AN ITERATIVE APROACH TO IMPROVE MODEL PREDICTIONS AND SITE CONCEPTUAL MODELS

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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

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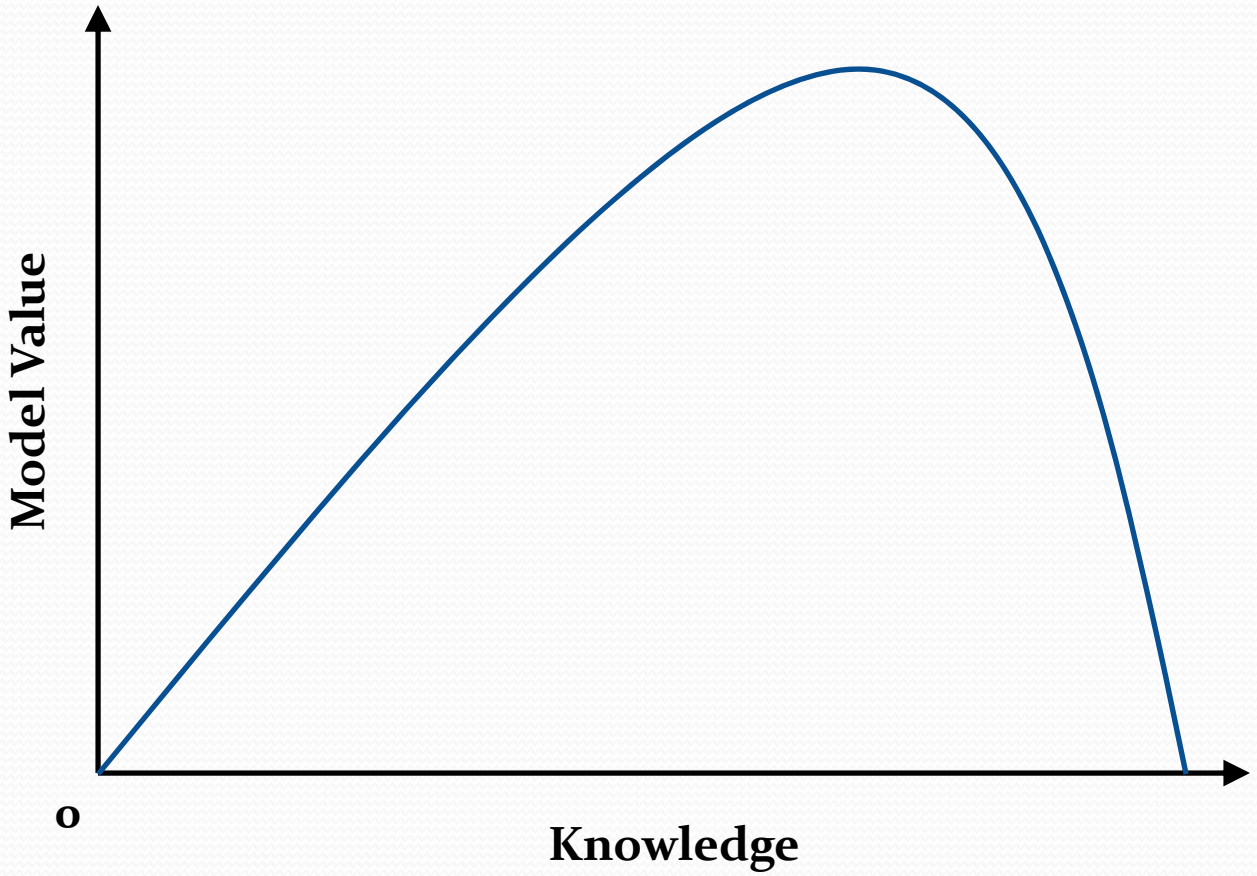

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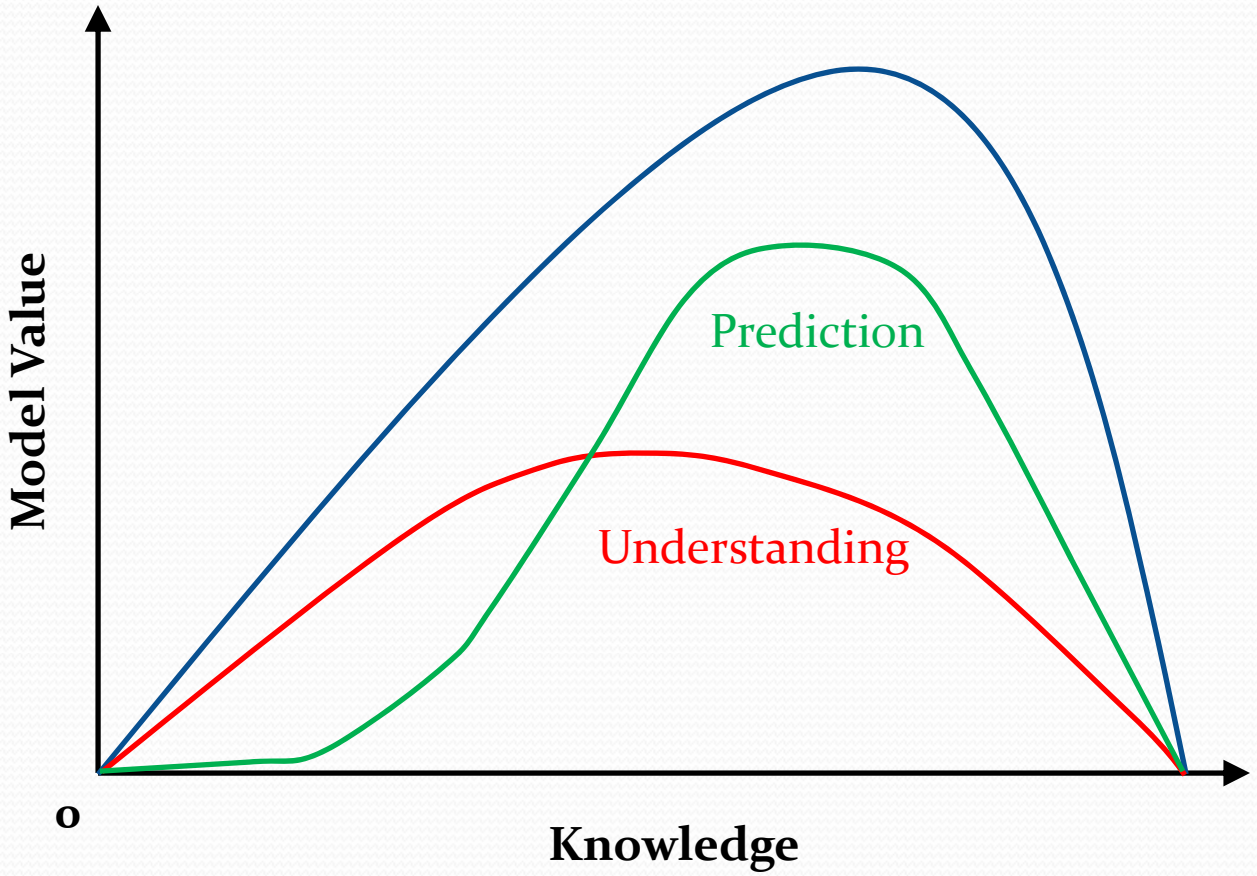

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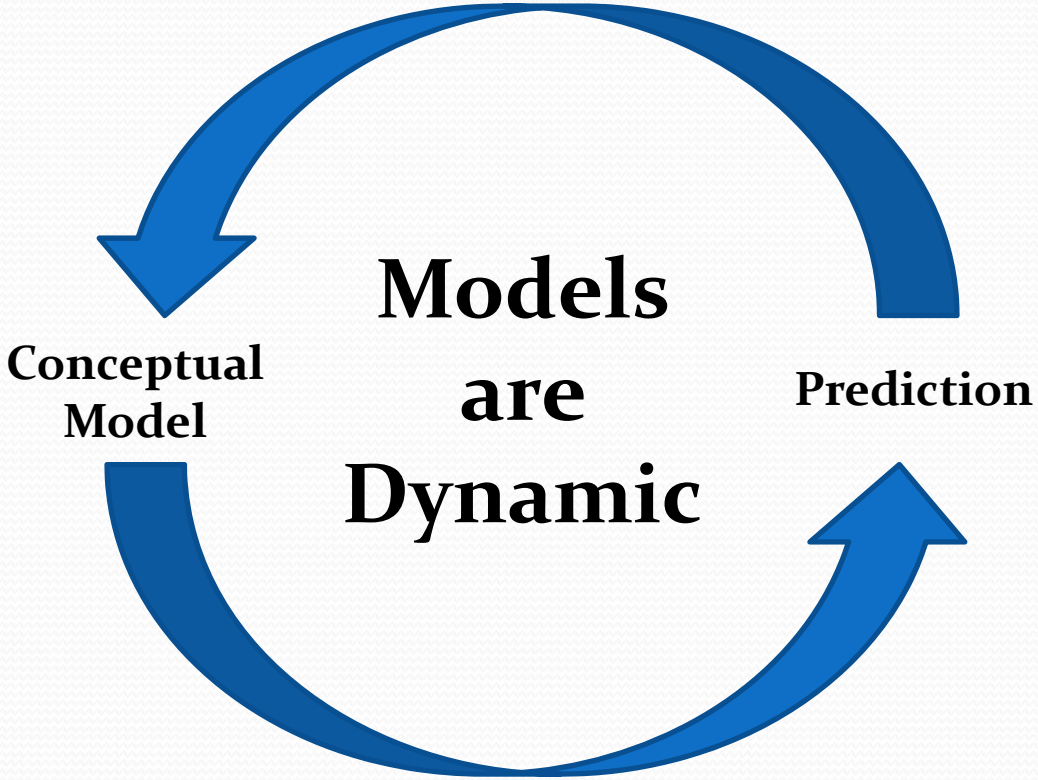

Model prediction shortcomings guide conceptual model revisions

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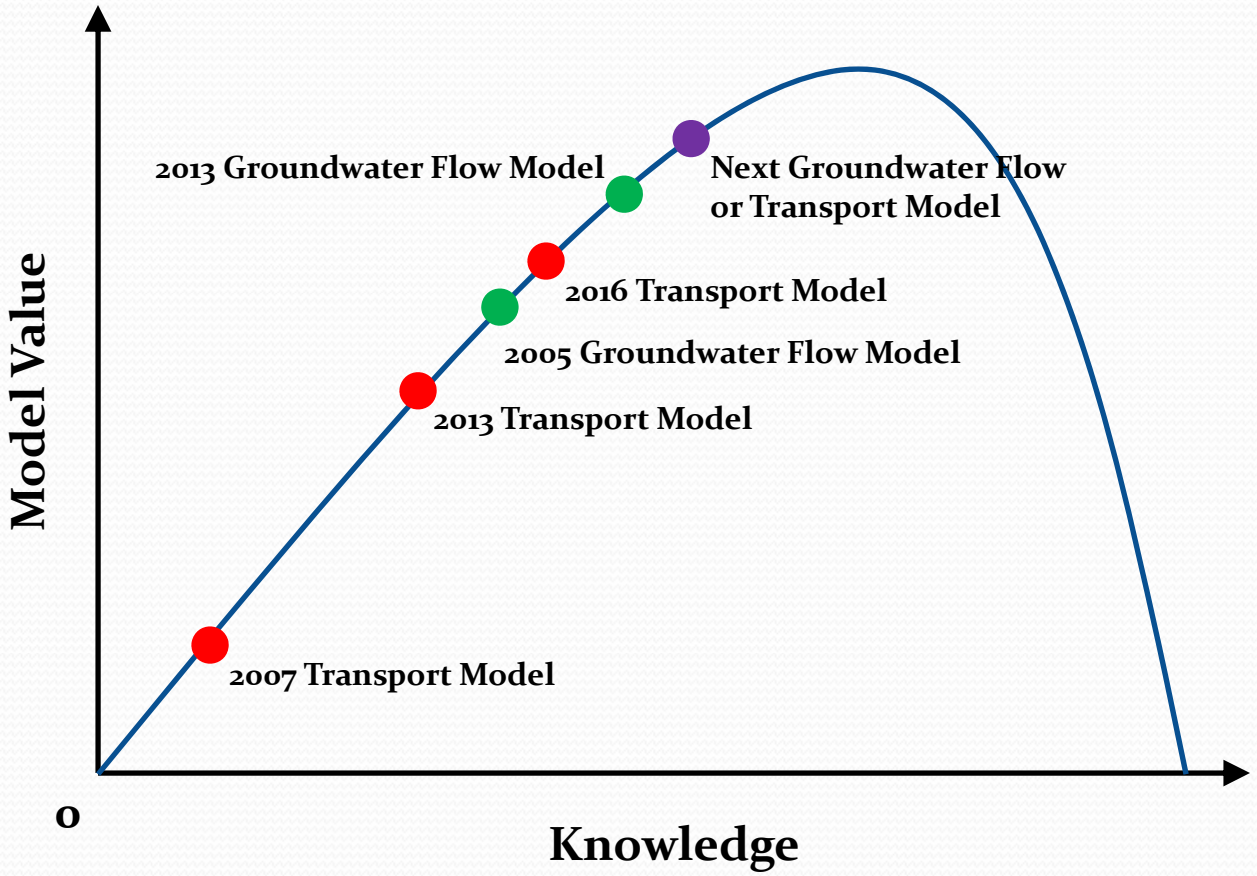

Orica Modeling Odyssey

- 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)

Orica Modeling Odyssey

Conceptual Model → 2007 Transport Model

- 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)

Model Calibration

Model Predictions

Observed

Orica Modeling Odyssey

Conceptual Model

Model Calibration

Model Predictions

Observed

- 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

Observed

- 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, ≤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 ≤0.1 mg/L everywhere in the aquifer

Orica Modeling Odyssey

Conceptual Model

Model Calibration

Model Predictions

Observed

2013

Constant Source Term

Model Layer	January 2005 EDC Plume Mass, kg	September 2013 EDC Plume Mass, kg	Difference, kg	Difference, %
1	65,220	92	65,128	99.9
2	190,220	10,012	180,208	94.7
3	669,760	57,079	612,681	91.5
4	647,469	116,266	531,202	82.0
TOTAL	1,572,668	183,449	1,389,219	88.3

Orica Modeling Odyssey

Conceptual Model → 2013 Transport Model

- Source areas are active and source loading is declining at an uncertain rate
- Kd is homogeneous
- Degradation rate is unknown but is <1500 days

Model Calibration

Model Predictions

Observed

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

Orica Modeling Odyssey

Conceptual Model

Model Calibration

Model Predictions

Observed

- 2013 Transport Model
  - Calibration resulted in degradation half lives of:

Model Layer	Degradation Half-Life, days
1	25
2	175
3	500
4	625

  - 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

Observed

- 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

Orica Modeling Odyssey

Conceptual Model → 2016 Transport Model

- Source area loading can be characterized by:

$$C(t) = C_o e^{-kt}$$

- Geosyntec characterized the expected k range for individual source areas
- K_d is possibly different for each of the four model layers

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_o 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

Orica Modeling Odyssey

Conceptual Model

Model Calibration

Model Predictions

Observed

- 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

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Model Calibration

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Model Predictions →

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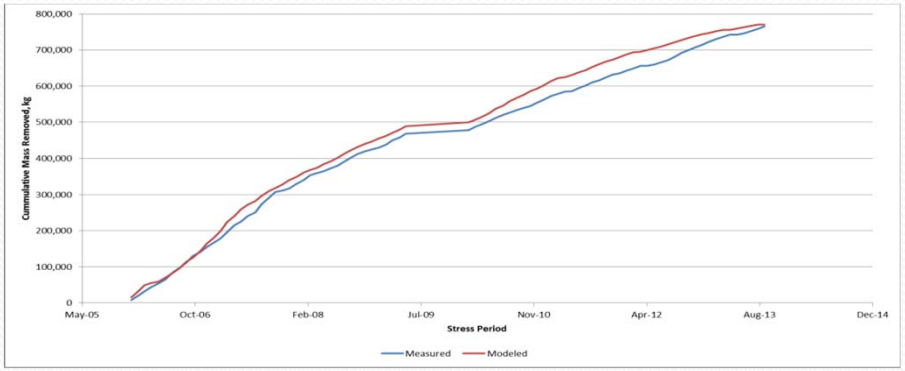
Observed

- 2016 Transport Model

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



Orica Modeling Odyssey

Conceptual Model

Model Calibration

Model Predictions

Observed

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

Model Layer	Degradation Half-Life, days	
	2016	2013
1	145	25
2	593	175
3	952	500
4	784	625

  - 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?