**Manual calibration tool (for Modflow models)**

1. **Get data from: HOB\_OUT**

* Search for the corresponding model calibration file 🡪 for MODFLOW the file is named name\_of\_model.HOB\_OUT
* Load the data so that you have a list with
  + Simulated values
  + Observed values
  + Observation well names
  + point arrays (simulated, observed, observation name)

*Structure of example HOB\_OUT data file*

"SIMULATED EQUIVALENT" "OBSERVED VALUE" "OBSERVATION NAME"

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-2.15291500092E+01 -1.93500003815E+01 Q\_63\_2

-2.13394184113E+01 -1.93299999237E+01 Q\_63\_3

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-2.06876773834E+01 -1.97399997711E+01 Q\_63\_12

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1. **Calculate statistics** 
   1. Number of data points n
   2. Maximum residual RMAX
   3. Minimum residual RMIN
   4. Residual mean RMEAN
   5. Absolute residual mean ∣RMEAN∣
   6. Standard error of the estimate SSE
      1. SSE =
   7. Root Mean Squared Error RMSE
   8. Normalized Root Mean Squared Error NRMSE
   9. Correlation Coefficient (Pearson`s R) R
      1. Simulated mean:
      2. Observed mean:
      3. Simulated standard deviation:
      4. Observed standard deviation:
      5. Covariance between calculated and observed:
   10. Coefficient of determination R²

* The received statistical parameters should be displayed next to or at least on the same page as the following graphs.

*For the example data you should get:*

|  |  |  |
| --- | --- | --- |
| Number of data points: |  | 288 |
| Maximum Absolute Residual | RMAX | 3.44 |
| Minimum Absolute Residual | RMIN | 0.01 |
| Residual Mean | RMEAN | -0.38 |
| Absolute residual Mean | IRMEANI | 1.05 |
| Standard error of estimation | SSE | 0.07 |
| Root Mean Squared Error | RMSE | 1.31 |
| Normalized Root Mean Squared Error | NRMSE | 0.05 |
| Correlation Coefficient Pearson R | R | 0.99 |
|  |  | -9.32 |
|  | -8.95 |
|  | 8.32 |
|  | 7.51 |
|  | 61.81 |
| Coefficient of determination | R² | 0.97 |

1. **Plot simulated vs. observed values**

* Plot simulated on y-axis, observed heads on x-axis
* Automatic scale for x- and y-axis
  + Calculate overall max, min of plotted values (x,y) and apply to both axis same max/min (maybe + threshold?)
* Plot every well with different colour
  + Well names defined in file “HOB\_OUT” , 3rd column “Observation Name”
* Include in plot: off/on for different wells
  + Well names defined in file “HOB\_OUT”, 3rd column “Observation Name”
* Include Line of equality (1:1)
* A feature which would be nice:
  + If you click on a specific data point, more information such as well name, stress period (time) and heads are shown
* *[include 95% confidence interval ?*
  + *🡪 95% confidence interval for observed mean*
  + *“Z is the value of standard normal variable that puts α/2 percent (here 2.5%) in each tail of the Student-t-distribution” 🡪 Z=1.96*
  + *Confidence interval for regression line 🡪 see file example calibration statistics]*

*Example Simulated vs. observed scatter graph:*

1. **Plot (weighted) residuals vs. simulated heads**

* Include in graph:
  + (weighted) residuals vs. simulated heads
  + Linear regression line with equation
  + Bold marked 0-line

🡪 Weighted residuals should be evenly distributed about zero for all weighted simulated values, and should display no trends with the weighted simulated values.

🡪 trends or unequal variances are indicators of model bias

*Example: residuals vs. simulated head (not weighted as only one kind of data is used for calibration)*

1. **Check for Normal Distribution**

* Rank residuals
* Calculate Normal Probability Function
  + - for *i* = 1, 2, ..., *n*, where
    - *a* = 3/8 if *n* ≤ 10 and
    - 0.5 for *n* > 10,
    - Φ−1 is the standard normal quantile function (PROBIT).
* Plot ranked residuals against NPF
* Calculate linear regression line and R²

🡪 Residuals should plot on straight line 🡪 normally distributed

*Example: Ranked residuals against normal probability*

1. **Time-series graph**

* Plot simulated, observed heads versus simulation time/stress periods
* Option to select/unselect wells

*Example Time-series graph:*

1. **ask user whether satisfied with calibration** 
   1. *Here we can give suggestions when calibration can be regarded satisfactory (define thresholds for statistical parameters??) but the final decision can only make the user*
   2. YES 🡪 model is calibrated
   3. NO 🡪 go back to soil model

***Some general aspects to consider for calibration:***

“It is the insight and skill of the investigator dur­ing a trial and error calibration that will control how well a model represents the ground-water system under investigation.

Questions to be addressed in evaluating the adequacy of calibration of a model using either trial and error or automatic methods are:

1. Is the conceptual model of the system under investigation reasonable?

2. Are the mathematical representations of the boundary conditions reasonable for the objectives of the study?

3. Does the simulated head and flow distribution mimic the important aspects of the flow system, such as magnitude and direction of the head contours?

4. Does some quantitative measure of head and flow differences between the simulated and observed values seem reasonable for the objectives of the investigation?

5. Does the distribution of areas where simulated heads are too high and areas where simulated heads are too low seem randomly distributed? If they are not randomly distributed, then is there a hydrogeologic justification to change the model and make the residuals more random areally?

Just because a model is constructed and calibrated, does not ensure that it is an accurate representation of the system. The appropriateness of the boundaries and the system concep­tualization is frequently more important than achieving the smallest differences between simulated and observed heads and flows.” (Reilly and Harbaugh, 2004)

* Include scaled sensitivities to identify what parameters and observations are important for model 🡪 dimensionless scaled sensitivities & parameter correlation coefficients
* Include confidence intervals for parameters