An Iterative Approach to Improve Model Predictions and Site Conceptual Models

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Background/Objectives.
Orica Botany Site groundwater flow and transport models are routinely updated and simulation results are used to guide management decisions. Initial transport model predictions were erroneous when compared to concentration data collected in the years following the modeling exercise. Rather than discontinue modeling, which is commonly the case when model predictions are significantly different to observed data, Orica instead collected data to refine the site conceptual model and correspondingly improve model predictive capabilities. The cycle of modeling and data collection has been repeated a number of times with model predictive capability and site understanding improving with each iteration. More accurate predictions support the adaptive remediation strategy underpinning the cleanup project.

Approach/Activities.
Modeling at the Orica Botany Site is guided by the understanding that models have two purposes; to make predictions and to improve understanding of the site groundwater flow and contaminant transport conceptual models. The two purposes are interrelated, a prediction failure indicates an erroneous conceptual model and the best way to improve the model's predictive capability is to refine the site conceptual model through targeted data collection. Initial transport modeling in 2007 predicted many decades of continuous operation of the 113 well extraction system would be required to reduce dissolved 1,2-dichloroethane (1,2-DCA) below established standards. Eight years after pumping began (in 2013), observed 1,2-DCA mass is the aquifer had been reduced by 88%, a declination rate not predicted by the initial transport simulations. Follow-on transport modeling using constant sources reasonably matched concentration trends by using dissolved phase degradation rates between 25 days and 625 days, rates not supported by characterization efforts. A post audit of the transport model suggested that the model could be improved by using temporally variable source term degradation rates and calibrating to treatment system temporal 1,2-DCA influent concentrations. To improve the site conceptual model, characterization efforts were undertaken to better understand 1,2-DCA dissolved phase degradation rates and source term degradation rates. The improved understanding of 1,2-DCA source term and dissolved phase degradation, combined with application of innovative transport calibration targets, resulted in model-predicted 1,2-DCA concentrations matching observed temporal trends. The updated transport model predicted that 1,2-DCA concentrations under the influence of pumping will decline below established standards within a third of the 2007 predicted duration.

Results/Lessons Learned.
Orica recognized groundwater flow and transport models are dynamic, not static, and routine cycles of data collection and model updates are necessary for improving model predictive capability.