AN ITERATIVE APPROACH TO IMPROVE MODEL PREDICTIONS AND SITE CONCEPTUAL MODELS

Al Laase, Navarro Research and Engineering
Grand Junction, Colorado  laase@navarro-inc.com

James O. Rumbaugh III (Environmental Simulations, Inc. Leesport, PA, USA)

James Stening (Orica Pty Ltd, Botany, NSW, Australia)
Orica Modeling Tenets

Why Model?

- Understanding
  - Site conceptual model development
  - Parameter sensitivity evaluation
  - Remedial strategy comparison
- Predictions
  - Plume trends and duration
  - Remedial design performance
  - Capture zone evaluation
Orica Modeling Tenets

Model Value

Knowledge

0
Orica Modeling Tenets

Model Value

Knowledge

Prediction

Understanding
Orica Modeling Tenets

Models are Dynamic

Model prediction shortcomings guide conceptual model revisions

Conceptual Model

Prediction
Orica Modeling Tenets

Model Value vs Knowledge Diagram:

- 2007 Transport Model
- 2013 Transport Model
- 2016 Transport Model
- 2005 Groundwater Flow Model
- Next Groundwater Flow or Transport Model

These models represent different stages of knowledge and model value in the Orica modeling process.
- Orica Botany site is located south of Sydney, Australia
- More than a century of industrial operations by multiple companies in the area have contaminated the Botany Aquifer with a variety of chemicals
- ICI Australia/Orica have been in operation for approximately 70 years at the Botany site
- In 2005 a remedial extraction well field consisting of 113 extraction wells pumping a cumulative 7 ML/d became operational
- Focus of this presentation is 1,2-dichloroethane (1,2-DCA)
Source areas are active and source loading is declining at an uncertain rate.

- $K_d$ is homogeneous.
- Degradation occurs but is limited due to high contaminant concentrations (assume 1500 day degradation half life).
Orica Modeling Odyssey

Conceptual Model

Model Calibration

Model Predictions

2007 Transport Model

- Used transient groundwater model as basis for transport simulations
- Calibrated the model to 347 concentration measurements collected at 48 locations between 1990 and 2004
- Calibrated 36 source area temporal loading rates from inception through 2004 using super position techniques
- Assumed fixed attenuation rate and $K_d$

PEST used to calibrate transport model
Orica Modeling Odyssey

- **Conceptual Model**
- **Model Calibration**
- **Model Predictions**
- **2007 Transport Model**
  - Simulated a variety of source remediation scenarios for combinations of extraction wells and reactive barriers
  - Depending on the timing and % reduction in the source area loading rates, \( \leq 0.1 \) mg/L concentrations could be achieved as soon as 2055 everywhere in the aquifer
  - Likely scenario was many 100s of years would be required to achieve \( \leq 0.1 \) mg/L everywhere in the aquifer
## Orica Modeling Odyssey

### Conceptual Model

### Model Calibration

### Model Predictions

### Observed

#### Constant Source Term

<table>
<thead>
<tr>
<th>Model Layer</th>
<th>January 2005 EDC Plume Mass, kg</th>
<th>September 2013 EDC Plume Mass, kg</th>
<th>Difference, kg</th>
<th>Difference, %</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>65,220</td>
<td>92</td>
<td>65,128</td>
<td>99.9</td>
</tr>
<tr>
<td>2</td>
<td>190,220</td>
<td>10,012</td>
<td>180,208</td>
<td>94.7</td>
</tr>
<tr>
<td>3</td>
<td>669,760</td>
<td>57,079</td>
<td>612,681</td>
<td>91.5</td>
</tr>
<tr>
<td>4</td>
<td>647,469</td>
<td>116,266</td>
<td>531,202</td>
<td>82.0</td>
</tr>
<tr>
<td>TOTAL</td>
<td>1,572,668</td>
<td>183,449</td>
<td>1,389,219</td>
<td>88.3</td>
</tr>
</tbody>
</table>
Source areas are active and source loading is declining at an uncertain rate.

- Kd is homogeneous
- Degradation rate is unknown but is <1500 days
Orica Modeling Odyssey

- **Conceptual Model**
- **Model Calibration**
- **Model Predictions**
- **Observed**

**2013 Transport Model**
- Used transient groundwater model as basis for transport
- Calibrated the model to 671 concentration measurements collected at 48 locations between 1990 and 2013
- Calibrated constant loading rates for 36 source area
- Calibrated individual degradation rates for each model layer

PEST used to calibrate transport model
2013 Transport Model

- Calibration resulted in degradation half lives of:

<table>
<thead>
<tr>
<th>Model Layer</th>
<th>Degradation Half-Life, days</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>25</td>
</tr>
<tr>
<td>2</td>
<td>175</td>
</tr>
<tr>
<td>3</td>
<td>500</td>
</tr>
<tr>
<td>4</td>
<td>625</td>
</tr>
</tbody>
</table>

- With the exception of the source areas, ≤0.1 mg/L concentrations could be achieved as soon as 2030
Orica Modeling Odyssey

- Conceptual Model

- Model Calibration

- Model Predictions

- 2013 Transport Model
  - Source area concentrations are declining; assumption that source area concentrations are constant is not realistic
  - Calibrated degradation half lives are much faster than previously characterized at the site

- Observed
Orica Modeling Odyssey

2016 Transport Model
- Source area loading can be characterized by:
  \[ C(t) = C_0 e^{-kt} \]
- Geosyntec characterized the expected \( k \) range for individual source areas
- \( K_d \) is possibly different for each of the four model layers

Conceptual Model

Model Calibration

Model Predictions

Observed
Orica Modeling Odyssey

- Conceptual Model
  - Model Calibration
  - Model Predictions
  - Observed

- 2016 Transport Model
  - Used transient groundwater model as basis for transport
  - Calibrated $C_0$ and $k$ for 36 source area
  - Calibrated individual degradation rates and $K_d$ for each model layer
  - Used BEOPEST to perform calibration in parallel

PEST used to calibrate transport model
2016 Transport Model
- Calibrated targets included:
  - 671 concentration measurements collected at 48 locations between 1990 and 2013
  - Temporal mass removed at the treatment plant
  - 2013 bulk plume statistics for each model layer:
    - Dissolved mass
    - Plume volume
    - Concentration distribution statistics

PEST used to calibrate transport model
Orica Modeling Odyssey

Conceptual Model

Model Calibration

Model Predictions

Observed

### 2016 Transport Model

<table>
<thead>
<tr>
<th>Model Layer</th>
<th>Observed EDC Plume Mass, kg</th>
<th>Model-Predicted EDC Plume Mass, kg</th>
<th>Difference, kg</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>92</td>
<td>960</td>
<td>-868</td>
</tr>
<tr>
<td>2</td>
<td>10,814</td>
<td>11,617</td>
<td>-803</td>
</tr>
<tr>
<td>3</td>
<td>57,079</td>
<td>12,339</td>
<td>44,740</td>
</tr>
<tr>
<td>4</td>
<td>116,266</td>
<td>145,446</td>
<td>-29,180</td>
</tr>
<tr>
<td>TOTAL</td>
<td>184,251</td>
<td>170,362</td>
<td>13,889</td>
</tr>
</tbody>
</table>

![Graph showing measured vs. modeled EDC plume mass over time.](image)
Orica Modeling Odyssey

- Conceptual Model
- Model Calibration
- Model Predictions
- Observed

2016 Transport Model
- Calibration resulted in degradation half lives of:

<table>
<thead>
<tr>
<th>Model Layer</th>
<th>Degradation Half-Life, days</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>2016</td>
</tr>
<tr>
<td>1</td>
<td>145</td>
</tr>
<tr>
<td>2</td>
<td>593</td>
</tr>
<tr>
<td>3</td>
<td>952</td>
</tr>
<tr>
<td>4</td>
<td>784</td>
</tr>
</tbody>
</table>

- Time to ≤0.1 mg/L
  - 2016 transport model - 2055
  - 2013 transport model - ≥2030
Orica Modeling Odyssey

**Conceptual Model**

**Model Calibration**

**Model Predictions**

**Observed**

---

- **2016 Transport Model**
  - Based on discrepancies between layer 1 and 3 modeled and observed plume mass, studies are being undertaken to characterize the spatial distribution of $K_d$ and degradation half lives within the aquifer.
  - Additionally, the study results will confirm the representativeness of the calibrated half lives.
  - Results of the studies will be used to update the next transport model.
Questions?