Model Calibration and Sensitivity Analysis
Calibration Criteria

1. Mean Error (ME)
\[ ME = \frac{1}{n} \sum_{i=1}^{n} (\text{cal}_i - \text{obs}_i) \]

2. Mean Absolute Error (MAE)
\[ MAE = \frac{1}{n} \sum_{i=1}^{n} |\text{cal}_i - \text{obs}_i| \]

3. Root Mean Squared (RMS)
\[ RMS = \left[ \frac{1}{n} \sum_{i=1}^{n} (\text{cal}_i - \text{obs}_i)^2 \right]^{1/2} \]

4. Correlation Coefficient (\( \gamma \))
\[ \gamma = \frac{\sum_{i=1}^{n} (\text{cal}_i - \bar{\text{cal}})(\text{obs}_i - \bar{\text{obs}})}{\sqrt{\sum_{i=1}^{n} (\text{cal}_i - \bar{\text{cal}})^2} \sqrt{\sum_{i=1}^{n} (\text{obs}_i - \bar{\text{obs}})^2}} \]
Presentation of Calibration Results

- qualitative comparison of calculated and observed contour maps
- tabulated results with summary statistics
- scatter diagrams
- comparison of observed and calculated breakthrough curves
- spatial distribution of residual errors
- comparison of observed and calculated mass distributions
Observed concentrations superimposed on calculated contours
Table 10-1. Example of tabulated calibration results with summary statistics

<table>
<thead>
<tr>
<th>Well Number</th>
<th>Model Layer</th>
<th>Model Row</th>
<th>Model Column</th>
<th>Observed Heads (H0)</th>
<th>Calculated Heads (H0)</th>
<th>Residual (H0 - H0)</th>
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<td>41</td>
<td>110.47</td>
<td>114.04</td>
<td>3.57</td>
</tr>
</tbody>
</table>

Mean Error: 0.65
Standard Deviation: 2.61
Correlation Coefficient: 0.94

A Framework for Model Applications 4
Comparison of calculated and observed discharge from 4 pumping wells
A Framework for Model Applications
NATS Site, Columbus, MS

(Julian et al., 2001)

A Framework for Model Applications
Observed and Calculated Bromide Concentrations
Scatter diagram of observed versus calculated bromide peak concentrations. Snapshots 3 and 4 correspond to observation times of 152 and 278 days after source emplacement.
Methods for Model Calibration

1 by trial-and-error procedures
   a) select one or more calibration criteria
   b) adjust one input parameter at a time
   c) compare values of calibration criteria

2 by “automated” procedures
   a) parameter values
   b) parameter structures
   c) available codes

3 points to ponder
   a) perform transient calibration, if possible at all
   b) calibrate flow rates, if possible
   c) much can be gained from calibration against transport data
Model Calibration as an Optimization Problem

Minimize objective function

$$S = \sum \omega_i (obs_i - cal_i)^2$$

subject to one or more specified constraints

Example of simple objective function
Example of more complex objective function with multiple local optima
Illustrative Example

Figure 4-1. Configuration of the two-dimensional test problem. The solid dots and open circles indicate the locations of pumping and monitoring wells where hydraulic heads and/or concentrations are used to estimate hydraulic conductivity in the three zones.
True head distribution

True concentration data at 3 wells

A Framework for Model Applications
Objective Functions for Parameter Estimation

Head data only

\[
\text{Minimize } S = \sum_{i=1}^{NH} \left[ \alpha_i \left( h_i - \hat{h}_i \right) \right]^2
\]

Both head and concentration Data

\[
\text{Minimize } S = \sum_{i=1}^{NH} \left[ \alpha_i \left( h_i - \hat{h}_i \right) \right]^2 + \sum_{j=1}^{NC} \left[ \beta_j \left( C_j - \hat{C}_j \right) \right]^2
\]

<table>
<thead>
<tr>
<th></th>
<th>(K_1) (m/d)</th>
<th>(K_2)</th>
<th>(K_3)</th>
<th>Obj. Func.</th>
<th># Generations</th>
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</thead>
<tbody>
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<td>200</td>
<td>0</td>
<td>200</td>
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<tr>
<td>H only</td>
<td>150</td>
<td>50</td>
<td>200</td>
<td>0</td>
<td>200</td>
</tr>
<tr>
<td>H &amp; C</td>
<td>150</td>
<td>50</td>
<td>200</td>
<td>0</td>
<td>200</td>
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</table>
Sensitivity Analysis

- sensitivity coefficient

measure of the effect of change in one factor on another factor

\[ X_{i,k} = \frac{\partial \hat{y}_i}{\partial a_k} \approx \frac{\Delta \hat{y}_i}{\Delta a_k} \]

normalized with respect to \( a_k \),

\[ X_{i,k} = \frac{\partial \hat{y}_i / \hat{y}_i}{\partial a_k / a_k} \approx \frac{\Delta \hat{y}_i / \hat{y}_i}{\Delta a_k / a_k} \]

dimensionless,

\[ X_{i,k} = \frac{\partial \hat{y}_i / \hat{y}_i}{\partial a_k / a_k} \approx \frac{\Delta \hat{y}_i / \hat{y}_i}{\Delta a_k / a_k} \]
Procedure for Sensitivity Analysis

- base case: calibrated model
- change a parameter by a certain percentage from the base case ($\Delta a/a$)
- run the model again
- calculate the change in model response ($\Delta y$) which could be any variable of interest, such as head, flow rate, concentration at a receptor, etc.
- calculate sensitivity coefficient and evaluate the results
Examples of Sensitivity Analysis

![Bar chart showing sensitivity analysis results for different parameters and aquifers.](chart.png)
Table 10-4. Ranking of the sensitivities of the calibration index (RMS) with respect to model parameters.

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Location of Observation Wells</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Aquifer 1</td>
</tr>
<tr>
<td>Recharge Rates (R)</td>
<td>1</td>
</tr>
<tr>
<td>Horizontal Hydraulic Conductivity</td>
<td>2</td>
</tr>
<tr>
<td>for Aquifer 1 ($K_1$)</td>
<td></td>
</tr>
<tr>
<td>Horizontal Hydraulic Conductivity</td>
<td>3</td>
</tr>
<tr>
<td>for Aquifer 2 ($K_2$)</td>
<td></td>
</tr>
<tr>
<td>Horizontal Hydraulic Conductivity</td>
<td>6</td>
</tr>
<tr>
<td>for Aquifer 3 ($K_3$)</td>
<td></td>
</tr>
<tr>
<td>Vertical Hydraulic Conductivity</td>
<td>4</td>
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<tr>
<td>between Aquifers 1 and 2 ($K_4$)</td>
<td></td>
</tr>
<tr>
<td>Vertical Hydraulic Conductivity</td>
<td>5</td>
</tr>
<tr>
<td>between Aquifers 2 and 3 ($K_5$)</td>
<td></td>
</tr>
</tbody>
</table>

Note: The sensitivity ranking is relative, with 1 indicating the highest sensitivity and 6 the lowest sensitivity.
Observed plumes of BTEX and electron acceptors at the Hill Air Force Base (Lu et al., 1999)

Results of sensitivity analyses for total BTEX mass and BTEX plume front (Lu et al., 1999)

<table>
<thead>
<tr>
<th></th>
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</tr>
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<td></td>
<td></td>
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<td>-0.047</td>
<td>-0.036</td>
<td>-0.058</td>
<td>-0.031</td>
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<td>Front of BTEX plume$^a$</td>
<td>+0.563</td>
<td>-0.088</td>
<td>-0.419</td>
<td>-0.077</td>
<td>-0.331</td>
</tr>
</tbody>
</table>

$^a$ Sensitivity analysis performed on 0.05 mg/l contour line of BTEX plume

A Framework for Model Applications 22
Prediction and Uncertainty

- simulation of future conditions
evaluation/assessment
vs.
prediction

- sources of uncertainty
  ⇒ conceptual
      related to the mathematical model
  ⇒ geological
      harder to quantify
  ⇒ stress and other conventional parameters
      targets of most uncertainty analysis studies
Methods for Uncertainty Analysis

- sensitivity analysis
  ⇒ simple, straightforward, but cannot examine correlation between parameters

- first-order error analysis
  ⇒ in the simplest form

\[
\text{Var}[y] = \sum_{i=1}^{N} \text{Var}[x_i] \left( \frac{\partial y}{\partial x_i} \right)^2
\]

⇒ approximation

- Monte Carlo simulation
  ⇒ most general, but computationally intensive
Procedure for Monte Carlo Analysis

1. Generate samples (or realizations) for each uncertain input parameter
2. Assemble input files and run the simulation model, once for each realization
3. Construct histogram (or frequency plot) for the model output variable under study
4. Convergence test passed?
   - Yes: Print cumulative probability distribution of the model output variable
   - No: Repeat steps 1-4
Example of Monte Carlo Analysis
Woldt et al. (1992)
Only $K$ as random variable

Only Initial Plume as random variable

Both $K$ and Initial Plume as random variables