 1 0.0 0.0 23.01
H2 1 2 2 1 1 0.0 0.0 23.01
H3 1 2 3 1 1 0.0 0.0 23.01
H4 2 2 4 1 1 0.0 0.0 23.01
H5 1 2 5 1 1 0.0 0.0 23.01
H6 1 2 6 1 1 0.0 0.2 22.39
H7 1 2 7 1 1 -0.25 0.0 22.08
H8 1 2 9 1 1 0.0 0.0 22.99
H9 1 2 10 1 1 0.0 0.0 23.00
```

rvob package

т	3	Τ,	(22)	
1.	. 0		$\overline{}$	
1	-:	3		
Q1	L :	L 1	L.0	-7.0
1	1	8	1.0	
1	2	8	1.0	
1	3	8	1.0	

RUN MODFLOW AND OBSERVE _os file

OBSERVATION_GROUPS BLOCK Chapter 8 (p81)

Follow tutorial/see Ucode_main.in

DECTN	OBSERVATION GROUPS
	_
grou	ıpname=Heads
plot	symbol=1
grou	upname=RIV_flows
plot	symbol=2
END OF	SSERVATION_GROUPS

Use groups to define common characteristics

We could extract some values but not "use" them as simulated equivalents, rather we might calculate simulated equivalents with those values

Notice other possible input items

Chapter ¹	Purpose	Blocklabel	Default col- umn order ²
		Options	No
		Merge Files ³	No
46	Define UCODE_2005	UCODE_Control_Data3	No
0	operation	Reg_GN_Controls ³	No
		Reg_GN_NonLinInt ^{3,4}	No
		Model_Command_Lines	No
		Parameter_Groups ³	No
7	Define parameters	Parameter_Data ³	Yes
,	Define parameters	Parameter_Values ³	Yes
		Derived_Parameters ³	Yes
	<	Observation Groups	No
	Define observations	Observation_Data ⁵	Yes
8	One or	Derived_Observations	Yes
0	the other	Prediction_Groups	No
	Define predictions	Prediction _Data ⁶	Yes
		Derived_Predictions	Yes
9	Define prior information	Prior_Information_Groups	No
,	Define prior information	Linear_Prior_Information	Yes
	Define variance-covariance		
	matrices to weight groups		
10	of observations or prior	Matrix_Files	No
	information with correlated		
	errors.	_	
11	Interact with process-model	Model_Input_Files	Yes
11	input and output files.	Model_Output_Files	Yes
12	Run process model(s) using	Parallel_Control	No
12	multiple processors	Parallel_Runners	Yes

Follow tutorial/see Ucode_main.in

OBSERVATION_DATA BLOCK - Chapter 8 (p83)

BEGIN OF	SERVATION	_DATA TABLE		
NROW=10	NCOL=5	COLUMNLABEL	S	
obsname	obsvalue	statistic	statflag	groupname
h1	23.01	0.0025	var	heads
h2	23.00	0.0025	var	heads
h3	23.01	0.0025	var	heads
h4	23.00	0.0025	var	heads
h5	22.78	0.0025	var	heads
h6	22.39	0.0025	var	heads
h7	22.08	0.0025	var	heads
h8	22.99	0.0025	var	heads
h9	23.00	0.0025	var	heads
Q1	-7.0	0.05	cv	RIV_flows
END OBSE	ERVATION_D	ATA TABLE		



Follow tutorial/see Ucode_main.in

MODEL_INPUT_FILES BLOCK - Chapter 11 (p108)

BEGIN MODEL_INPUT_FILES
MODINFILE=ep.pval TEMPLATEFILE=ep_pval.jtf
END MODEL_INPUT_FILES

Any file names are OK

I use jtf or tpl to help myself identify files

The modinfile must be what the process model expects to use

Template files start with jtf and a symbol. They are copies of process model input files with values where estimated parameters should go replaced by parameter names from the PARAMETER_DATA block bounded by the symbol. Leave room for lots of significant figures

Chapter ¹	Purpose	Blocklabel	Default col- umn order
		Options	No
		Merge Files ³	No
46	Define UCODE_2005	UCODE Control Data ²	No
.0	operation	Reg GN Controls	No
		Reg GN NonLinInt ^{3,4}	No
		Model Command Lines	No
		Parameter_Groups	No
		Parameter Data	Yes
7	Define parameters	Parameter Values ³	Yes
		Derived Parameters ³	Yes
8	Define observations	Observation Groups	No
		Observation Data	Yes
		Derived Observations	Yes
		Prediction_Groups	No
	Define predictions	Prediction Data	Yes
	Decar section (4)	Derived_Predictions	Yes
9	Define prior information	Prior_Information_Groups	No
2	Deime price micensagon	Linear_Prior_Information	Yes
10	Define variance-covariance matrices to weight groups of observations or prior information with correlated errors.	Matrix_Files	No
11	Interact with process-mode		Yes
	input and output files.	Model_Output_Files	Yes
12	Run process model(s) using	Parallel_Control	No
***	multiple processors	Parallel_Runners	Yes

Follow tutorial/see ep_pval.jtp

Make your template files - Chapter 11 (p109)

Template files start with jtf and a symbol. They are copies of process model input files with values where estimated parameters should go replaced by parameter names from the PARAMETER_DATA block bounded by the symbol.

Leave room for lots of significant figures

It is convenient to use the pval file because all of the parameters we might want to estimate are there.

<u>pval</u> package 8	jtf @ 8	
K1 0.01	K1 @K1	@
K2 10.0 KVA 1.0	K2 @K2 KVA @KVA	@
KVCB 1E-5	KVCB @KVCB	@
rch1 0.1 rch2 0.05	rch1 @rch1 rch2 @rch2	@
rch3 0.01	rch3 @rch3	@
Kriv 1e-3	Kriv @Kriv	@

Follow tutorial/see Ucode main.in MODEL_OUTPUT_FILES BLOCK - Chapter 11 (p111) Blocklabel Chapter Purpose Options Merge_Files³ UCODE_Control_Data³ Reg_GN_Controls³ Reg_GN_NonLinlnt³ Model_Command_Lines Define UCODE_2005 BEGIN MODEL_OUTPUT_FILES MODOUTFILE=ep._os INSTRUCTIONFILE=ep._os.jif Parameter Groups Parameter Data¹ Parameter Values Yes Yes Define parameters category=obs END MODEL_OUTPUT_FILES Derived_Parameters Observation_Data Define observations Yes Prediction Data Prediction Data Any file names are OK Define predictions Yes The modoutfile must be what the file the Prior_Information_Groups Linear_Prior_Information Define prior information No Yes process model produces with the results you Define variance-covariance matrices to weight groups of observations or prior information with correlated want to extract No 11 input and output files. Model Output Files Run process model(s) using Parallel_Control multiple processors Parallel_Runners

Follow tutorial/see ep._os.jif

INSTRUCTION FILE - Chapter 11 (p 113 115)

The way we have MODFLOW set up now we can use a standard instruction file. Far more complicated extractions can be made.

```
StandardFile 1 1 10
H1
н2
нз
н4
н5
Н6
н7
н8
н9
01
```

There is great flexibility to address most any situation you encounter. Chapter 11 has much detail on this.

Batch file to run UCODE EXECUTE UCODE in a FORWARD RUN

Follow tutorial/see RunUcode epMM.bat

Path-to-ucode-executable ucode-input-file root-calib-output root-pred-output

See UCODE Manual Chapter 4 (p29) for executing UCODE & associated codes

See and _files

What new files were created? Ucode_main_out.#uout Drag them into the text editor Read through their contents

VERY IMPORTANT USE YOUR COMMON SENSE

Have expectations for the results, question all aspects of the situation when calculations do not match expectations

Fix Problems

If you do not have a pause in the batch file. you may be confused about what might have gone wrong Go to the command window

Type "cd" space and drag the model folder in, enter Now drag the batch file in, enter Note what is on the screen for clues to any problems

REMEMBER

- When you run a code, you should <u>expect that there will</u> <u>be errors</u> and be pleasantly surprised if there are not. When you see an error:
- 1) look closely at the error message, try to understand it, use any clue that may be provided (paths, directories, file names, numbers) to explore it
- 2) check the directory to see what files were created and view their contents, look at the dates and times on files to determine what was created recently
- 3) delete outputs and try it again and look at the new outputs
- 4) as Winston Churchill once said, "never, never, give up". If you do not find the error, keep thinking and experimenting to decipher the situation. Utilize "show me" skills.

Follow tutorial/see Ucode_main_out.#uout and _files

EVALUATING OUTPUT

Notice any errors in the command window and read the file to confirm everything is what you expected

The most common error is related to paths and file names Next common error is improper substitution or extraction

Check that the UCODE input items are echoed correctly.

View the output (see Chapters 14 and 16)

fn.#uout & DataExchange files: fn._*

Note GWChart works for ucode _ files

Follow tutorial and use GWChart

Follow tutorial and use GWChart

EVALUATING OUTPUT

fn.#uout includes statistics, top portion of Fit Statistics Table 28

These reflect model fit given the initial model configuration and starting values USE GWChart for convenient viewing of files

Exceptionally large discrepancies between simulated and observed values may indicate that there is a conceptual error either in the model configuration or in the calculation of the simulated values

Fixing these now can eliminate many hours of frustration.

Data exchange files include residual informations at starting values

Table 31

It is essential for UCODE to perform correctly in the forward mode. Proceeding with errors will result in an invalid regression and wasted time.

Resolve any problems and continue

Due this week:

UCODE files set up using modelmate for your project and preliminary analysis of output

Include the associated mtc file and the modflow files

Follow tutorial for sensitivity run / see ep_Ucode_main.in & Ucode_main_out.#uout

SENSITIVITY of the SIMULATED EQUIVALENTS to the PARAMETER VALUES

Sensitivities serve two functions:

indicators of

importance of the observations to the estimation of the different parameters

importance of each parameter to the simulated values

needed by the modified Gauss-Newton method to

determine parameter values that produce the best fit

The sensitivities are determined

[simulated(current b values)simulated(perturbed b values)]/ [(current b's) - (perturbed b's)]

i.e.

simulated(b_o)- simulated(b') b_o- b'

They form a 2D array (ND,NP) i.e.

(#observations × #parameters)

Notation:

1D array, single underscore 2D array, double underscore

Follow tutorial for sensitivity run / see Ucode_main.in & Ucode_main_out.#uout

Evaluate SENSITIVITY of the SIMULATED EQUIVALENTS to the PARAMETER VALUES

 Δ SimulatedEquivalent/ Δ ParameterValue

with perturbation sensitivities

ucode1

UCODE_Control_Data Block (p55)
sensitivities = yes

Choose printing options or default

Notice other possible input items

Chapter ¹	Purpose	Blocklabel	Default col- umn order ²
		Options	No
		Merge Files ³	No
46	Define UCODE_2005	UCODE_Control Data ³	No
ľ	operation	Reg_GN_Controls ³	No
		Reg_GN_NonLinInt ^{3,4}	No
		Model_Command_Lines	No
		Parameter_Groups ³	No
7	D-f	Parameter_Data ³	Yes
'	Define parameters	Parameter_Values ³	Yes
		Derived_Parameters ³	Yes
		Observation_Groups	No
	Define observations	Observation Data	Yes
8		Derived Observations	Yes
δ		Prediction_Groups	No
	Define predictions	Prediction _Data ^b	Yes
		Derived_Predictions	Yes
9	Define prior information	Prior_Information_Groups	No
9	Deime phoi information	Linear_Prior_Information	Yes
	Define variance-covariance		
	matrices to weight groups		
10	of observations or prior	Matrix_Files	No
	information with correlated		
	errors.	_	
11	Interact with process-model	Model_Input_Files	Yes
- 11	input and output files.	Model_Output_Files	Yes
12	Run process model(s) using		No
12	multiple processors	Parallel_Runners	Yes

Follow tutorial for sensitivity run / see Ucode_main.in & Ucode_main_out.#uout

EXECUTE UCODE in the SENSITIVITY MODE

Look for the differences in the #uout file What are the sensitivities?

Are there some parameters that will be difficult to estimate?

Dimensionless scaled sensitivity - 1 for each obs and parameter

dss = unscaledsens * (PARAMETER_VALUE * (wt**.5))

Composite Scaled Sensitivities - 1 for each parameter.

Composite Scaled Sensitivities - 1 for each parameter css = ((SUM OF THE SQUARED DSS) / ND)**.5

Generally should be >1 AND

within ~ 2 orders of magnitude of the most sensitive parameter

Notice statistics are calculated for the starting parameter values as if they were optimal his can be useful if you want to regenerate the statistics for

This can be useful if you want to regenerate the statistics for an optimal parameter set

Follow tutorial for sensitivity run / see Ucode_main.in & Ucode_main_out.#uout

See "Perturbation Sensitivities" starting on p15 Accuracy of Sensitivities Depends on:

number of accurate significant figures in extracted simulated values (print many significant figures and extract them all)

magnitude of the simulated values

magnitude of the substituted parameter values

size of the parameter perturbations, for nonlinear parameters

What if Sensitivities are zero?

If more than a few sensitivities equal zero, it may indicate extracted perturbed & unperturbed values are identical (given the significant figures) or perhaps the model did not execute

See "What to Do When Sensitivities Equal Zero" (p37) of the UCODE manual.

If sensitivities are zero for a Parameter:

If many other sensitivities are nonzero, observation is not very important, NO corrective action needed

If all sensitivities are zero, corrective action is needed (if there is a hydraulic reason for lack of sensitivity, do not estimate the parameter)

If many sensitivities are zero, corrective action MAY OR MAY NOT be needed

What if Sensitivities are zero?

Five possible corrective actions:

- 1) smaller solver convergence criteria can be specified in the application codes;
- 2) the extracted values can be printed with more significant figures in the application model output file if the values are calculated with sufficient accuracy;
- 3) the datum of the problem can be changed or a normalization can be applied;
 4) the perturbation for the parameter can be changed; too small perturbations may result in negligible differences in extracted values, or differences that are obscured by round-off error; too large may yield inaccurate sensitivities for nonlinear parameters
- 5) the methods for coping with insensitive parameters discussed later can be employed.
- Reconsider the model construction
- Modify the defined parameters
- Eliminate observations or prior information, if biased
- Adjust weights either for groups of, or individual, observations

Sensitivities calculated for the values of the parameters just prior to failure can be investigated by substituting these parameter values as starting values in the prepare file and executing UCODE with sensitivities=yes, optimize=no. (add SenMethod=2 to also evaluate correlation)

Sensitivities for all intermediate sets of parameter values can be investigated by setting IntermedPrint=sensitivities in the input file and executing UCODE again with optimize=yes.

Follow tutorial for parameter estimation run/see Ucode_main.in & Ucode_main_out.#uout

Estimate Optimal Parameter Values & Associated Uncertainty

UCODE_Control_Data Block (p55)

optimize = yes

EXECUTE UCODE in the OPTIMIZE MODE

Have a look at the output to see the troubles

This is what you will need to do to get your projects going in the future at work

The regression control defaults work OK in this case In other cases use a Reg_GN_Controls Block (p60)

To override defaults, most commonly

BEGIN REG_GN_CONTROLS KEYWORDS tolpar=0.01 maxiter=10 maxchange=2.0 stats_on_nonconverge=yes END REG_GN_CONTROLS

Notice other possible input items

EVALUATING PARAMETER ESTIMATION OUTPUT

View fn.#uout

Consider Progress of the Regression Table 29 (p 178)
Parameter Statistics Table 30 (p179)

Follow tutorial for parameter estimation run/see Ucode_main.in & Ucode_main_out.#uout

Read through the resulting files

VERY IMPORTANT: USE YOUR COMMON SENSE

Most common trouble is lack of convergence, or progress toward it. Consider how to tackle that.

<u>Have expectations</u> for the results, question all aspects of the situation when calculations do not match expectations

Fix Problems

Evaluate Results

What do you make of the estimated parameter values?

What of the confidence intervals?

EVALUATING PARAMETER ESTIMATION OUTPUT

OVERALL FIT, SUM OF SQUARED ERRORS

$$S(\underline{b}) = \sum_{i=1}^{ND} \omega_i \left[y_i - y_i'(\underline{b}) \right]^2$$

CALCULATED ERROR VARIANCE (cev)

$$cev = s^2 = \frac{S(b)}{ND - NP}$$

STANDARD ERROR sqrt(cev)

$$s = \sqrt{s^2}$$

Model Selection Criteria

MLOF / AIC / AICc / BIC / KIC

The regression is not extremely sensitive to the weights, thus the casual approach to their definition is not a problem

The weighting can be evaluated at the end of the regression by considering the cev (calculated error variance)

smaller values of s 2 and s indicate a better fit

values close to 1.0 indicate the fit is consistent with the data accuracy as described by the weighting

cev > 1 (eg 95% confidence intervals on cev completely above 1) indicates the modeler globally underestimated the variances (i.e. the model does not fit the observations as well as the variances assigned by the modeler would reflect)

cev < 1 (eg 95% confidence intervals on cev completely below 1) indicates the modeler globally overestimated the variances (i.e. the model fits better than expected)

The 95% confidence intervals on cev are calculated using the ChiSq distribution. Deviations from 1.0 are significant if 1.0 falls outside of the confidence limits.

The modeler could adjust weights to obtain 1, but it is not necessary as long as the cev is discussed along with the input variances

CONSIDER HOW THE PARAMETER UNCERTAINTY IS CALCULATED

Variance Optimal Parameters:

$$V(b) = \frac{\text{Sum of Squared Weighted Residuals}}{\text{\#Observations - \#Parameters}} \left[\underline{X}^T \underline{w} \underline{X} \right]^{-1}$$

$$V(b) = \text{cev } \left[\underline{X}^T \underline{w} \underline{X} \right]^{-1}$$

vector of optimal parameters (e.g. K,S,R,H,Q)
 sensitivity matrix
 w weight matrix for observations

Results in NPxNP matrix, with variances on the diagonal

$$V(\underline{b}) = \text{cev} \left[\underline{X}^T \underline{w} \underline{X} \right]^{-1} = V(\underline{b}) = \begin{pmatrix} var1 & cov12 & cov13 \\ cov21 & var2 & cov23 \\ cov31 & cov32 & var3 \end{pmatrix}$$

 $[NP \times NP] = constant [NP \times ND] [ND \times ND] [ND \times NP]$

e.g. If NP=3 and ND=12 then V(b) is a 3x3:



VARIANCE (K)

$$VAR(K) = \underbrace{\left(\underline{X}^{T} \underline{\omega} \underline{X}\right)^{-1}}_{L,1} (EVAR)$$

Std Dev = \sqrt{VAR} (K) 95 % Confid = K + /-2*StdDev

VARIANCE (H)

$$VAR(H) = \underbrace{\left(\underline{X}^{T} \underbrace{\omega X}\right)^{-1}}_{==24,4} (EVAR)$$

Std Dev = \sqrt{VAR} (H) 95 % Confid = H + /-2*StdDev

CORRELATION (normalized variance)

$$CORR(i, j) = \frac{COV(i, j)}{\sqrt{VAR(i)} * \sqrt{VAR(j)}}$$

$$j=1$$
 • $j=NP$
 $i=1$
[1,1 1,2 • 1, NP
2,1 2,2 • •
 $i=NP$
 $NP,1$ 4,2 $NP,3$ NP,NP

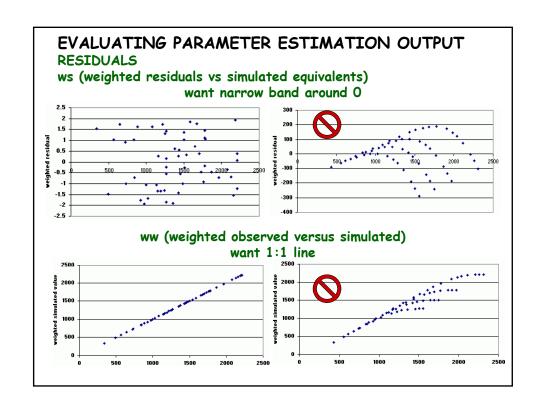
Follow tutorial for parameter estimation run/see Ucode_main.in Ucode_main_out.#uout and _files

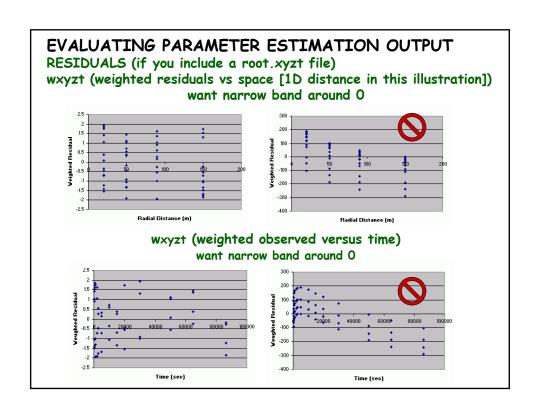
As before view residual statistics / sensitivities

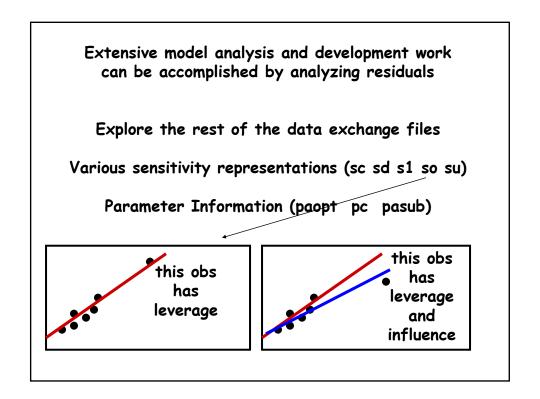
Using GWChart also

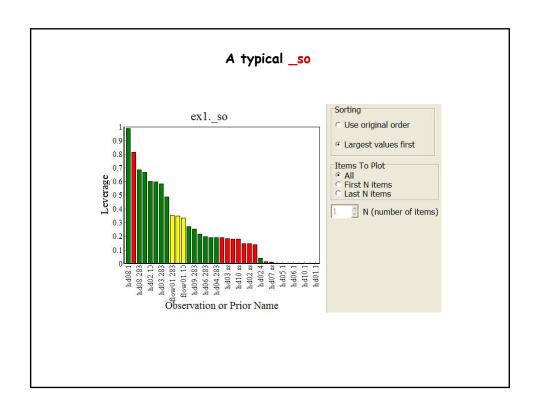
See previous items and more from

Tables 28 (p 176) and 31 (p 180)









If the PARAMETER ESTIMATION is successful:

Further EVALUATE RESULTS

with UCODE's Residual_Analysis (p159 and on)

It only needs the data exchange files, but there is optional input described in the ucode manual

Create batch file for residual_analysis OR run in ModelMate

Additional Residual Analyses can be obtained running

residual_analysis.exe >>> fn.#resan

VIEW RESULTS WITH GW_CHART

_nm - want normally distributed residuals

If not a straight line compare to realizations of residuals:

Uncorrelated _rd - if these look like your nonlinear nm plot

the cause is too few residuals

Correlated _rg - if these look like your nonlinear nm plot it is OK, due to correlation in the regression

ALSO see rdady of residual_analysis_adv.exe on next slide

Create a batch file to run residual analysis adv or run in ModelMate

View _rdadv in GW_Chart

to see the theoretical confidence limits on the weighted residuals

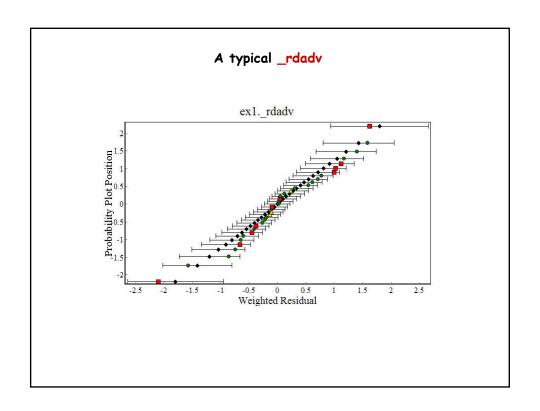
#resanady

Mean Weighted Residual should be ~ 0 Slope should be ~ 0

INTRINSIC NONLINEARITY << Sum of Squared Residuals

If large Corfac_plus correction factors may not be accurate

CED correlation of weighted residuals and means of synthetic residuals PROB - probability that a correlation would be <= CED if the residuals were normally distributed



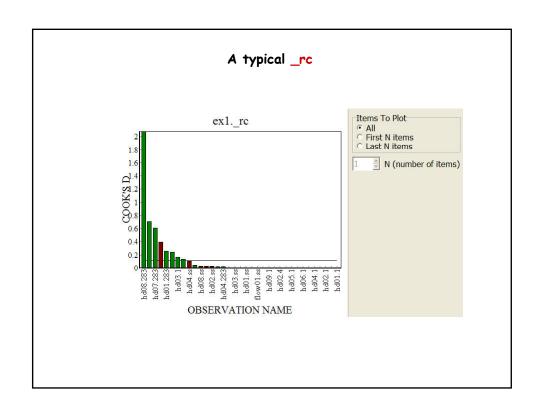
Back to:

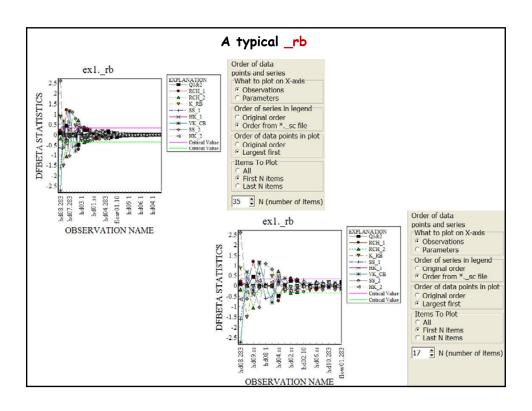
EVALUATING PARAMETER ESTIMATION OUTPUT from Residual_analysis fn.#resan _rc _rb

Cook'sD large values indicate observations that most influence all estimated parameter values

DFBetaS large values indicate observations important to individual parameters

Do you understand why the flow observation is so important? What would you be able to say about the parameter values without that observation?





Туріс	al #resan results
******	**********
ANALYSIS OF COOKS D	
FOR PLOTTING, COOKS D STATISTICS ARE LISTED IN THE _RC	OUTPUT FILE
INFLUENTIAL OBSERVATIONS WITH COOKS D > CRITICAL VALUE	(4/(NOBS+MPR)) = 0.114
OBS# OBSERVATION PLOT-SYMBOL COOK'S D	
3 hd01.283 2 0.19920774E+00	
- 10 hd03.1 2 0.16229212E+00	
11 hd03.283	
23 hd07.283 2 0.69218923E+00	
25 hd08.1 0.77273656E+00	
26 hd08.283 0.19342235E+01	
27 hd09.ss 0.41209141E+00	
29 hd09.283 2 0.15028790E+00	***************************************
NUMBER OF INFLUENTIAL OBSERVATIONS IDENTIFIED:8	ANALYSIS USING DFBETAS
	FOR PLOTTING, DFBETA STATISTICS ARE LISTED IN THE _RB OUTPUT FILE
	PARAMETER NUMBERS AND NAMES:
	Q162 RCH 1 RCH 2 K RB SS 1
	6
	HK_1 VK_CB SS_2 HK_2
	INFLUENTIAL OBSERVATIONS WITH DFBETA >
	CRITICAL VALUE (2/(NOBS+MPR)**0.5) = 0.
	PARAMETERS INFLUENCED IDENTIFIED BY #
	PARAMETER NUMBER
	OBS# ID PLOT-SYMBOL 1 2 3 4 5 6 7 8 9
	3 hd01.283
	4 hd02.ss 1 - # #
	10 hd03.1 2 #
	11 hd03.283 2 # # - # # -
	12 hd04.ss 1 # # # # #
	23 hd07.283 2 # # - # # -
	25 hd08.1 2
	26 hd08.283 2 # # - # # #
	27 hd09.ss 1 # # # # #
	NUMBER OF INFLUENTIAL OBSERVATIONS IDENTIFIED: 9

EVALUATING PARAMETERIZATION

High parameter correlations calls for either Additional data that will break the correlations

Or

Reparameterization

Barring the availability of additional data, consider reparameterization e.g. USING DERIVED_PARAMETERS Block
As an example you could define rch2=0.5*rch1 and rch3=0.1*rch1

However, notice that the true values do not have those ratios

To evaluate if correlations are too high try starting from different values USE PARAMETER_VALUES Block

If results are the same (parameter values fall within one standard deviation of those determined with different starting values) correlation is not an issue

Thus parameters are being independently estimated