GEOS 5311 Lecture Notes: Model Calibration

Dr. T. Brikowski

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Why Calibrate?

- numerical model and field data are imperfect representations of the real world, e.g. well tests cannot sample the full range of heterogeneity
- the goal is to obtain a reasonably accurate representation that is at least internally consistent
- this is done by calibrating or adjusting the model until errors are minimized, as measured by qualitative or quantitative means
What is Calibration

- Model calibration is solution of an inverse problem
  - Forward problem: model parameters $\rightarrow$ model $\rightarrow$ prediction of data
  - Inverse problem: data $\rightarrow$ model $\rightarrow$ prediction of model parameters (AKA parameter estimation)
- Calibration: given observed data (usually head), adjust model parameters (usually $K$) until model reproduces observation "closely enough"
- Remember perfect accuracy is impossible, especially since some errors cannot be reduced in the model, e.g. measurement errors inherent in well test results
- see Hill and Tiedeman (2007) for entire textbook on this topic
Calibration Options

- Check model against analytic solution results (verification, only possible for extremely simple cases)
- Utilize global or local water mass balance within code (e.g. Modflow, Harbaugh et al., 2000) or add-ons (ZONEBUDGET, Harbaugh, 1990)
- Compare to observations (usually head or flux) and adjust parameters
  - Use visual error indicators (e.g. “calibration targets”, EMRL, 2003b)
  - Use sensitivities for guidance (e.g. Modflow Observation-Sensitivity Process, Hill et al., 2000)
  - Use formal parameter-estimation program, e.g. built in to Modflow, or universal tools like UCODE (Poeter and Hill, 1999) or PEST (Doherty, 1994)
Inverse “Protocols”

- a formal, pre-determined inverse modeling procedure is best Hill (1998) or Hill et al. (Modflow2K 2000)
- formal mathematical approaches are available (“automated”, e.g. Menke, 1984)
- Trial-and-error calibration: the typical approach in hydrology, “try things until it works”
Calibration Data: Head

- Head observations usually represent incomplete view of transient variations
- Error sources
  - transient variations, try to get a dataset that represents a single time (synoptic)
  - measurement error
  - scaling effects: measurements made over different scale/interval than used in model
  - interpolation error: measured heads not located at a model node
Calibration Data: Fluxes

- Flux data
  - observed or inferred fluxes are very useful calibration data
  - may have moderately large errors, use with caution
  - most useful in providing range of possible parameter values
  - also help to distinguish which of many parameters to adjust during calibration
Error Criteria

- Used to control iterative solutions
- Head error criterion: best to pick order of magnitude smaller than level of accuracy desired
- Water balance error
  - “residual” error in Modflow, an absolute error \( \left( \frac{L^3}{T} \right) \)
  - most codes set this as a relative error
  - 1% mass error acceptable, 0.1% better
  - Modflow doesn’t automatically use this (user must read output file, rerun if mass balance unacceptable)
- Note: GHB package in Modflow can lead to unintended mass errors if boundary conductance set too high
Trial-and-Error

▶ most common approach, easier now with graphical aids (Fig. 1)
▶ Method: repeatedly solve forward problem, with ad hoc adjustment of parameters until results match observations within tolerance
▶ strictly valid only if calibration goal specified in advance
▶ requires tens to hundreds of runs. In GMS be sure to use Display/Plot Wizard/Error vs. Simulation to monitor calibration progress
Graphical Calibration Tool

Figure 1: Graphical calibration target in GMS. Error bar is green if error less than interval, yellow if error is $< 100\%$, red if error is $\geq 200\%$. Other modeling packages such as GroundwaterVistas use similar icons. After EMRL (Fig. 11.2, 2003a).
Figure 2: Example of graphical calibration targets. Results indicate model head too low to right, too high in middle, acceptable on the right (Brikowski and Faid, 2006). $K$ might be adjusted in the opposite direction to produce better results during trial-and-error calibration.
Automated Calibration

- theoretically better approach, in practice can be unsatisfactory because it ignores hydrologist’s “intuition”

- proper zonation is the key to a successful automated inverse solution

Method:
- user divides model area into a number of homogeneous zones, characterized by one or more parameters, which may vary from zone to zone
- program (e.g. **Modflow**2K Parameter Estimation/Sensitivity process) repeatedly solves forward problem, adjusting parameters in prescribed fashion to minimize an objective function

Implementation:
- objective function is usually the squared residuals (e.g. least-squares difference between observed and modeled)
Automated Calibration (cont.)

- inverse codes vary mostly in the method used to find the minima in the objective function, and secondarily in the choice of objective function
- best-fit value or sensitivity (effect on model of small changes in parameter) of parameters is reported
- most accessible code: **Modflow2K** with Parameter Estimation/Sensitivity process enabled (Hill, 1998; Hill et al., 2000)
Evaluating the Calibration

▪ Qualitative
  ▪ show map(s) of difference between calculated and observed head
  ▪ be sure errors are distributed \(\sim\) randomly in space

▪ Quantitative (calibration criterion)
  ▪ best to include a quantitative measure of calibration. This is already calculated during automatic calibration
  ▪ Error measures:
    ▪ Mean error: average difference between measured heads. Negative and positive errors may cancel out, giving misleading indication of minimum error.
    ▪ Mean absolute error: average of absolute value of difference between measured heads. Avoids the canceling-out problem.
    ▪ Root Mean Squared Error (standard deviation). Square root of average of squared difference in heads. Weights large errors higher, best measure of error in general.
Traditional Sensitivity Analysis

- Quantifies uncertainty in the final calibrated model
- Procedure:
  - vary calibrated values through plausible range of values (established before calibration)
  - plot change in calculated variable (e.g. head) as a function of calibrated parameter
  - also examine change in spatial distribution of error
- Highlight or re-examine the most sensitive parameters
Figure 3: Traditional parameter sensitivity plot showing % change in parameter value vs. % change in head (right) and leakage from stream (left). Computed head is most sensitive (depends most) on Recharge and $K_h$. After Anderson and Woessner (Fig. 8.15a, 1992).
MF2K Summary

- invoked by enabling the Sensitivity and/or Parameter Estimation processes in Modflow2K (see Modflow/Global Options in GMS)

- Observation Process must also be active (i.e. create an observation coverage in GMS using Map Module/Coverages). Typically observed head at wells will be used, but flux or other observations are possible.

- plot sensitivity (in GMS using Display/Plot Wizard/Parameter Sensitivities to determine which parameters are best constrained (most sensitive) by observation data (Fig. 4)

- my current approach:
  - trial-and-error calibration to “get used to system”
  - sensitivity run to determine which parameters are realistically constrained by observations
MF2K Summary (cont.)

- parameter estimation run to get best automatic model (done outside of GMS, since I haven’t paid for the inverse module)
- fine-tune using trial-and-error incorporating hydrogeologic “intuition” (soft information)
Figure 4: GMS parameter sensitivity/calibration plot showing hydraulic conductivity parameter sensitivities (top) and results of trial-and-error calibration (bottom). Zones HK.100 and HK.300 are best constrained by observed heads, other parameters may be controlled by other model features (e.g. streamflow for HK.200).
Sensitivity/Estimation Without GMS

- sensitivity information is stored in the Global file (*.glo)
  - find and plot the “COMPOSITE SCALED SENSITIVITY” (same information that is plotted by GMS “Parameter Sensitivity” plot, top of Fig. 4)
  - peruse the “ONE-PERCENT SCALED SENSITIVITIES”, which give the
  - contour the 1% sensitivity arrays to determine where new observations would be most likely to improve the model (not possible in GMS?)
- best-fit parameter values
  - these are tabulated at the bottom of the global file (“FINAL PARAMETER VALUES”)
  - **Modflow**2K also makes a forward run using these values, which are tabulated at the top of the output file (*.out)
  - use these with caution, since they may be hydrologically absurd if observations contain significant error, were insufficient in number or distribution, or you’re just unlucky.
Follow the procedures in Hill (1998) for further evaluation of parameter estimates/sensitivity.
References


EMRL: GMS 4.0 Tutorials. Environmental Modeling Research Laboratory, Brigham Young University, Provo, UT, 4.0 edn. (2003a)


