

## Groundwater modelling to help diagnose contamination problems

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**Abstract:** Aquifer remediation for a contaminated site is complex, expensive, and long-term. Groundwater modelling is often used as a tool to evaluate remedial alternatives and to design a groundwater remediation system. Groundwater modelling can also be used as a useful process to identify aquifer characteristics and contaminant behaviour that are not realized prior to modelling, to help diagnose what happened and why it happened at contaminant sites. Three real-world modelling cases are presented to demonstrate how groundwater modelling is applied to help understand contamination problems and how valuable the improved understanding is to decision-making and/or to remedial design.

**Keywords:** Groundwater modelling; Groundwater contamination; Aquifer remediation; Groundwater remediation

### Introduction

Groundwater flow models and solute transport models are often developed to support aquifer remediation at contaminated sites. Groundwater modelling is a process, which has three major components, conceptual model development, numerical model development and calibration, and model prediction. Among these, conceptual model development is most important, however it is often overlooked. Numerical groundwater modelling is often thought of as a useful tool to evaluate various remedial alternatives or to design a remedial system, but it is not commonly considered as a useful process to help improve the understanding of site conditions.

This paper emphasizes the importance of detailed evaluation and revision of the conceptual

model prior to and during a modelling process. Groundwater modelling is a process that integrates various types of data or information (geology, hydrogeology, groundwater flow, and contaminant behavior) into a dynamic system that is governed by groundwater flow and solute transport principles. It provides an opportunity to systematically identify data gaps, to logically- examine the conceptual model, and to verify or update the conceptual model.

This paper also demonstrates that improvement of a conceptual model has significant impacts on decision-making for aquifer remediation. Groundwater model prediction results cannot avoid having uncertainty due to uncertainty in model parameters and/or in future hydrologic conditions. If a conceptual model is representative of site hydrogeological and contaminant conditions, some uncertainty of model predictions (especially for contaminant concentrations) is less important,

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which should not affect selection of remedy. However, if a conceptual model is not representative of site conditions, then the selected remedial alternative may not be appropriate, or the remedial system design may not be effective.

Three real-world modelling cases are presented below. To maintain confidentiality, actual project names and locations are not identified, however the site conditions and issues described are based on actual site hydrogeological conditions.

## **1 Case 1-an atypical groundwater PCE plume**

Case 1 discusses mystery and challenges accounted during groundwater modelling for a fractured bedrock aquifer that serves as a water supply source. The model initially could not simulate the historical plume migration because the observed groundwater PCE concentration distribution is very different from a typical groundwater PCE plume. We were forced to re-visit the conceptual model and to figure out what mechanism causes an atypical groundwater PCE plume. The final modelling results indicate that even though the contaminant source zone is occupied by a large amount of dense non-aqueous phase liquid (DNAPL), there is no need to conduct additional active DNAPL remediation to protect groundwater quality. The modelling results saved the client significant time and money.

### **1.1 Problem description**

Roughly 400 000 lb (180 000 kg) of chlorinated solvents were disposed in a small leach pit from a former vapor degreasing facility during the early 1950s to 1972, resulting in a large amount of DNAPL in the subsurface and a

dissolved contaminant plume in groundwater. Since 1995, multiple remedial activities have been conducted in the source area. During 2009 to 2011, in-sit thermal treatment was implemented to remove DNAPL in the source zone.

Subsequent investigations found that thermal treatment removed the majority of DNAPL from the subsurface within the treatment zone, but left approximately 100 000 lb (45 000 kg) of DNAPL in the surrounding area, some of which was not identified prior to treatment. Groundwater tetrachloroethene (PCE) concentrations increased following thermal treatment and the PCE mass flux increased by approximately three times in the aquifer immediately downgradient of the treatment zone. This was likely due to mobilization of DNAPL from the less permeable shallow aquifer into the underlying permeable intermediate aquifer.

Immediately downgradient of the source zone, a relatively small PCE plume [500 feet (152 m) by 350 feet (106 m)] is present in the shallow aquifer with PCE concentrations up to 50 000 microgram per liter ( $\mu\text{g/L}$ ). The shallow PCE plume primarily migrates downward into the thin, permeable intermediate aquifer, resulting in a larger PCE plume [1 000 feet (300 m) by 400 feet (120 m)] with concentrations up to 10 000  $\mu\text{g/L}$ . A groundwater extraction well is located at the distal end of the intermediate PCE plume ( $> 5 \mu\text{g/L}$ ) and has been in operation since 2004. This hydraulic containment system was installed to prevent the plume from moving into the downgradient fractured bedrock that is a major water supply aquifer for the area.

Beyond the extraction well, the PCE plume ( $>5 \mu\text{g/L}$ ) appears to rapidly dissipate, only trace-level (0.01 to 1  $\mu\text{g/L}$ ) groundwater PCE

concentrations are found over a large down-gradient area from 1991 to 2013 in more than 20 monitoring wells. These wells are located in the fractured carbonate bedrock aquifer, with multiple well screens/FLUTe™ systems, sparsely located in an area of approximately two square miles (5 km<sup>2</sup>). Further downgradient about six miles (10 km) away, the surface water sampling results at springs, seeps, and a creek have shown trace-level PCE concentrations (0.01 to 0.18 µg/L) since 2006. The flow rates at these locations range from 0.5 to 30 cubic feet per second (cfs) (0.014 to 0.85 m<sup>3</sup>/s), which suggests that PCE concentrations in surface water are highly diluted.

## 1.2 Is existing groundwater extraction necessary?

The objective of groundwater modelling is to predict, after DNAPL removal by thermal remediation, whether the existing groundwater extraction system at the leading edge of the intermediate PCE plume (> 5 µg/L) is necessary to protect groundwater quality beyond the property boundary, which is approximately 2 miles (3 km) downgradient from the high-concentration PCE plume.

## 1.3 What mechanism reduced PCE concentrations?

To meet the modelling objectives in this highly heterogeneous environment, it is necessary to understand what happened at and downgradient of the site and what caused such an atypical PCE plume where the PCE concentrations rapidly dissipated downgradient.

At this site, it was difficult to conceptually understand:

(1) Why the high-concentration PCE plume

(>5 µg/L) suddenly dissipated 1 000 feet (300 m) downgradient of the source zone; where the plume exactly went, and what the groundwater preferential pathways are?

(2) What mechanism could suddenly reduce the high PCE concentrations to trace levels in the fractured bedrock? and

(3) Is it possible that contaminant mass is trapped in the fractured bedrock? But if so, how does the trace-level PCE get transported in groundwater over a long distance [six miles (10 km)] and then detected in highly diluted surface water samples?

To understand what happened and why, all available data, including geology, hydrogeology, groundwater levels, and historical groundwater and surface water sampling results, as well as well completions and boring logs, were compiled into a database and evaluated, and numerous site characterization and remediation reports over the last 20 years were reviewed. The previous conceptual model was revised, but the above questions were not adequately addressed.

A numerical groundwater flow model, using MODFLOW-NWT (Niswonger *et al.* 2011), was developed to simulate a quasi-steady state flow condition. The steady state groundwater flow model was calibrated to the average groundwater water levels and average groundwater discharge fluxes between the high and low flow conditions in 2002. A groundwater solute transport model was developed using MT3DMS (ZHENG and WANG 1999) for history matching simulation of the PCE plume over totally 60 years (period 1 from 1954 to 2003 and period 2 from 2004 to 2013). The history matching simulation of the PCE plume migration successfully matched the small-scale high-concentration PCE plumes, but failed to match the plume shape, plume extent, or the observed

trace-level PCE concentration distributions in the downgradient area.

This posed a question-If the historical PCE plume cannot be approximately simulated, how could the model be used to reasonably predict future PCE concentrations?

Effort for improving the numerical models was tried. An alternative solute transport modelling approach was tried using a dual-domain mass transfer model, which is recommended in the literature for fracture flow systems. This approach only provided a minor improvement compared to the commonly used advection-dispersion model. The hydraulic conductivity distribution in the flow model was also revised in detail based on geologic interpretations, which only provided limited improvement in the contaminant distribution along the flow pathways.

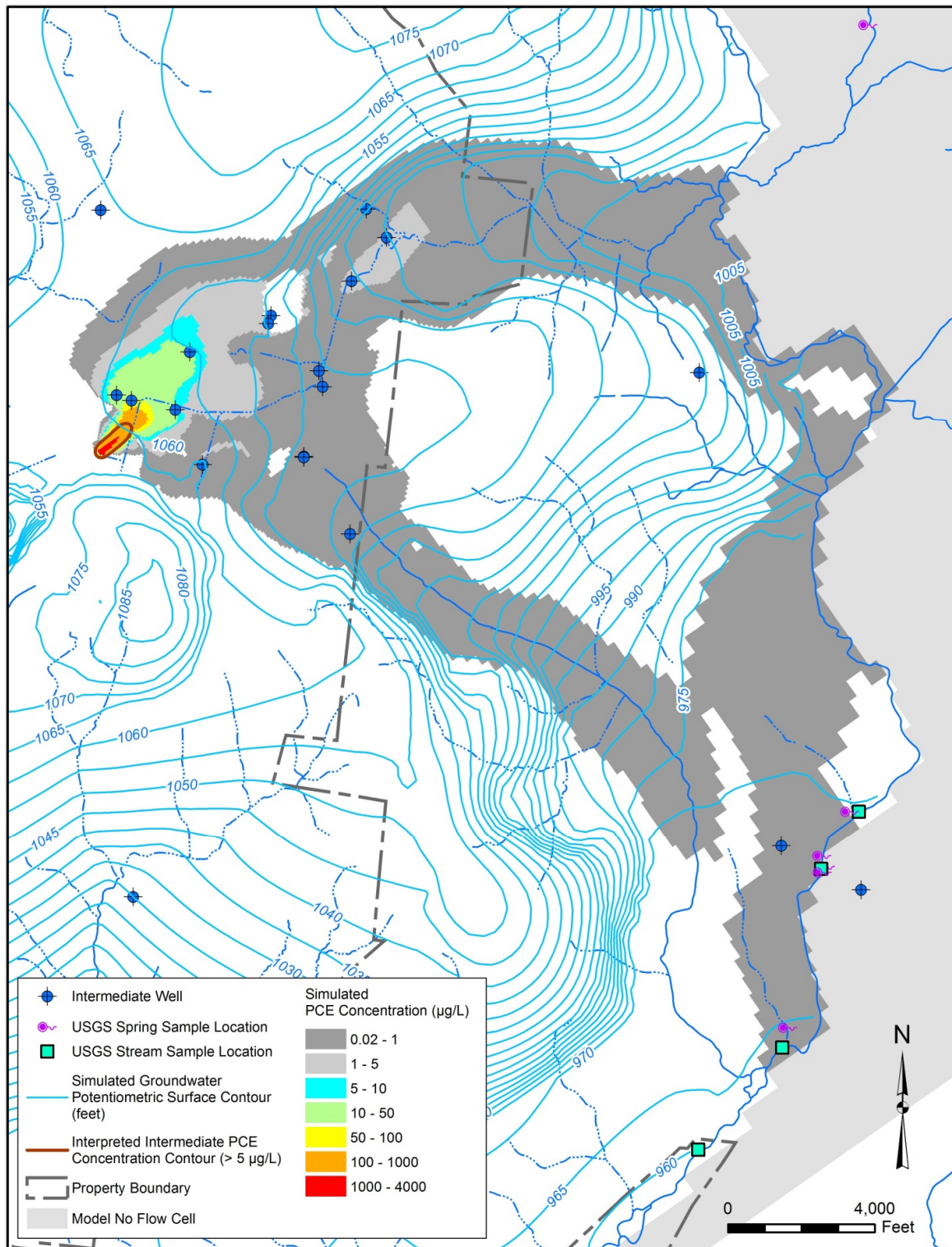
The conceptual model was re-visited. The available groundwater level data for 2002 and 2013 were reviewed again. Seasonal water level fluctuations between May (high levels) and October (low levels) for 2002 were posted on a topographic surface map. It was found that the seasonal fluctuations varied significantly in space, from less than 5 feet (1.5 m) to more than 30 feet (9 m), which suggests that groundwater levels do not increase the same amount in the aquifer after each rainfall event as most aquifers do. Seasonal groundwater potentiometric surfaces of 2013 were then developed for high and low flow conditions based on more available data within the study area. It was found that the groundwater flow directions and hydraulic gradients vary seasonally. During the high flow season, groundwater flows to the northeast, east, and southeast and diverges over a broad area, and then converges along two surface water drainages, one to the northeast and the other

to the southeast. During the low flow season, groundwater flows to the northeast and east, and converges to the northeast surface water drainage, but not to the southeast drainage. The vertical groundwater flow gradients also change the direction during seasons as shown by the multi-zoned/multi-screened FLUTE™ water level measurements.

The findings of the seasonal change of groundwater flow directions and hydraulic gradients in highly fractured bedrock helped explain the rapid dissipation of the PCE plume downgradient of the extraction well.

Two significantly different parts of the groundwater PCE plume are recognized: A small high-concentration plume ( $>5 \mu\text{g/L}$ ) [0.015 square miles ( $0.039 \text{ km}^2$ ) in area] and a large trace-concentration plume ( $0.02$  to  $5 \mu\text{g/L}$ ) [6 square miles ( $15 \text{ km}^2$ ) in area]. The entire plume is similar to the simulated PCE plume of period 1 by 2003 (1954-2003) shown in Fig. 1. The small plume includes the DNAPL source zone and the high-concentration PCE plume; both are present in the fine-grain regolith and located along a groundwater division. The large plume includes trace PCE concentrations over a broad groundwater stagnation zone in the highly fractured bedrock and then along two surface water drainages, which are eventually discharged at springs/seeps along the creek.

Seasonal rainfall variations [annual average precipitation of 50 inches ( $1270 \text{ mm}$ )] and areal recharge variations cause seasonal variations of groundwater flow directions and hydraulic gradients in the fractured bedrock aquifer, resulting in seasonal variations of preferential groundwater flow paths in the fractured bedrock within the groundwater stagnation zone.



**Fig.1** History matching of simulated PCE plume by 2003 for period 1 (1954-2003)

Extensive spreading of the PCE plume occurs within the large groundwater stagnation zone in the fractured bedrock, which is immediately down-gradient of the extraction well. During high flow season, the PCE mass flux into the fractured

bedrock is spread laterally over a broad area by the divergence of groundwater flow; while during low flow season, the contaminated groundwater flow converges along a relatively narrow path and is transported further downgradient.

However, the impact of seasonal rainfall in the area of contaminant source and high-concentration plume is limited, because the source zone and the high-concentration plume are present in the thick fine-grain regolith.

#### **1.4 Improved conceptual model helped decision making**

A quasi-steady state flow model is not possible to provide a variable flow field for the subsequent fate and transport simulations; however, the existing data were not adequate for developing a transient groundwater flow model.

The extensive spreading effect on the PCE plume due to the varying groundwater flow directions and hydraulic gradients was equivalently simulated using large longitudinal and transverse dispersivities [300 feet (100 m)] in the solute transport model. The history matching simulation results reasonably and conservatively matched the shape, the extent, and the PCE plume concentrations in both the high-concentration part and trace-concentration part of this atypical plume, as well as in the groundwater discharge zone along the creek (Fig. 1). The model then was used to predict the PCE concentrations for various remediation scenarios for the next 160 years.

The modelling results conservatively addressed several key questions regarding future remedial actions, including (1) the hydraulic containment system can be turned off and (2) there is no need for any additional active remediation in the DNAPL source zone or the high concentration PCE plume to protect groundwater quality in the water supply aquifer beyond the property boundary.

Large amount DNAPL will remain in the subsurface for a long time; however, the low

groundwater velocity in the fine-grained, lower permeability regolith will limit the DNAPL dissolution rate. The dissolved PCE mass flux into the fractured bedrock aquifer is small [around 30 lb/year (14 kg/year)], which has been and will continue to be significantly attenuated by extensive spreading mechanism that is caused by seasonal variation of groundwater flow direction and hydraulic gradients as well as by other natural attenuation mechanisms including naturally occurring biodegradation. The predicted extent of the groundwater PCE plume 160 years later is not significantly different from the history matching simulation by 2003 (Fig. 1), indicating that the present PCE distribution is reasonably stable and poses no long-term threat to the water supply.

The modelling conclusions provide a significant potential cost savings by showing that no additional remedial actions are needed at the site to protect future groundwater quality. The cost spent on the modelling, although higher than usual, is only a small cost compared to continuing remediation at the site. Although there is uncertainty in the model predicted future PCE concentrations in the fractured bedrock aquifer, the model results along with the improved conceptual model and field evidence provided a clear rationale that helped final decision making. The model recommended alternative, turning off the existing pumping, has been accepted and implemented in the field.

#### **2 Case 2-a groundwater discharge zone**

A hydraulic containment system with 13 extraction wells has been operated since 2002 to intercept several large-scale groundwater conta-

minant plumes in an agriculture area. In order to optimize the existing hydraulic containment system, the groundwater model was updated during 2006 to 2008. A natural groundwater discharge zone was identified in the middle of a large-scale trichloroethene (TCE) plume during the modelling process. Additional field work confirmed presence of this groundwater discharge zone. The modelling demonstrated that the groundwater discharge zone naturally and effectively intercepts a major portion of the TCE plume, which prevented the potential plume migration towards two large-scale water supply well fields. It also suggested a nearby extraction well is no longer needed.

## 2.1 Problem description

Four large-scale groundwater contaminant plumes, including TCE and Hexahydro-1,3,5-trinitro-1,3,5-triazine (RDX), have been identified in an alluvial aquifer. These plumes occupy an area of approximately 20 square miles ( $50 \text{ km}^2$ ) with variable TCE concentrations up to  $10\,000 \mu\text{g/L}$ . A groundwater hydraulic containment system with 13 extraction wells was designed in 1998 and modified in 1999 and 2002. The design was based on a simple rectangular numerical groundwater flow model, which covered all the plumes. In this simple model, constant-head boundary was prescribed along the upgradient and downgradient boundaries and no-flow boundary was specified on both sides of the model domain. Extensive surface water and groundwater interactions at the site were not initially given enough attention in the model. The design was based on particle tracking simulation results.

## 2.2 A groundwater discharge zone

### directly intercepts contaminant plume

Prior to the groundwater model update, all available geologic, hydrogeological, and historical groundwater sampling data for contamination were thoroughly reviewed. The model was reconstructed to represent the hydro-stratigraphy of the two linked alluvial aquifers and hydrogeological conditions, including natural interior and exterior boundary conditions. The groundwater flow model was rigorously calibrated to observed hydraulic heads and estimated fluxes under both steady state and transient conditions.

Among the interior boundaries, a small creek passes through one of the major TCE plumes. In the early model design, it was uncertain whether the creek was gaining or losing and an extraction well was installed next to the creek with the intent to intercept the contaminant plume.

Groundwater flow model calibration suggested that there were upward hydraulic gradients along the small creek and that groundwater discharged into agriculture drain tiles surrounding the small creek in an approximately one square mile area ( $2.5 \text{ km}^2$ ). This area appears to be the confluence of two alluvial aquifers, *i.e.* where groundwater from the two aquifers converges and discharges to ground surface.

A follow-up field investigation was conducted during the winter of 2007 to 2008. Field evidence indicated that contaminated groundwater discharged to an artesian well, several sustained seeps, a wetland, and several small ponds on a private property. These small ponds did not freeze during the winter even though the surrounding area was frozen, which confirmed the groundwater discharge.

The groundwater modelling results indicated that pumping at the extraction well next to the

creek only increased the local cone of depression but did not change the converging groundwater flow and consequent groundwater discharge to the ground surface in this area. The natural groundwater discharge zone directly intercepts the contaminant plume, and the extraction well is not necessary. Groundwater modelling indicated that public water supply well fields were not in danger of being contaminated by the contaminant plume.

### **3 Case 3-unexpected depletion of contaminant in a NAPL source zone**

Two creosote-dominated NAPL source zones in the subsurface have been targets for active remediation for years. Groundwater modelling focused on dissolved phase constituents to protect downgradient groundwater users. The modelling results show that the dissolved chemical of concern in half of one of the source zones was largely flushed away, which was not expected, as NAPL has always been observed in that source zone. Post modelling groundwater sampling confirms that the modelling results are reasonable. This finding will help the decision-makers by reducing the need for remediation in that source zone. Without modelling, a much larger source zone with a much larger remediation effort and cost probably would be assumed at this site.

#### **3.1 Problem description**

Treated wood constituents were used at a former lumber mill from 1946 to 1969. The wood treating fluids consisted of complex mixtures of different blends of chemical products used over time, product process residues, and spent mixtures. The primary wood treating compounds used at the

site were pentachlorophenol (PCP) and creosote. Creosote predominantly consists of polynuclear aromatic hydrocarbons (PAHs). PCP and PAHs are the primary contaminants of concern (COCs) at the site and they exist as both NAPL and dissolved phase constituents in groundwater. The NAPL at the site is predominantly a dense NAPL (DNAPL), a NAPL denser than water, but some light NAPL (LNAPL) also exists. The dissolved PCP is the most widespread contaminant that exceeds its respective groundwater cleanup level of 1 µg/L.

The historical NAPL disposal was primarily in source zones A and B. The size of each source zone is approximately 500 feet (150 m) by 300 feet (100 m). Source zone A is located hydraulically downgradient of a fire pond that receives water from a creek and stores water for fire protection. Source zone B is located hydraulically cross-gradient of the fire pond. Field tests in 1988 estimated that the fire pond leakage to the aquifer was approximately 5 cfs (0.14 m<sup>3</sup>/s). Large amounts of data were collected from source zone B in 2012, including soil and groundwater sampling for both NAPL and dissolved phases, which improved the understanding of the properties and behavior of the NAPL and dissolved phases in the subsurface.

#### **3.2 Simulation approach for source depletion**

In the solute transport model using MT3DMS (ZHENG and WANG, 1999), the PCP dissolution process from the two NAPL source zones was simulated using an equivalent mass transfer method. In this method, the relationship between NAPL and dissolved PCP was specified using an equivalent NAPL-water partitioning coefficient, which is similar to a soil-water distribution coefficient.

cient for adsorbed soil contaminant.

Compared to the commonly used constant-concentration source or specified-variable-concentration source, this approach allows the following advantages in:

- Specifying a finite mass of contaminant in a source zone based on available site estimates,
- Simulating depletion of the source mass based on calibrated groundwater flow conditions, and
- Reasonable assumptions for source zone parameters based on available sampling data (groundwater and NAPL/soil concentrations).

Using this approach the solute transport model can be used to approximately simulate dissolution of dissolved phase contamination from a finite NAPL source in the aquifer.

### 3.3 Unexpected depletion of contaminant in source zone

A history matching simulation for groundwater PCP plume fate and transport over a 40-year period from 1973 to 2012 was conducted. In the two source zones, the initial PCP concentration was assumed to be 6 000 µg/L (in the range of PCP water-solubility), and the equivalent NAPL-water partitioning coefficient was assumed to be 10 liters per kilogram (L/kg), based on the data collected from source zone B. The simulated PCP concentrations in source zone A decreased from the initial 6 000 µg/L to 0.5 to 10 µg/L in half of the source area after 40 years, while the simulated PCP concentrations in source zone B were still high, varying up to 5 000 µg/L. The significant differences in the simulated PCP concentrations in the two source zones are attributed to: (1) the hydraulic gradient relationship to the fire pond and (2) the calibrated hydraulic conductivity distributions in the two source zones. Source zone A is more permeable and receives a large amount of

fresh water from the upgradient fire pond, while source zone B is less permeable and only receives a small amount of fresh water laterally from the fire pond.

The simulated PCP concentrations in 2012 in source zone A were unexpected, as it was believed that groundwater PCP concentrations must be high because NAPL was always observed in the monitoring wells. No sampling was conducted for source zone A for almost 20 years, partially due to earlier groundwater sampling results being influenced by NAPL presence in the monitoring well. To verify the model predicted PCP concentrations, groundwater sampling was conducted in 2013 within source zone A using an improved sampling technology. The 2013 groundwater sampling results were surprisingly consistent with the model predicted PCP concentrations, including the local distribution of concentrations within source zone A. This finding also suggests that NAPL presence does not necessarily mean that high dissolved PCP concentration can be expected to occur.

The close match of the model prediction to the unexpected field conditions can be primarily attributed to: (1) Rigorous groundwater flow model calibration to the independently estimated fire pond leakage and to the observed hydraulic heads, and (2) reasonable simulation of the dissolution of PCP from the NAPL phase using the equivalent NAPL-water partitioning coefficient method with appropriately estimated parameters based on understanding of the NAPL composition and properties.

## 4 Conclusions

The real-world modelling cases presented above suggest that as long as a model is developed

rigorously for the stated purpose, groundwater modelling is a valuable process for gaining insight of site conditions. The improved understanding of contaminant conditions represents a significant time and cost savings for groundwater remediation projects.

Whether a groundwater model is useful depends on whether the conceptual model represents the field reality with respect to its intended objective. For real-world modelling projects, there are always limitations in data availability, budget, and schedule. Within these limitations, a conceptual model can be improved during the modelling process depending on the modeler's motivation and professional experience. Improvement of a conceptual model requires the modeler to search through all available data for evidence and to figure out rational explanation. The advantage for a modeler is that he or she can

use a numerical groundwater model as a convenient tool to help logical thinking.

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