MIKE SHE PP – User Manual

Calibration Statistics Utility

CONTENTS

1 GENERAL DESCRIPTION

The calibration statistic utility is a tool tailored to produce performance statistics (goodness or fit) for a MIKE SHE simulation.

The main purpose is to calculate statistics on the residuals between observed and simulated data. The current version enables the user to compare observed and simulated groundwater heads.

The present utility is developed under the project "Developing a Small Scale Integrated Surface Water and Groundwater Model for the South Florida Hydrogeologic System". The calibration utility was developed based on SFWMD traditions when calibrating a MODFLOW ground water model.

The main input is time-series files (T0-files) of observed groundwater heads. These files must include information on the location for the observation. A simulation result file including results from the saturated zone is required too.

The main output is statistical measures for each observation location and statistics on the number of locations to fulfil a number of criteria. Output can optionally be chosen as table, scattered data (.dig) or a plot macro (.plt).

2 TECHNICAL DOCUMENTATION

The calibration utility calculates the following basic statistical measures. Symbols and notations can be found in the list in the end of this section:

The residual or difference between observed and simulated values for each observation

$$RES_{i,j} = \left(H_{OBS,i,j} - H_{SIM,i,j}\right)$$

For each location (time series) the average residual and the average of the absolute residuals

$$\overline{RES_j} = \frac{\sum RES_{i,j}}{n}$$

$$\left|\overline{RES_j}\right| = \frac{\sum \left|RES_{i,j}\right|}{n}$$

Root mean square of the residuals

$$RMS_j = \frac{\sqrt{\sum RES_{i,j}^{\ 2}}}{n}$$

Standard deviation on the residuals and on the observed data

$$STD_j = \sqrt{\frac{\sum \left(RES_{i,j} - \overline{RES_j}\right)^2}{n}}$$

$$STD_{OBS,j} = \sqrt{\frac{\sum \left(H_{OBS,i,j} - \overline{H_{OBS,j}}\right)^2}{n}}$$

The Nash-Sutcliffe coefficient is calculated as

$$R5_j = \frac{\sum \left(H_{OBS,i,j} - H_{SIM,i,j}\right)^2}{\sum \left(H_{OBS,i,j} - \overline{H_{OBS,j}}\right)^2}$$

These statistical measures are checked against different criteria. Four criteria have been implemented:

The R1 criterion ensures that the difference between residuals and the standard deviation on the residuals is kept within limits relative to the range of observed values. T_{R1} determines the acceptable range of deviation.

$$R1: \left|\left|RES_{i,j}\right| - STD_j\right| < T_{R1}\left(H_{OBS,\max,j} - H_{OBS,\min,j}\right)$$

The R2 criterion ensures that the acceptable difference between observed and simulated values is less than the standard deviation of observations.

$$R2: H_{OBS,i,j} - STD_{OBS,j} < H_{SIM,i,j} < H_{OBS,i,j} + STD_{OBS,j}$$

The R3 criterion is applied to avoid that simulated values drop below observed minimum or exceed maximum values.

$$R3: H_{OBS,\min,j} < H_{SIM,i,j} < H_{OBS,\max,j}$$

The R4 criterion provides an absolute measure of the maximum allowable difference between observed and simulated values. The allowable difference, T_{R4}, is specified in meters.

$$R4: H_{OBS,i,j} - T_{R4} < H_{SIM,i,j} < H_{OBS,i,j} + T_{R4}$$

The R1-R4 criteria are checked at discrete observations within the simulation period. Often field observations and simulation results are not available at exactly the same time and normally simulation results are stored with a higher frequency. Simulated values are interpolated (linear) in time to calculate the residuals for a specific observation.

At each well location percentage of residuals to fulfil the four criteria is calculated. These percentages are checked against specified global fit criteria to determine the number of observed time series that satisfies it. Statistics on the number of observation time series satisfying the global fit criteria are determined (P_{R1-R4}).

Definitions	***Description***	***Unit***
i	Index for time	
j	Index for location	
$H_{OBS,i,j}$	Observed value at time i at location j	m
$H_{SIM,i,j}$	Simulated value at time i at location j	m
$RES_{i,j}$	Difference between observed and simulated values	m
$\| RES_{i,j} \|$	Absolute difference between observed and simulated values	m
n	Number of observations at one location	
N	Number of observation locations	
STD_j	Standard deviation of $RES_{i,j}$	m
$STD_{obs,j}$	Standard deviation of $H_{obs,i,j}$ at location j	m
RMS_j	Root mean square of $RES_{i,j}$	m
$H_{obs,max,j}$	Maximum value of $H_{obs,i,j}$ at location j	m
$H_{obs,min,j}$	Minimum value of $H_{obs,i,j}$ at location j	m
R1, R2, R3, R4	Numerical criteria for goodness of fit	
R5	Nash-Sutcliffe coefficient	
T_{R1}, T_{R4}	Tolerance constants used for criteria R1 and R4	frac., m
P_{R1}, P_{R2}, P_{R3}, P_{R4}	Percentage of observation where R1-R4 is meet.	%
C_{R1}, C_{R2}, C_{R3}, C_{R4}	Success criteria for percentages P_{R1}-P_{R4}	frac.

Figure 1 Definitions.

3 USER'S GUIDE

3.1 General

In every project the calibration and verification procedures are crucial to the accuracy and reliability of the model results. The results of the calibration should be evaluated both qualitatively (visual comparison) and quantitatively (mathematically). In the beginning of a modelling study, before any modelling is done, it is useful and sound to assess the precision required by the model and to formulate calibration targets on that basis. Calibration targets can seldom be considered strict success criteria, but they should serve a quality measure. In most model calibrations some observations will not meet the targets. This is not necessary because the mathematical model is wrong. It is however the modeller's responsibility to identify a justified explanation of the problem and to suggest means to overcome the problem and to assess the importance of this on the overall model performances. The reason may be, for instance, errors in field data used for calibration or perhaps small scale features that are not accounted for by the model.

A programme for calculating statistical measures is provided – and the use of it is described in the following. The utility is aimed for projects where time-series of observed potential head constitutes a major calibration reference. As described in the technical documentation the goodness of fit of simulated potential heads are checked for a number of criteria. The criteria provides help when considering the dynamics of the ground water table with respect to both correct mean level and short and long term temporal variations.

In order to run the calibration statistics programme – the menu U.10 (Calibration Statistics) must be accessed, see Figure 2. It is a sub-menu to the general utility menu (menu U) – accessible from the main menu.

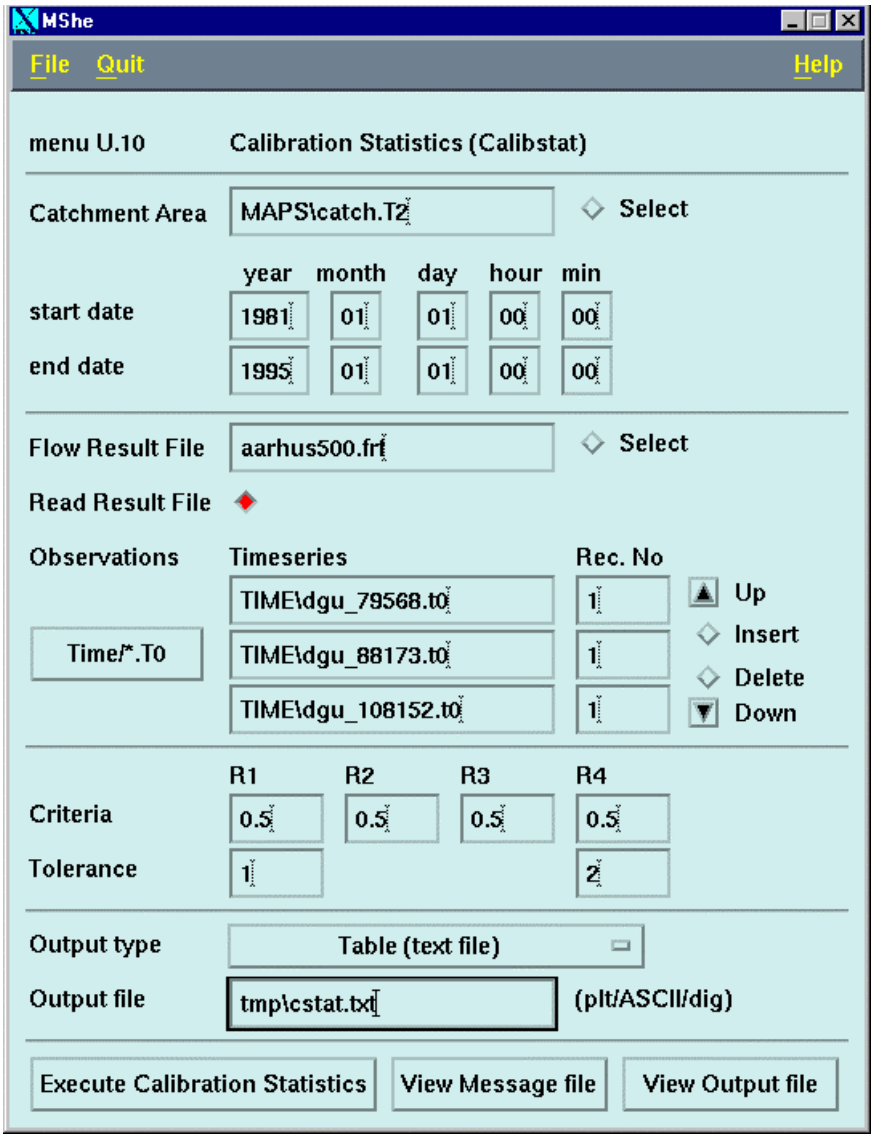


Figure 2 Menu U.10 Calibration Statistics Utility.

3.2 Input

The basic input observed and simulated groundwater levels. Observed head must be specified in time-series files (T0-files) and simulated heads are extracted from a simulation result file. Including the information on the position of the individual observation locations together with the observed time-series (time-series files type 3, see PP Manual) enables the programme determine the corresponding location in the model – thereby making comparison with simulated heads possible.

Catchment area (T2-file)
Specify a T2 file delineating the area of interest. Calculations are performed for observation wells placed within the area. Grids included in the area should have a integer code 1 and boundary grids should have a integer code 2 - i.e. if the whole model area is of interest the catchment grid code file can be specified.

'Select' gives the opportunity to import a file from a list of files in the maps-directory. Use the file-selection box to browse to other directories if needed.

Start and end date
Specify here start and end date within which comparison between observed and simulated groundwater levels should be performed. The period must be within the simulation period – i.e. the start date should be equal or later than simulation start date and the end date must be equal to or earlier than the simulation end date.

Flow Result File (frf-file)
Specify here the name of the flow result file. The flow-simulation must include storing of the potential head in the saturated zone (datatype 15).

'Select' gives the opportunity to choose a flow result file from a list of files in the res-directory. You can only select files within the res-directory – even though using the file-selection box to browse to other directories seems to work – the calculation of the calibration statistics will not work.

Read Result File
Activating 'Read Result File' will result in retrieving simulated potential head for grid cells corresponding to where observations are measured. Retrieved data is placed in the tmp-directory.

There will be placed one file for each observation location in the tmp-directory containing the simulated time-series of the potential head. The names of these files will use the syntax – Hi_j_k.T0. Where i,j,k refers to the calculation cell in the saturated zone corresponding to the location of the observation well.

Retrieving data can be time consuming, and if different output type is chosen just after one another retrieving are only needed the first time. Without 'Read Result File' switched on information in the tmp-directory is used.

Observation time-series and record no
Specify here filenames of the time-series of observed groundwater levels. Indicate by the record number what time-series in the file to

use. If one file contains several time-series the file name must be repeated for each record to be used.

Only three time-series are visible – but many more can be used in the calculation of statistics. Use the 'Up' and 'Down' buttons to browse the list of specified time-series. Use the 'Insert' and 'Delete' buttons to make changes in the list. For adding time-series to the end of the list it is not necessary to use the 'Insert' – simply specify the new time-series in the empty field at the end of the list.

Time-series file names can either be typed – using a path relative to the application directory- or be selected using the 'TIME/*.T0' button. A file-selection box will be evoked by default showing the content of the time-directory. Selecting a T0-file and pressing OK will close the file-selection box and store the filename in a buffer. Point to the field where you want the filename to be pasted and press the mouse-select button.

R1, R2, R3, R4 criteria and tolerance

The criterion is the fraction of observations in one time-series that must satisfy the different formula (R1-R4). The observations within the specified period are checked against the R1-R4 measures and the percentage of observation to fulfil the measures is calculated for each well. These percentages are then checked against the criteria to summarise the number of observation wells where the criteria are meet.

The formulations of the different measures can be found in the technical documentation section.

For the R1-criterion a tolerance constant must be specified – it is merely a multiplication number used to multiply on the difference between the maximum and the minimum head observation.

For the R4-criterion a tolerance constant must be specified. The values is used directly in the R4-measure as an absolute measure of the maximum allowable difference between observed and simulated values. Unit of the tolerance is [m].

Output type
Select here the desired output type.

Table gives a text file containing calculated criteria for each observation well. Results about R1-R4 are listed along with data of the residuals and R5 (Nash-Sutcliffe coefficient).

The different calculated data can be stored in dig files. These files contain the x and y location of the observation wells and the calculated statistical data for each well.

An option for generating a plot-macro for the graphical presentation programme is also available. Due to limitations in the plot programme the number of time series should not exceed 50.

Output file
Enter here a file name of the output data file. For dig files and plot macros it is recommended to use suffixes .dig and .plt respectively to comply with other parts of the MIKE SHE system.

Execute Calibration Statistics
Press this button to make the calculation of the calibration statistics.

View Message file
Press this button to view the message file. The message file will contain error messages if any.

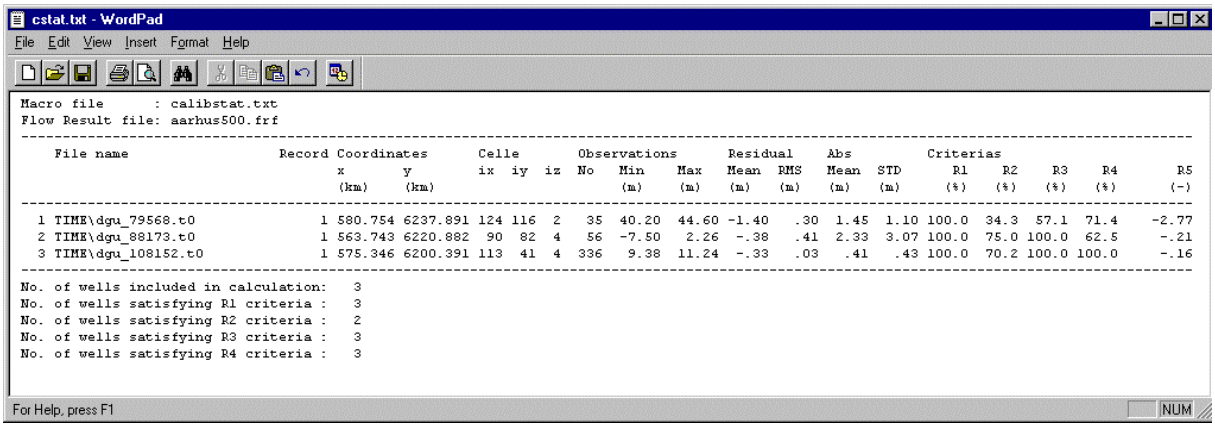
View Output file
Press this button to view the result file. This is most relevant is output type is chosen to 'Table'.

3.3 Output

Output in a table will result in generation of a text file. The file consists of header specifying information on which flow result file was used and some headlines. Then follows a line for each time-series specifying information about observation location and the statistical data about how well the simulation performs compared to the observations. The statistical data listed are number of observation, min. and max. observation, mean residual, RMS, STD and the percentages of observations fitted by simulated values in accordance with the R1-R4 measures and in the end is found the R5-value (Nash-Sutcliffe).

Finally statistics on how many wells fulfilled the different criteria is written. An example is found in Figure 3.

If the statistics are not calculated a message is found “No criteria calculated - check input data !”. Typically there are no observations inside the specified period.



cstat.txt - WordPad

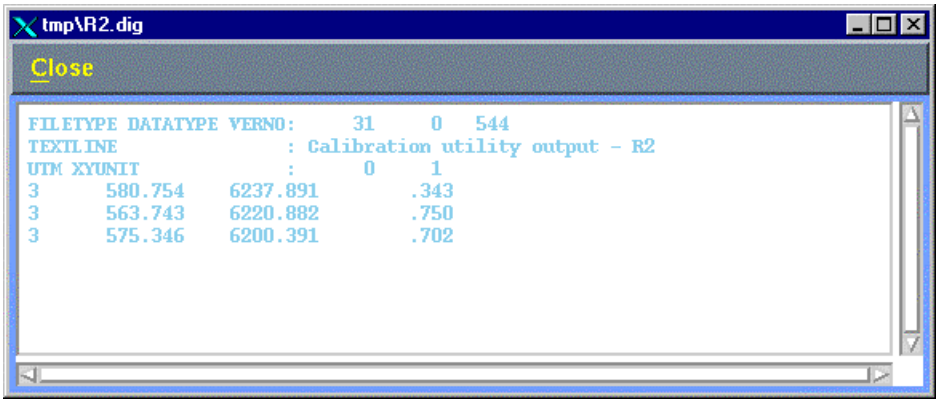
File Edit View Insert Format Help

```
Macro file      : calibstat.txt
Flow Result file: aarhus500.frf
-------------------------------------------------------------------------------------------------------------------------------
    File name                    Record Coordinates      Celle       Observations      Residual    Abs          Criterias
                                        x       y        ix  iy  iz  No   Min    Max   Mean  RMS   Mean  STD     R1    R2    R3    R4     R5
                                        (km)    (km)                     (m)    (m)   (m)   (m)   (m)   (m)     (%)   (%)   (%)   (%)    (-)
-------------------------------------------------------------------------------------------------------------------------------
  1 TIME\dgu_79568.t0              1 580.754 6237.891 124 116  2   35  40.20  44.60 -1.40   .30  1.45  1.10 100.0  34.3  57.1  71.4   -2.77
  2 TIME\dgu_88173.t0              1 563.743 6220.882  90  82  4   56  -7.50   2.26  -.38   .41  2.33  3.07 100.0  75.0 100.0  62.5    -.21
  3 TIME\dgu_108152.t0             1 575.346 6200.391 113  41  4  336   9.38  11.24  -.33   .03   .41   .43 100.0  70.2 100.0 100.0    -.16
-------------------------------------------------------------------------------------------------------------------------------
No. of wells included in calculation:   3
No. of wells satisfying R1 criteria :   3
No. of wells satisfying R2 criteria :   2
No. of wells satisfying R3 criteria :   3
No. of wells satisfying R4 criteria :   3
```

For Help, press F1 NUM

Figure 3 Example of table output.

A number of .dig files can be produced containing the location of the observation wells and a statistical number for each well. The selection can be made between 9 number – the percentage of observation to fulfilled by simulations according to R1, R2, R3, R4 criteria and residual mean and standard deviation of the residuals and root mean square of the residuals and the average of the absolute residuals and finally the Nash-Sutcliffe number.
The digfiles can be overlayed on a grid plot or imported to ArcView to assess the spatial distribution of the various calibration criteria.



tmp\R2.dig

Close

```
FILETYPE DATATYPE VERNO:     31     0   544
TEXTLINE                : Calibration utility output - R2
UTM XYUNIT              :      0     1
3       580.754    6237.891         .343
3       563.743    6220.882         .750
3       575.346    6200.391         .702
```

Figure 4 Example of .dig output.

The last output option is the generation of a plot macro, which can be used in the Graphical Presentation tool. The plot macro will be constructed by placing 6 figures on each page. Due to limitations in the plotting programme this option only allows up to 50 time-series. If the plotting is activated through the Graphical Presentation menu the number of time-series should be restricted to 15 only.

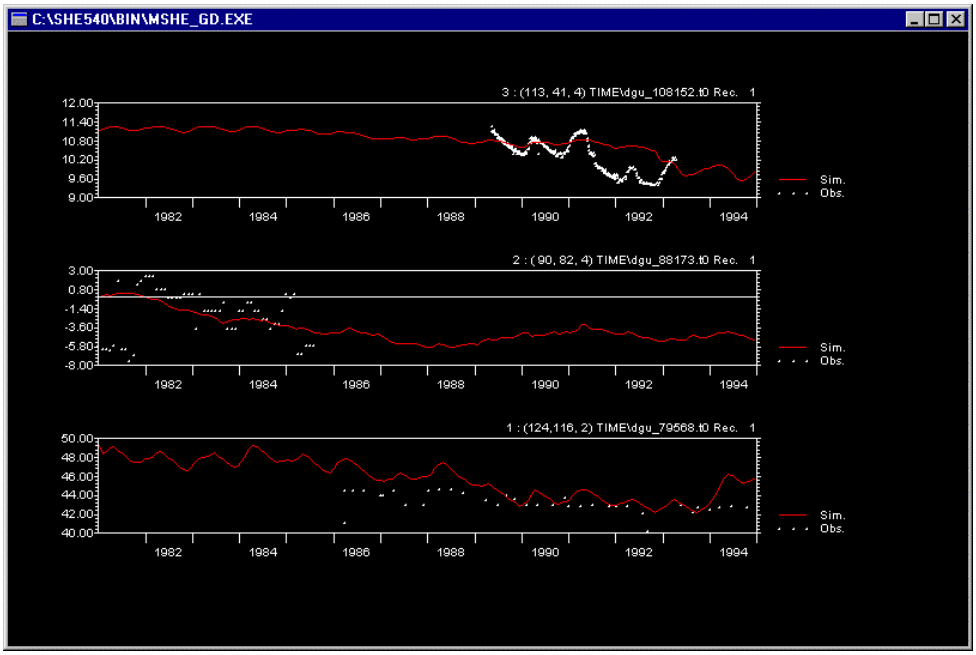


Figure 5 Plot made by using auto-generated the plot macro.