# Multiphase Simulation of DNAPL Migration for Site Characterization

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ABSTRACT
Chlorinated solvents, which are low-viscosity, dense non-aqueous liquids (DNAPLs), have been released over approaching the past hundred years into the subsurface both intentionally and unintentionally. Such solvents have caused widespread ground-water contamination, incurred huge costs and have produced complex subsurface characterization problems for those involved in remedial design and risk assessment. To date, few attempts have been made to employ multiphase simulators to predict the migration, trapping and dissolution of spilled DNAPLs in order to assist in site characterization operations. This paper demonstrates how it is possible to use multiphase computer models to design characterization plans for implementation at DNAPL sites based upon limited knowledge of the geology, release rates and the physical-chemical properties of the DNAPL.

RÉSUMÉ
Les solvants chlorinés, qui ont une viscosité basse et sont des liquides denses non-aqueux (DNAPL), ont été relâchés sous la surface de la terre au courant des preseque dernières cent années intenionnellement et non-intentionnellement. Ces solvants ont déjà causés de nombreuses contaminations d'eaux souterraines, ont entraîné des coût énormes et ont produits des problèmes pour la caractérisation des régions souterraines pour ceux et celles impliqués dans l'atténuation et la gestion des risques. À date, peu d'essais ont été entrepris pour effectuer des simulations multiphasiques pour prédire la migration, le piégeage et la dissolution des DNAPL répandus pour assister avec les opérations de caractérisation d'un site. Cet article démontre comment il est possible d'utiliser des modèles informatiques multiphasiques pour conçevoir des plans de caractérisation et les implanter aux sites contaminés par des DNAPL en utilisant des connaissances limitées de la géologie, des taux de relâchement et des propriétés physicaux-chimiques du DNAPL.

## 1 INTRODUCTION

The characterization of DNAPL sites poses difficult problems that become more complex and much more costly as the size of the potential DNAPL zone increases due to the expense of drilling, coring and chemical analysis. While it is quite difficult to *detect* dense non-aqueous liquids (DNAPL) contamination in alluvium, whether they are viscous DNAPLs such as creosote and coal tar or low-viscosity solvents such as trichloroethylene, the *quantitative mapping* of the spatial distribution of chlorinated solvents in the subsurface is a far more stubborn problem. Such quantitative information is needed to determine the costs and duration of DNAPL remediation, whether it be pump-and-treat or some method of DNAPL recovery.

## 2 THE USE OF MULTIPHASE SIMULATORS FOR PREDICTING DNAPL MIGRATION

Although it is possible to interpret soil chemical data from borehole cores quantitatively to yield the DNAPL saturation (i.e., volume of DNAPL per unit volume of pore space), e.g., Mariner et al. (1997), such an approach depends on mapping DNAPL sites using exploratory drilling and coring, which becomes prohibitively expensive at sites where the DNAPL zone exceeds a few tens of cubic meters of alluvium. Because of the heterogeneity of alluvial sediments, all experimental research to date (see Pankow and Cherry, 1996) points to the conclusion that the DNAPL distribution itself must also be strongly spatially heterogeneous and therefore not amenable to a simple drilling and coring approach if quantitative mapping of DNAPL is the goal. Furthermore, the common techniques in use for characterizing core samples only indicate the presence or absence of DNAPL within a borehole, not its concentration (i.e., saturation) either at that point in space or even over short distances away from it. Consequently, the quantitative characterization of DNAPL zones by drilling, coring and sampling alone can cause long-term uncertainties in the cost of – or even the need for – DNAPL remediation.

While geophysical tools are critical for stratigraphic definition, claims that geophysical methods are able to identify DNAPL source zones at depth -- including the claim made for the same DNAPL zone as is considered in this paper (Temples et al, 2001) -- have been contradicted by field confirmation drilling that found the geophysical anomalies “do not indicate the presence of DNAPL-rich zones” (Rohay et al., 2002). Therefore, partitioning tracer testing has been used at some sites to quantify the spatial distribution of DNAPL in-situ over interwell distances of 10-40 meters (30-110 feet) but, although it has been demonstrated to be reliable in quantifying DNAPL volumes even in low-permeability lenses in both the saturated and unsaturated zones of aquifers, it is both costly and complex (Jackson and Jin, 2005 and references therein).

In their review of multiphase flow and transport modeling, Adeel et al. (2000), indicate that the “evaluation of historical migration of NAPL and its present occurrence" is a potential use of multiphase simulators. They describe the use of one- and two-dimensional simulations of two-phase flow beneath the S-Area Landfill in Niagara Falls, New York in the 1980s. However, such predictive simulations have not become commonplace in site characterization practice, consequently a useful tool may have been neglected by hydrogeologists and geoenvironmental engineers.

This neglect is likely because of the specialized nature of multiphase simulators and the requirement for multiphase parameter values and field data as inputs to the models. However, these parameters and data can be obtained or estimated to allow the use of such simulators when the need arises.

Consequently, when soil-vapor and ground water analyses indicate widespread contamination in alluvial aquifers and the geometry of the DNAPL source zone is unclear, it may become desirable to use multiphase (i.e., DNAPL, water, air) simulation to guide site characterization plans so that drilling and coring operations can be conducted in an optimal manner. This is particularly the case where the groundwater systems are large and correspondingly large dissolved-phase plumes of chlorinated hydrocarbons derived from solvent releases have been mapped but the source zones containing the DNAPL remain poorly understood (Jackson, 1998).

A further complication arises from the depth of the regional water table in semi-arid areas, such as the Western US states, which necessitates the use of three-phase simulation. In this context, multiphase simulation is used to model various scenarios of DNAPL migration and re-distribution in the alluvium, and embedded capillary barriers within the alluvium, to allow the development of site investigation programs that will identify the present distribution of DNAPL within the alluvial aquifer – both saturated and unsaturated zones – so that remedial operations may be optimized and risks estimated.

The example used in this study is to develop a conceptual model of the distribution of carbon tetrachloride (CT) in the subsurface at the Hanford Site, a former nuclear-materials processing site in Washington State, USA operated by the US Department of Energy (DOE). Majer et al. (2002) reported that drilling costs at Hanford for a 50 m deep borehole exceed $1 million because of the presence of radioactive contamination, consequently geophysical and simulation tools are essential to reduce site–characterization costs. Through the numerical simulation and subsequent sensitivity studies, the simulation results provide a best estimate of the distribution of mass of CT beneath the disposal areas.

The simulation results also can be used to answer the questions of whether the DNAPL resides primarily above the aquitard that protects the regional aquifer system and whether there is a continuing source of DNAPL contamination to ground water, and, if so, what is the position of the source in relation to the water table. Lastly, the simulation results can be used to determine whether the bulk of DNAPL resides below the disposal trenches and whether the remaining DNAPL will influence compliance levels in the future.

## 3 DESCRIPTION OF THE FLOW SYSTEM

The Hanford Site is a U.S. Department of Energy (DOE) facility on the Columbia Plateau of south-central Washington State, where nuclear materials were produced during World War II and the Cold War that followed. Carbon tetrachloride (CT), a chlorinated solvent DNAPL, was used in the nuclear-materials separations process at the Hanford site. From 1955 to 1973, an estimated total of between 363,000 to 580,000 L of liquid carbon tetrachloride in solution with other compounds were disposed into the soil at three disposal facilities in the 200 West Area, in particular, the 216-Z-9 trench area. CT disposal has caused the contamination of an area of over 11 km$^2$, in which ground water exceeds the drinking water standard of 5 µg/L, and groundwater samples collected 30 years after disposal ended contain high CT concentrations (3-5 mg/L; see Figure 1) that indicate CT DNAPL is still present in the saturated zone. Although approximately 53,500 L of CT has been removed from the subsurface by soil vapor extraction and ground water pump-and-treat operations as of 2001, the CT plume continues to increase in size and modeling shows that contamination is moving from the 200 Area Plateau towards the Columbia River, which is approximately 20 km downgradient of the leading edge of the plume.

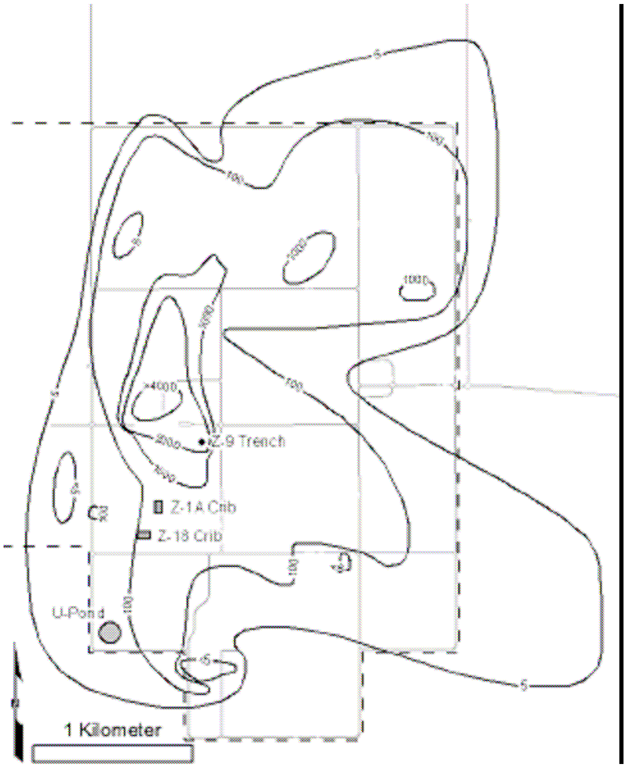

Figure 1: The carbon tetrachloride plume in the Ringold aquifer at US DOE Hanford Site, Washington state. The principal source of the CT plume is the Z-9 trench.

This contamination has caused DOE to consider various approaches to the development of a new site characterization plan for the DNAPL zone. However, all approaches must consider the very difficult drilling environment due to the presence of very large boulders transported by the Ice-Age floods that inundated the Hanford area of Washington and which are difficult to penetrate with conventional drilling tools. The Cold Creek Carbon-Rich Unit, a relatively low-permeability layer of caliche upon and within which much of the CT is suspected to be trapped (Rohay et al., 2002), is ~45 m below ground surface (bgs). Vapor concentrations of >10,000 ppmv have been measured directly below the DNAPL entry location but above the Cold Creek Unit at the 216-Z-9 trench area and at ~100 ppmv beneath the Cold Creek Unit but above the water table.

The water table is ~70 m deep and continues to drop due to groundwater extraction to contain the CT plume, which may be causing continuing drainage of DNAPL as pores convert from two-phase (ground water and DNAPL) to three-phase (ground water, DNAPL and air) conditions (Jackson et al., 2006). Aqueous CT concentrations at the top of the water-table aquifer beneath the 216-Z-9 trench area are currently ~3,000 µg/L, although they are reach 4,000 µg/L in several wells 400 m northwest of the 216-Z-9 trench area (Dresel et al., 2005). Without an understanding of the spatial distribution and quantity of CT, DOE is not in a position to develop a long-term remediation strategy that will prevent target concentrations from being exceeded at the compliance boundary.

## 4 HYDROSTRATIGRAPHY

The Hanford site is positioned above a regionally unconfined aquifer comprising four principal geologic units; the Holocene sands and silts; the Hanford Formation, the Cold Creek Unit; and the Ringold Formation. A plan view of the 200 West Area including the CT disposal areas is shown in Figure 1 together with the CT plume in the Ringold aquifer at > 70 m depth. A generalized geologic cross-section through the CT disposal sites is shown in Figure 2. Holocene-aged aeolian sand and silt and some anthropogenic backfill overlie the Hanford formation sediments throughout the 200 West Area. The Hanford formation was deposited during the Pleistocene-age Lake Missoula floods. Locally, the Hanford formation can be divided into four sub-units, of which three are present at the Z-9 site.

The Cold Creek or Plio-Pleistocene Unit is a quasi-continuous feature limited to the 200 West Area. The importance of this unit lies in its potential to impede the vertical migration and promote the lateral distribution of waste fluids emanating from the source areas.

Beneath the Plio Pleistocene Unit is the Ringold aquifer – Ringold E in Figure 2 – consisting of fluvial gravels and sands, overbank deposits, and lacustrine silty sands, silts and clays deposited by the ancestral Columbia River. Underlying the Ringold aquifer is the Ringold Lower Mud sequence, which defines the bottom of the regional unconfined aquifer.

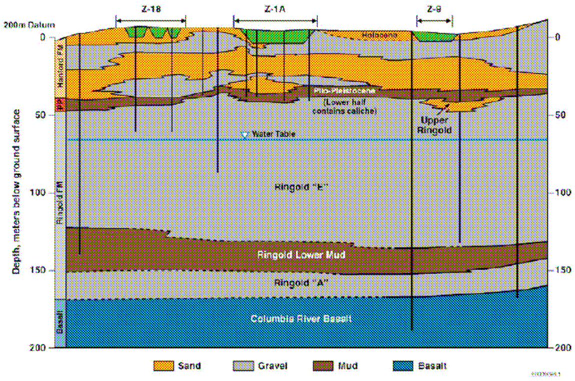

Figure 2: Hydrostratigraphic model of the Hanford Site.

## 5 HYDROGEOLOGY

The unconfined aquifer lies almost entirely in Ringold Unit E gravels. Estimates of saturated hydraulic conductivity range from 2.9 x $10^{-2}$ to 8.8 cm/sec at Hanford. The water table is approximately 106 meters (350 feet) beneath the center of the site. Perched water was identified in association with the Cold Creek Unit during the drilling of two wells in the vicinity of the 216-Z-9 Trench and in several wells nearby (Rohay et al. 1994). Based on interpretation of geologic logs, the Cold Creek Carbonate-Rich Unit is the confining layer in 216-Z-9 Trench area wells.

Regional groundwater flow is generally west to east, however the direction of ground water flow within the 200 West Area has been greatly influenced by ground water mounding due to the disposal of large volumes of waste water some 3000 feet southeast of the CT source areas at the U pond (see Figure 1). Wastewater disposal at the U pond ceased in 1984 and ground water levels beneath the CT source areas have since been declining at an approximate rate of 0.6 to 0.8 metres per year. The natural recharge rate used in previous modeling studies ranged from 5 mm/yr (Oostrom et al., 2003a) to 50 mm/yr (Piepho et al., 1993).

## 6 UTCHEM MODEL DEVELOPMENT

Simulations of CT DNAPL release were conducted with UTCHEM (Delshad et al., 1996; Pope et al, 1999), which is a three-dimensional, multi-component, multiphase, compositional simulator originally developed for use in enhanced oil recovery. It is capable of simulating (1) organic component dissolution into ground water, (2) multiphase flow including three-phase flow in the unsaturated zone and two-phase flow in the saturated zone, (3) aqueous-phase solute advection and dispersion and (5) organic solute biodegradation.

### 6.1 Stochastic Permeability Model Construction Methodology

The development of the detailed site-specific model was approached in four stages. First, a site-wide three-dimensional hydrostratigraphic model was constructed based on the geology and hydrostratigraphic information presented in the previous section. The data for individual boreholes was interpreted in coordination with cross-borehole correlations and the geologic contacts ('picks'). The model developed in this stage is called the solid model.

The next step in the model development was the creation of local-scale solid model to support detailed flow and transport simulations of a single disposal site, i.e. the 216-Z-9 Trench. The local-scale solid model was developed by sub-griding the regional solid model. Thirdly, a stochastic permeability field was generated for each geological unit based upon its stochastic properties, i.e., the mean and standard deviation of hydraulic conductivity, and correlation length. Finally, the permeability fields thus generated were populated into the non-uniform simulation grid.

Stochastic-based permeability fields are a significant refinement over previous simulation studies (Piepho et al., 1993, Oostrom et al., 2003a) as they more realistically account for field-scale heterogeneities. Whereas these models are premised on the assumption that each stratigraphic unit is homogeneous, the saturated hydraulic conductivity of each stratigraphic unit is varied over a range of values in each of the stochastic-based models. Each stratigraphic unit is divided into grid blocks, the size of which is based on correlation lengths derived from the variogram, which was based upon data presented in Oostrom et al. (2003a), and a different conductivity is assigned to each block. Therefore, to the extent that data variability accurately reflects field conditions (rather than measurement error), the stochastic distribution simulates variability in the hydrogeologic system.

The hydraulic conductivity distributions are based on stochastic properties presented in Oostrom et al. (2003a,b) and summarized in Table 1. A Fast Fourier Transform (FFT) stochastic permeability field generator was used for this purpose (courtesy of J. Jennings, Bureau of Economic Geology and University of Texas at Austin). The permeability field assumes a lognormal permeability distribution and an exponential variogram.

Figure 3 shows a three-dimensional view of the solid model for the 216-Z-9 trench area. This model covers an area of 244 m x 244 m with the trench located at the center of the domain. The top of the model domain represents the bottom of the trench at an elevation of 198 m above mean sea level (amsl). The bottom of the model domain represents the top of the Ringold Lower Mud at 76 m amsl. A non-uniform simulation grid was used in order to minimize computational requirements with finer discretization used near the trench at stratigraphic unit boundaries. Figure 4 is a view of the 216-Z-9 trench model populated with a stochastic permeability field. A statistical summary of the porosity and hydraulic conductivity distribution of this model is provided in Table 2.

Table 1: Summary of statistics used to generate stochastic hydraulic conductivity distributions.

| Hydro-stratigraphic Unit | Hydraulic Conductivity (m/s) | | Correlation Length (m) | |
|---|---|---|---|---|
| | Mean | Std. Dev. | Lateral | Vertical |
| Hanford Upper Coarse (Hc) | 5.04E-5 | 3.69E-4 | 15 | 1.8 |
| Hanford Middle Fine (Hf) | 5.81E-6 | 4.70E-5 | 15 | 1.8 |
| Hanford Lower Coarse (Hlc) | 3.00E-5 | 2.70E-2 | 15 | 1.8 |
| Hanford Lower Fine (Hlf) | 1.93E-5 | 1.30E-4 | 15 | 1.8 |
| Cold Creek Silt (PPlz) | 1.55E-7 | 4.00E-6 | 50 | 1.8 |
| Cold Creek Carbonate Rich (PPlc) | 6.69E-6 | 4.21E-4 | 50 | 1.8 |
| Ringold | 7.95E-6 | 1.20E-4 | 15 | 1.8 |

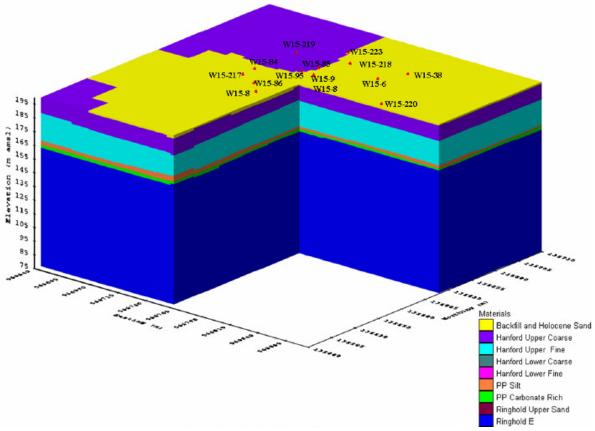

Figure 3: Solid model of the hydrostratigraphic units.

Table 2: Porosity and stochastic hydraulic conductivity distribution for the 216-Z-9 Trench Model. K in m/s.

| Hydrostratigraphic Unit | Porosity | K (mean) | K (std dev) |
|---|---|---|---|
| Hc | 0.17 | 5.04E-4 | 3.69E-3 |
| Hf | 0.37 | 5.81E-5 | 4.70E-4 |
| PPz | 0.42 | 1.55E-6 | 4.00E-5 |
| PPc | 0.32 | 6.69E-5 | 4.21E-2 |
| Ringold | 0.24 | 7.95E-5 | 1.20E-3 |

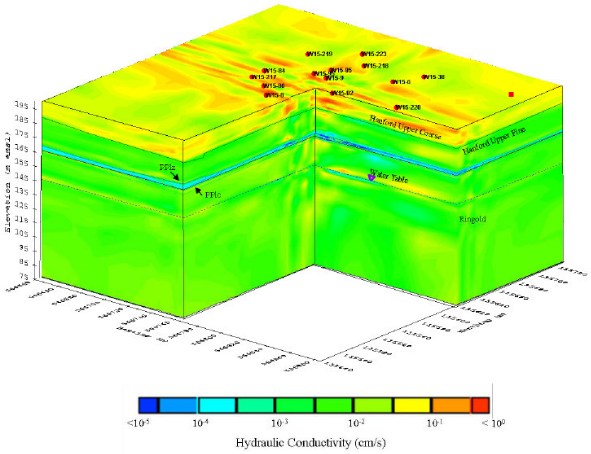

Figure 4: Upscaled stochastic permeability field.

## 7 SIMULATION OF DNAPL RELEASES

The process of simulating various scenarios of DNAPL migration was an iterative one. There are a number of parameters that have a major influence on the CT distribution but their exact values are uncertain. Sensitivity studies are conducted by adjusting these variables within their ranges of uncertainty. For this investigation study, in addition to the “Base Case”, a total of 15 additional sensitivity simulations were conducted to study the fate and transport of the CT under different conditions to formulate the potential distribution scenarios. The results of these sensitivity studies were then used to determine the most likely distribution scenarios.

During the course of the sensitivity studies, it was concluded that: (a) the PP or Cold Creek units were of considerably lower permeability than represented in Table 2; (b) the CT DNAPL was diluted with machining oil that would raise its viscosity and lower its density significantly; and (c) the residual CT DNAPL saturations in the vadose zone would be very low due to film drainage caused by a positive spreading coefficient (Dwarakanath et al., 2002). Therefore, to represent the most probable scenario for the fate of the CT DNAPL beneath the Z-9 trench, the permeabilities in the Cold Creek units were reduced from the permeabilities presented in Table 2 by a factor of 10.

### 7.1 Model Input Parameters

The UTCHEM model input data fall into two major categories: the model data and the process data. The model data include:

- Aquifer properties (hydraulic conductivity distribution and sediment texture)
- Fluid properties (density, viscosity, interfacial tension and composition of water and DNAPL)
- Source terms (CT release history, i.e., volumes, composition and rates)
- Boundary conditions (control the direction of flow and the hydraulic gradient)
- Initial conditions (e.g., water saturations in the vadose zone beneath the disposal areas and the elevation of the water table)

These input parameters are assembled by synthesizing the information obtained from previous site characterization activities, numerical simulation and laboratory studies. The following is a brief summary of the sources of information from which the input parameters were obtained.

The hydrogeological and petrophysical properties were believed to be well known due to previous work (e.g., Oostrom et al., 2003b; Piepho, 1996), although the effect of heterogeneity was obviously considerable.

We surmised that the DNAPL itself had very different properties from those found in the literature for carbon tetrachloride solvent. The interfacial tension for CT was set a 10 dynes/cm rather than the literature value of 40 dynes/cm. This is because field samples of chlorinated solvents, such as CT, have much lower interfacial tensions than laboratory reagent-grade samples of the same solvent (e.g., Dwarakanath et al., 2002). It is believed that this is due to the incorporation of other organic liquids within the solvent that partition to the interface of the solvent with water and cause a reduction in interfacial tension. In the case of the Hanford CT, it is well established that machining oil oil was present in the effluent solvent that was likely to cause a significant reduction in interfacial tension as well as in the DNAPL density, while the DNAPL viscosity would increase. The solubility of CT was left unchanged from literature values, although it is likely that the presence of oil in the DNAPL would have reduced it by 10-50%.

The Brooks and Corey (1966) model was used to calculate the capillary pressure between the three phases – air, water and DNAPL. Capillary pressure in the Brooks and Corey capillary pressure-saturation relationship is scaled for interfacial tension, permeability, and porosity (Leverett, 1941).

The DNAPL spill event in the vadose zone is assumed to be in the imbibition direction, i.e., the DNAPL displaces air and, to the limit of its residual saturation, water. The DNAPL spill event in the saturated zone is taken to be in the first drainage direction for the entire spill process, i.e., the system remains water wet while water drains from the pores. Implicit in the capillary pressure formulation for the vadose zone where three phases exist, is that the direction of descending wettability is water, CT, and air, and that the water phase is always present.

The Brooks-Corey model is

$$\left(\frac{P_b}{P_{cw\ell}}\right)^{\lambda} = 1 - \frac{S_\ell - S_{\ell r}}{1 - S_{ar} - S_{wr} - S_{or}} \quad [1]$$

where $l$ = a (air) or w (water), $P_{cwl}$ is the capillary pressure between water and phase $l$, $\lambda$ is a measure of the pore size distribution of the medium, $S_l$ is the saturation of phase $l$, $S_{lr}$ is the residual saturation of phase l, and $S_{ar}$, $S_{wr}$ and $S_{or}$ are the residual saturations of air, water and DNAPL (oil), respectively.

The entry pressure ($P_b$) is given by:

$$P_b = C_{pci} \frac{\sigma_{w\ell}}{\sigma_{wo}} \sqrt{\phi / k} \quad [2]$$

where $l$ = a or w, $C_{pci}$ is the UTCHEM input parameter, $\sigma_{wl}$ is the interfacial tension between water and phase $l$, $\sigma_{wo}$ is the interfacial tension between water and DNAPL, $\Phi$ is the porosity, and $k$ is the formation permeability. The input parameter $C_{pci}$ was obtained by fitting the equation to experimental data presented by Oostrom et al. (2003b).

The entrapped DNAPL saturation for three-phase (air/DNAPL/water) flow is based on a function by Fayers and Matthews (1982) which uses the two-phase entrapped saturation values:

$$S_{or} = S_{orw}\left(1 - \frac{S_a}{1 - S_{wr} - S_{ora}}\right) + S_{ora}\left(\frac{S_a}{1 - S_{wr} - S_{ora}}\right) \quad [3]$$

where $S_{orw}$ and $S_{ora}$ are the entrapped DNAPL saturations to flowing water and air phases, respectively. The residual saturations from the Brooks and Corey model are the input parameters in the relative permeability function.

## 7.2 Relative Permeability

The multiphase relative permeabilities were modeled based on Corey-type functions (Brooks and Corey, 1966). In the vadose zone, it was assumed that water and air relative permeabilities are unique functions of their respective saturations only. DNAPL relative permeability, however, is assumed to be a function of two saturations. These assumptions are consistent with relative permeability measurements (e.g., Oak *et al.*, 1990).

$$k_{r\ell} = k_{r\ell}^{o} \left(S_{n\ell}\right)^{n_\ell} \quad [4]$$

where $l$ = w, o, or a and the normalized saturations are defined as

$$S_{n\ell} = \frac{S_\ell - S_{\ell r}}{1 - S_{wr} - S_{or\ell} - S_{ar}} \quad [5]$$

for $l$ = w or a. For DNAPL

$$S_{no} = \frac{S_o - S_{or}}{1 - S_{wr} - S_{or} - S_{ar}} \quad [6]$$

The relative permeabilities in the saturated zone for water and DNAPL are

$$k_{rw} = k_{rw}^{o}\left(\frac{S_w - S_{wr}}{1 - S_{wr}}\right)^{n_w} \quad [7]$$

and

$$k_{ro} = k_{ro}^{o}\left(\frac{S_o}{1 - S_{wr}}\right)^{n_o} \quad [8]$$

The residual saturations, relative permeability endpoints, and exponents are input parameters. The residual saturations vary from 0.02 for $S_{ora}$ to 0.245 for the Cold Creek or PPlc carbonate aquitard. The relative permeability endpoints for groundwater are 0.5 for the sand and gravel units and 0.1 for the aquitard; the relative permeability for DNAPL is everywhere 0.9 and 1.0 for the air phase. The exponent is 2.5.

## 7.3 Source Terms

The description of the source release histories was presented in the 1994 Conceptual Model report for 200 Area West (Rohay et al., 1994). The release histories were used to generate the CT DNAPL source terms for the simulations. Infiltration of water and DNAPL began in 1955 and was estimated at 700 and 10 L/day, respectively. This rate increased during the Cold War to 1900 and 130 L/day in 1961 before decreasing and then ending in 1962 by which time 3780 cubic metres of water and 232 cubic metres of CT solvent had been discharged to the Z-9 trench.

## 7.4 Boundary and Initial Conditions

The saturated zone boundary conditions consist of constant pressure heads on the west and east ends of the model domains allowing water to flow into or out of these boundaries. No-flow boundaries were used at the north and south ends of the models. A hydraulic gradient of 0.001 in the saturated zone was used for flow from the west side toward the east side of the model domain. An interpreted 1954 average water table elevation of ~ 145 m above mean sea level (m amsl) was assumed. Seasonal fluctuations of the water table or the changing of ground water flow direction due to the operation of the pump-treat system were not considered. Air pressure was fixed at one atmosphere at the ground surface for the unsaturated zone with no barometric pressure oscillations included. The initial air and aqueous phase pressure distributions in the domain were obtained by conducting equilibrium simulations using the interpolated water levels, the specified boundary conditions, and a recharge rate of 0.5 cm/year for 100 years. It was assumed that no CT was present in the domain at time zero.

## 8 MOST PROBABLE SCENARIO

In addition to the base case, some 15 scenarios were simulated. Figure 5 shows the most probable scenario of CT migration, trapping and dissolution in three dimensions (3D) in 2003. The results were post processed using EarthVision software. This particular scenario was based upon the work of Oostrom et al. (2003a) and others who had conducted earlier simulations without employing stochastic permeability fields. However, as noted above, the permeabilities in the Cold Creek units were reduced to account for the field distribution of CT. Otherwise, this scenario resembled earlier scenarios in that it represented a consensus of opinion on the likely structure of the flow system beneath 200 West Area.

The results indicate that there is relatively small amount of CT reaching the Ringold aquifer and significant amount of CT lateral pooling and spreading on top of the Cold Creek Silt Unit. The CT penetrates the Cold Creek units only through high permeability 'windows' in the Cold Creek Unit to reach the Ringold (vadose and saturated zones) Formation. The results also indicate that high DNAPL saturations are located in the Cold Creek Silt (PP) Unit and small but significant saturations in the saturated zone of the Ringold fm.

Figure 5 shows the aqueous CT migrated eastwards towards the Columbia River, the regional groundwater discharge area. The simulation results indicate that there is a significant amount of spreading of aqueous CT plume in the saturated zone of the Ringold as well as in the vadose zone of the Cold Creek or Plio Pleistocene Unit. The minimum aqueous CT concentration contour is 0.1 µg/L and the maximum CT concentration (i.e., the aqueous solubility of CT) is located in the vicinity of where the CT residual resides. Away from the CT source, the concentrations decrease as a result of hydraulic mixing. The predicted values exceed 100 mg/L at the water table and decline to 0.1 µg/L approximately 50 m below the water table.

Measured CT concentrations in the Ringold aquifer beneath the source zone at the 216-Z9 trench are in the range of 1,000-4,000 µg/L (Dresel et al., 2005), however sampling is usually from wells with long (16-26 m) screens rather than from multi-level monitoring systems resulting in considerable in-well mixing and dilution. Furthermore, the presence of CT in mg/L concentrations in high-permeability alluvium over 30 years after CT disposal points to the continuing presence of DNAPL beneath the water table.

## 9 CONCLUSIONS

The use of the Hanford example points to an approach in other western ground water basins that would stress the value of improving information related to (a) the rate and volume of DNAPL released, (b) the geometry and physical-chemical properties of important capillary barriers to DNAPL migration, and (c) the measurement of the relative permeability and capillary pressure vs. DNAPL saturation in the alluvium defined with respect to its texture.

Unfortunately this information is so frequently absent from site-investigation reports that these conclusions are of little help to the geoscientist or engineer given the task of designing a characterization plan (Jackson, 1998). However, as with groundwater flow and transport modeling, the use of multiphase simulators provides a framework within which quantitative DNAPL migration models can be tested and DNAPL characterization planning put on a rational footing.

The critical issue that these simulations suggest for groundwater flow systems is whether the volume of DNAPL assumed released was sufficient to either (a) be laterally diverted by a capillary barrier present at depth or (b) penetrate it due to its exceedance of the entry pressure of the barrier. Given the typical uncertainty in the DNAPL volume released and the ubiquity of capillary barriers, this study indicates the need for the integration of hydrostratigraphic, geophysical and petrophysical investigations to constrain the uncertainty in the DNAPL migration pathways in these basins.

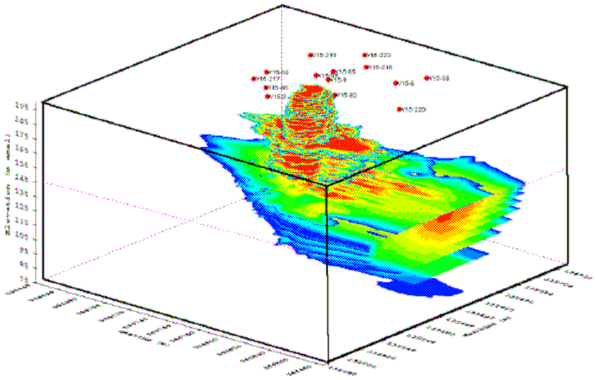

Figure 5: 3D structure of aqueous CT plume in 2003 emanating from the Z-9 trench. The red beneath the trench indicates concentrations approaching the aqueous solubility (800 mg/L) while blue at the base of the Ringold aquifer indicates a concentration of 1 µg/L.

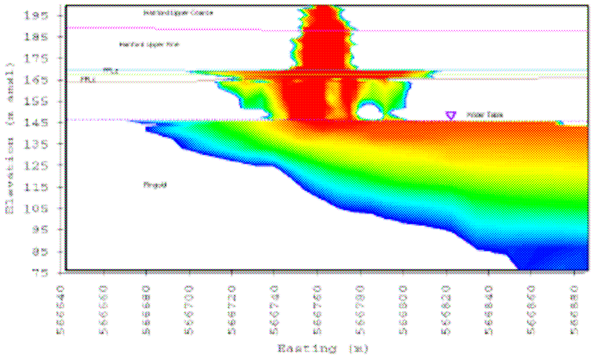

Figure 6: Cross-sectional (E-W) view of aqueous CT plume in 2003 emanating from the Z-9 trench.

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