Case Study:
Integrated Conceptual and Numerical Modeling
Chemwest Industrial Site
Objectives

- Design a conceptual model, consisting of
  - Geologic Structure
  - Hydrogeologic Properties
  - Boundary conditions and wells
- Simulate Groundwater Flow with MODFLOW and FEFLOW
- Compare simulated results with field data
- Demonstrate the value in having a grid and simulator-independent conceptual model that is *integrated* with the numerical model
Background - Site

- ChemWest Laboratories Ltd. manufactured inorganic and organic industrial chemicals
- Benzene was found in the groundwater 25 years ago
- Originated from an underground storage tank (UST) several hundred feet upgradient of the well.
- A pump and treat recovery program was initiated to hydraulically contain the benzene plume and to ultimately capture it.
- After more than ten years of continuous groundwater pumping substantially, the extent of the benzene plume has diminished substantially.
- Recent sampling revealed that only four monitoring wells in one area of the site contained benzene concentrations above the prescribed groundwater criteria.
- ChemWest proposed to the U.S. EPA that the pump and treat operations be terminated and allow natural biodegradation to eliminate the remaining benzene.
- SWS was asked to develop a numerical groundwater model to assess the feasibility of this plan.
Steps for Conceptual Modeling

1. Collect and Visualize Data
2. Design Geologic Structure
3. Define Flow Properties
4. Define Hydrologic Boundaries
1. Collect and Visualize Data

- **GIS Data:**
  - Locations of water bodies, roads, plant and property boundaries
  - Pumping and Observation wells
  - Borehole log data
- **Site Plan:** DXF file
- **Water table (initial heads)**
- **Cross-section interpretations**
  - Combine to define geologic surfaces
2D Views

Locations of:
- Norman River
- Deer Creek
- Bass Lake
- Salmon Pond
Cross sections

AA’, Vert Exag. 10

BB’, Vert Exag. 10
Generate Surfaces from XS and Log Data

Top Bedrock

Top Sand

Ground Surface
2. Design Geologic Structure

- Provide the model boundary (polygon)
- Provide Geologic Surfaces as Input
- Define Horizon Rules
- Interpret 3D Geologic bodies
Convert Surfaces to Horizons

Horizon Settings

<table>
<thead>
<tr>
<th>Surfaces</th>
<th>Name</th>
<th>Type</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ascii-Ground-Surf</td>
<td>Horizon1</td>
<td>Erosional</td>
</tr>
<tr>
<td>tcp_Sand2</td>
<td>Horizon2</td>
<td>Conformable</td>
</tr>
<tr>
<td>tcp_bedrock</td>
<td>Horizon3</td>
<td>Conformable</td>
</tr>
</tbody>
</table>

Horizon truncation rules:
- Erosional: Horizons below will be truncated.
- Base: Horizons above will be truncated.
- Discont: The horizon is both a base and an erosional. Horizons below and above will be truncated.
- Conformable: Horizons will be truncated by erosional, base and discont. Lower conformable horizons will be truncated by upper conformable horizons in the make horizon process.
Generate 3D Structural Model
3. Define Flow Properties

- Select the geometry (polygons, structural zones)
- Define the method (constant, shp attribute, 2D or 3D Grid)
- Provide the values/attributes (Conductivity, Storativity, Initial Heads, etc..)
Upper Formation:
Constant $K_x = 0.0006 \text{ m/s}$

Lower Formation:
Using Polygons:
1. $0.0009 \text{ m/s}$
2. $0.00025 \text{ m/s}$
3. $0.0003 \text{ m/s}$
4. $0.0012 \text{ m/s}$
4. Define Hydrologic Boundaries

- Select the geometry
- Define the method (constant, shp attribute, 2D or 3D Grid)
- Provide the values/attributes

Boundary Types Used:
- Constant head (west edge)
- River
- 2 Ponds (modeled as Lakes)
- Recharge
Constant Head

- Norman River modeled as a constant head:
  - 602 m; above the dam
  - 587 m; below the dam
River

- **Stage:**
  - 598 m stage at the eastern edge
  - 587 m at the discharge point to the western river boundary
- River bottom is 1.5 m below the surface of the river.
- Conductance estimated to 10 m\(^2/\text{day}\)
Ponds

- The 2 ponds as Type 3 Lake boundaries
- Stage: 599.0 m
- Bottom: 597.5 m
- Leakance: 100 m$^2$/day,
Recharge

- Uniform across top of model domain
- 254 mm/yr
Steps for Numerical Modeling - MODFLOW

1. Define Uniform Grid
2. Refine Grid
3. Populate Grid with Conceptual Model Data
4. Review, make cell based edits
5. Translate to MODFLOW Packages
6. Run Simulation
7. Analyze Results
8. Validate with Conceptual Model and Assumptions
MODFLOW Step 1: Generate MODFLOW Grid

- Initial uniform grid of 100 m x 100 m,
  - Results in 40 columns, 85 rows
- Upper formation is refined to create 2 layers
- Deformed grid layers follow conceptual model horizons

Plan view of the grid
Cross-sectional view of grid
MODFLOW Step 1: Generate MODFLOW Grid
Step 2: Refine MODFLOW Grid

- The grid is refined by a factor of 2 around the area of interest.
- Resulting grid is 119 Rows * 56 Col (Total 6664 cells)
Step 3: Populate Grid with Conceptual Model Data

- Define Inactive Cells
- Populate Cells with Properties and Boundary Conditions

Kx values in 2D, XS, and 3D View

Cell representation of Boundary conditions
Step 4: Review and Edit Cell Attributes
Step 5: Translate to MODFLOW Packages

![Image of MODFLOW package translation process]

Translate to MODFLOW Packages...
Step 6: Run Simulation

MODFLOW-2005 with PCG Solver
Step 7: Analyze Results

Heads Contours
XS View: Row 75

Head Contours,
Plan View: Layer2
Step 7: Analyze Results

Reasonable Calibration to Heads

Mass Balance <0.1%
Step 8: Compare Results with Field Data

Overlay heads (contours, colormap), pathlines, compare to conceptual model.
Steps for Numerical Modeling - FEFLOW

1. Define Superelement Mesh; Add-Ins (Points, lines, polygons)
2. Generate Mesh
3. Populate Mesh with Conceptual Model Data
4. Review, make element-based edits
5. Run Simulation
6. Analyze Results
7. Validate with Conceptual Model and Assumptions
FEFLOW Step 1: Define Superelement Mesh

- Provide Line and Point Add-Ins:
  - Calibration Points
  - Constant Head Boundary
  - River and Lakes
Step 2: Generate Mesh

- Using Triangle Mesh generator
- Est. 6500 elements
- Refine around lines and edge (flow boundaries)
Step 2: Generate Mesh
Step 3: Populate Mesh with Conceptual Model Data

- Provide run settings (date, type)
- Select the Options for representing boundaries
Step 4: Review Cell Attributes, and Adjustments
Step 5&6: Run Simulation and Analyze Results
Step 6: Analyze Results
Step 7: Compare Results with Field Data

Overlay heads (contours, colormap), pathlines, compare to conceptual model
Summary

- The conceptual model provides the ability to:
  - understand the site conditions before running a simulation
  - choose between MODFLOW or FEFLOW
  - Provides ability to select different grid types
- Grid and mesh is easily generated and populated from conceptual objects
- The MODFLOW and FEFLOW Simulation show reasonable likeness
- Integrated Conceptual and Numerical Modeling allows for:
  - Efficient design of multiple models to reduce uncertainty
  - Manage multiple modeling scenarios
  - Comparing simulated results with observed field data to improve model credibility