ABSTRACT

WARREN, KIMBERLY ANNE. A Fundamental Investigation of Well Injection Depth Extraction (WIDE) System Performance Aspects in Fine-Grained Soil Contaminated with Trichloroethylene. (Under the direction of Mohammed A. Gabr).

This research consisted of three components: the field demonstration, laboratory experimentation, and finite element analysis. Global WIDE system performance (in-situ ground water and contaminant transport) was investigated during the field demonstration, PVW performance was examined during laboratory experimentation, and contaminant partitioning tendencies were evaluated as a function of time and operational scheme during the finite element analysis.

The field demonstration was conducted at a site located in Ashtabula, Ohio. With the exception of a silt seam located approximately 1.8 m to 2.4 m below the ground surface, the subsurface consisted of clay (CL) and the in-situ permeability was determined to be approximately $1 \times 10^{-6}$ cm/s. TCE contamination levels as high as 300,000 µg/kg were detected on the soil, and concentrations as high as 475 mg/L were detected in the ground water. A 21.0 m by 18.3 m WIDE demonstration system was installed over an area that encompassed a TCE plume. The test area was divided into four quadrants and 494 PVWs were installed to a depth of 6.1 m. Concurrent injection extraction, alternating row extraction, and full quadrant extraction operations took place over a nine month demonstration. Vacuum pressure, injected and extracted fluid volumes, TCE concentrations (gas and soluble-phase), and water table levels were monitored.
A 10 kPa laboratory tracer test experiment was conducted using a 1.0 m$^3$ clay slurry sample with a high permeability soil seam, similar to field conditions. The test box was lined with a geocomposite to provide a constant head reservoir boundary around the test sample. Three settlement plates, 23 piezometers, and 27 tracer tubes were installed to monitor settlement, pressure head, and chloride (Cl) tracer concentration, respectively. The zone of influence and PVW geometry effects were evaluated.

NAPL Simulator (a three-dimensional finite element analysis model) was calibrated using hydraulic field data and then used to simulate soluble and gas-phase contaminant transport in saturated and unsaturated soil media. Using a reference case, a parametric evaluation was initially performed to establish the input variables that significantly affect contaminant transport. System performance and contaminant partitioning tendencies were evaluated as a function of time and operational scheme. Finally, a sensitivity analysis, consisting of 36 simulations, was performed to evaluate contaminant partitioning tendencies as a function of the PVW spacing, extraction water flow rate, and mass transfer coefficient.
A Fundamental Investigation of Well Injection Depth Extraction (WIDE) System Performance Aspects in Fine-Grained Soil Contaminated with Trichloroethylene

by

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BIOGRAPHY

Kimberly Anne Gates was born in Houston, Texas on July 22, 1974 and raised in Springfield, Virginia. She graduated from Robert E. Lee High School in 1992 and subsequently enrolled in the Civil Engineering Program at Virginia Tech. Beginning in the summer of 1993, she worked for G.K.Y & Associates (a Civil Engineering consulting firm located in Springfield, Virginia) as a cooperative education student for four semesters. She performed research in the hydraulics laboratory at the Federal Highway Administration Research Center, located in McLean, Virginia. In December of 1996, she received a Bachelor of Science Degree in Civil Engineering, with honors, from Virginia Tech.

Following graduation, Kimberly secured a geotechnical engineering position with Law Engineering in Raleigh, North Carolina, and initiated her graduate education at North Carolina State University during the fall semester of 1997. She was a teaching assistant for two semesters and received the Kimley-Horn Graduate Teaching Award for the 1998-1999 academic year. Kimberly received her Masters of Science Degree in Civil Engineering from North Carolina State University in August of 1999 and was offered a Dean Fellowship at North Carolina State University to continue her graduate education as a Ph.D. candidate.

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Kimberly was married to Bruce Warren on September 2, 2001. She will begin her career as an assistant professor at the University of Arkansas, located in Fayetteville.
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I would also like to acknowledge the efforts set forth by Reactive Metals Incorporated (RMI) employees in Ashtabula, Ohio and Nilex Corporation in Colorado Denver. RMI employees assisted the team from North Carolina State University during the field installation and data collection process. Nilex Corporation installed the field demonstration test pad.
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1. INTRODUCTION

1.1. Introduction

Contamination in low-permeability, fine-grained soils poses a significant technical challenge to in-situ remediation efforts. While conventional pump-and-treat systems can be effective for containment and has been proven to decrease contaminant levels in cohesionless soils, these systems typically exhibit tailing and rebounding effects over time in reactive fine-grained soils. Tailing refers to the progressively slower rate of decline in recovered contaminant concentration with continued operation of a pump-and-treat system, while rebounding refers to the rapid increase in contaminant concentration that occurs after pumping is discontinued for an extended period of time (EPA, 1996).

Contaminant diffusion, adsorption-desorption kinetics, and dissolution processes contribute to contaminant movement retardation. In addition, Non-Aqueous Phase Liquid (NAPL) zones existing in the subsurface can act as continual sources. Due to these limitations, most contaminated sites are unable to reach target maximum contaminant levels (MCLs) using conventional pump-and-treat remediation technology, as presented by the National Research Council (1994), the U.S. EPA (1989), Travis and Doty (1990), Haley et al. (1991), and Bartow and Davenport (1995).

In addition to the technical limitations, conventional pump-and-treat technology is expensive to design, install, and operate, and it must be maintained and operated for decades before accurate cleanup time projections can be made (Hoffmann, 1993). Recognizing that inadequate technology is a critical limiting factor in meeting federal
cleanup standards, the U.S. Environmental Protection Agency (U.S. EPA), Department of Defense (DOD), and the Department of Energy (DOE) initiated programs to develop new and innovative environmental remediation technologies (NRC, 1994).

1.2. Well Injection Depth Extraction (WIDE) Technology Overview

The Well Injection Depth Extraction (WIDE) system is an enhanced pump-and-treat remediation system that utilizes geosynthetic prefabricated vertical wells (PVWs) for in-situ remediation of contaminated, fine-grained soils. PVWs are also commonly referred to as wick drains or prefabricated vertical drains. Each PVW is a geosynthetic composite system consisting of (1) a flexible polypropylene core with flow grooves along the length of the PVW, and (2) a durable, non-woven geotextile filter jacket wrapped around the core. The core channels facilitate fluid injection and extraction transfer while the geotextile filter jacket prevents adjacent soil particles from impeding the channels of the core. A typical band-shaped PVW (100mm wide by 4mm thick) is displayed in Figure 1.1.

WIDE system PVWs are installed in a grid formation and the typical PVW spacing is approximately 1.0 m. PVW spacing is site specific and requires pilot scale testing prior to full operation to determine the zone of influence and maximum extraction depth for each PVW as a function of applied system vacuum. In-situ PVW installation is performed by Nilex Corporation (Denver, Colorado) using patented technology. Nilex Corporation uses a hollow steel mandrel, typically 11.7 cm by 3.0 cm in cross section, to install each PVW. The length of the mandrel can reach 30.0 m, depending on application requirements. Each PVW is positioned inside the hollow core of the steel mandrel, which
is hydraulically pushed into the subsurface at rates greater than 3 m/s in firm clay. An anchor plate is attached at the end of each PVW, prior to installation, to secure it during mandrel retrieval. An impermeable barrier sleeve can also be attached to the PVW prior to installation, to enable depth-specific extraction and injection capability, which can potentially accelerate the remediation process.

The PVWs are clamped to rows of PVC piping positioned at the ground surface and controlled by the main manifold. The manifold design enables WIDE technology to operate under extraction-only, injection-only, or concurrent injection-extraction procedures for full system flexibility and control. The PVC pipe network is engineered to distribute air vacuum from the vacuum extraction unit, receive extracted fluids, and inject flushing solutions from the positive injection system. An above-ground contaminant treatment system is utilized for soluble and gas-phase contaminants. WIDE can be used as a stand-alone technology or in conjunction with other methods to enhance recovery of contaminants.

Several key WIDE system design features provide distinct advantages over conventional pump-and-treat procedures:

1. The PVW redundancy and short installation spacing ensure accurate plume detection and coverage, accelerated soil flushing or ground water extraction, and advantageous hydraulic head control.

2. The impermeable barrier sleeve provides a unique depth specific remediation feature that can potentially enhance the process. For example, the barrier sleeve
can be attached to the PVW to prevent fluid extraction in areas that are not contaminated.

3. WIDE is installed without drilling, which minimizes contaminant exposure and release potential.

4. WIDE can operate under extraction-only operations (to simulate a vapor extraction system) or it can operate under concurrent injection-extraction operations (to simulate a vacuum enhanced soil flushing unit) depending upon the target contaminant and primary remediation objective. Additionally, the system can be operated in rotational sections to further increase system efficiency.

1.3. Research Objectives

WIDE technology is being evaluated for use in heterogeneous, fine-grained soils. The scope of this research includes field testing, laboratory experimentation, and a finite element analysis.

Nine months worth of field demonstration data collected at a TCE contaminated field test site located in Ashtabula, Ohio are evaluated to discern WIDE system performance issues. The 21.0 m by 18.3 m WIDE demonstration test area is positioned over the area of a former unlined evaporation pond used for disposal of spent solutions. 132 PVWs were installed 6.1 m deep. Vacuum pressures, displaced fluid volumes, TCE concentrations, and water table depth data are collected.

Laboratory experimentation is designed to determine the zone of influence, maximum extraction depth, and geometry effects of each PVW. A large-scale, 10 kPa test is performed using clay soil obtained from the field site. A high permeability seam,
similar to field conditions, is also included. The test soil and sample preparation procedures, experimental configuration, fluid flow rates, drawdown capabilities, zone of influence, and the NaCl tracer distribution are described.

The NAPL Simulator is the three-dimensional finite element analysis model used in the third component of this research. Hydraulic field data is used to develop and calibrate the model. Soluble and gas-phase contaminant transport is simulated in saturated and unsaturated soil media. The model test grid is 0.6 m deep and the PVW spacing is 1.0 m during the calibration procedure. One quarter of the total extraction flow rate is assigned to corner nodes located 0.150 m below the ground surface to simulate the impermeable sheathing. Atmospheric gas pressure head and contaminant concentration boundary conditions are assigned. Similar to field conditions, the global dry unit weight is 1.8 kN/m$^3$, the soil porosity is 0.4, and the global soil permeability is $1 \times 10^{-6}$ cm/s. Deviations to the global soil permeability ($1 \times 10^{-5}$ cm/s) correspond to the location of the silt seam detected during subsurface exploration in the field. The initially saturated model test grid also has an initial soluble phase contaminant concentration was equal to the solubility limit (1100 mg/L).

Using the calibrated model, a parametric evaluation is performed to establish the input variables that significantly affect contaminant transport. System performance and contaminant partitioning tendencies are evaluated as a function of time for two different operational schemes. Finally, a sensitivity analysis, consisting of 36 simulations, is performed to evaluate contaminant partitioning tendencies as a function of the PVW spacing, extraction water flow rate, and mass transfer coefficient.

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More specifically, the following objectives are identified:

1. To install and conduct the first full-scale WIDE system field demonstration testing program to collect valuable data and discern global WIDE system performance issues for future design considerations.

2. To determine fluid (air and water) extraction rates as a function of applied vacuum pressure and water table depth during extraction-only and concurrent injection-extraction field tests.

3. To measure soluble and gas-phase TCE concentrations in the field and determine the predominant mode of TCE extraction during extraction-only and concurrent injection-extraction field tests.

4. To estimate end-point remediation time intervals using calculated TCE extraction rates and contamination estimates generated during the subsurface investigation.

5. To develop a method and construct a large-scale slurry sample to investigate PVW performance during the laboratory test that simulates field conditions with the use of soil obtained from the field site.

6. To establish a method for which the PVW zone of influence and maximum extraction depth can be evaluated as a function of soil and vacuum pressure in the laboratory.

7. To investigate the effects of PVW geometry and design during laboratory experimentation.

8. To develop and calibrate a three-dimensional finite element analysis model that can handle soluble and gas-phase species in saturated and unsaturated soil media using hydraulic data acquired from the field demonstration testing sequence.
9. To determine the effects of varying select model input parameters on contaminant transport using a finite element analysis model.

10. To evaluate changes in mass as a function of the soluble-phase, gas-phase, and sorbed contaminant mass during an extraction-only and concurrent injection-extraction simulation using the finite element analysis model.

11. To determine the predominant mode of contaminant extraction during extraction-only and concurrent injection-extraction simulations using the finite element analysis model.

12. To determine the rate of change in soluble-phase, gas-phase, sorbed, and total system contaminant mass as a function of critical design parameters (PVW spacing, water extraction flow rate, and mass transfer rate) during extraction-only simulations.

1.4. **Research Scope**

This dissertation is organized as follows (equations and tables are included within the text, but figures are provided at the end of each chapter):

- A literature review is presented in Chapter 2.

- Chapter 3 details the field demonstration testing component of this research. The subsurface conditions, installation procedures, and field performance data obtained from the field for extraction-only as well as concurrent injection-extraction tests are presented in this chapter.

- Chapter 4 summarizes the laboratory experimentation. The laboratory sample preparation and installation procedures, experimental configuration, and the results from a 10kPa test are detailed in this chapter.
• Chapter 5 describes the finite element analysis model in detail and outlines the methods used to develop and calibrate the model using hydraulic data obtained during the field demonstration.

• Chapter 6 presents the approach and results from the finite element analysis.

• Chapter 7 summarizes the three components of this research, describes the contribution to the state of the art, and provides recommendations for future research.

• Chapter 8 lists all references.

• Chapter 9 (Appendix A) presents the field demonstration test sequence.

• Chapter 10 (Appendix B) displays the sample water vapor extraction rate calculations.

• Chapter 11 (Appendix C) summarizes the complete finite element analysis model input parameter set.
Figure 1.1. The Prefabricated Vertical Well (PVW) (Quaranta et al., 2000)
2. LITERATURE REVIEW

2.1. Conventional Pump-and-Treat

Pump-and-treat is one of the most widely used ground water remediation alternatives (used at approximately 75% of the Superfund sites) (U.S. EPA, 1996). For this method, extraction wells pump contaminated fluids from the subsurface, which are subsequently treated ex-situ. The design of a conventional pump-and-treat remediation system depends upon (1) the type and location of the extraction wells, pumps, and piping, (2) the drilling method, and (3) the design and construction of each extraction well (U.S. EPA, 1990c). Injection wells may be used concurrently if the soil permeability is high, drains may be used if the contaminated aquifer is shallow, and intercept drains may be used if a shallow aquifer is surrounded by low permeability material (U.S. EPA, 1990c). A schematic of a typical pump-and-treat system is displayed in Figure 2.1.

2.1.1. Case Studies

Conventional pump-and-treat remediation systems have been evaluated extensively in the literature. The following case studies were reviewed:

1. The National Research Council (1994) reviewed 77 pump-and-treat cases and determined that full cleanup was achieved at only eight of these sites. The committee concluded that conventional pump-and-treat systems were ineffective at locations that contained significant amounts of solvents, precipitated metals, contaminants that have
diffused into small pore spaces, and contaminants that adhere strongly to soils (NRC, 1994).

2. Data from 112 sites (Superfund, RCRA, EPA controlled industrial, and government-owned sites) were collected and organized in a data base for review (U.S. EPA, 1990b). Nineteen of these cases were identified as suitable candidates for evaluation (U.S. EPA, 1990a). Table 2.1 provides a list of all 19 case studies. The case studies were obtained from a variety of geographic locations and geologic conditions. The primary contaminants in all but two cases were volatile organic compounds (VOCs). Containment of contaminants was achieved at each site and removal was often significant (up to 130,000 pounds in one case) but the rate of contaminant mass removal declined quickly with time (Haley, Hanson, Enfield, and Glass, 1991). Tailing and rebounding problems were encountered at all sites and in many cases, the pump-and-treat remediation systems were operated longer than the estimated times (Travis and Doty, 1990). According to Haley, Hanson, Enfield, and Glass (1991), the factors that affected the performance of these systems fell into four major categories: (1) aquifer properties and subsurface heterogeneities/fractures, (2) contaminant sorption and mass transport kinetics, (3) adequacy of sources removal and size of plume, and (4) system design (pumping rate, well locations, and screened interval depths).
Table 2.1. Summary of Case Study Site Characteristics (partially taken from Haley, Hanson, Enfield, and Glass, 1991)

<table>
<thead>
<tr>
<th>Site</th>
<th>Site Name</th>
<th>Chemicals*</th>
<th>NAPLs</th>
<th>Soil Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Amphenol Corporation</td>
<td>Organics</td>
<td>No</td>
<td>Unconsolidated glacio-fluvial sediments</td>
</tr>
<tr>
<td></td>
<td>New York</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>Black and Decker</td>
<td>Organics</td>
<td>No</td>
<td>Glacial till and fractured sandstone</td>
</tr>
<tr>
<td></td>
<td>New York</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>Des Moines TCE</td>
<td>Organics</td>
<td>No</td>
<td>Unconsolidated glacio-fluvial sediments</td>
</tr>
<tr>
<td></td>
<td>Iowa</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>Dupont Mobile Plant</td>
<td>Organics</td>
<td>No</td>
<td>Alluvial sand and clay</td>
</tr>
<tr>
<td></td>
<td>Alabama</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>Emerson Electric Company</td>
<td>Organics</td>
<td>No</td>
<td>Sand</td>
</tr>
<tr>
<td></td>
<td>Florida</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>Fairchild Semiconductor</td>
<td>Organics</td>
<td>Possible</td>
<td>Alluvial sand and gravel with silt, and clay layers</td>
</tr>
<tr>
<td></td>
<td>California</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>7</td>
<td>General Mills, Incorporated</td>
<td>Organics</td>
<td>Possible</td>
<td>Peat, glacial deposits, and fractured rock</td>
</tr>
<tr>
<td></td>
<td>Minnesota</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>GenRad Corporation</td>
<td>L-Sorption</td>
<td>No</td>
<td>Glacial sand, gravel</td>
</tr>
<tr>
<td></td>
<td>Massachusetts</td>
<td>Organics</td>
<td></td>
<td></td>
</tr>
<tr>
<td>9</td>
<td>Harris Corporation</td>
<td>Organics</td>
<td>No</td>
<td>Sand and shell with a clay layer</td>
</tr>
<tr>
<td></td>
<td>Florida</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>IBM Dayton</td>
<td>Organics</td>
<td>Yes</td>
<td>Sand with clay layers</td>
</tr>
<tr>
<td></td>
<td>New Jersey</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>11</td>
<td>IBM San Jose</td>
<td>Organics</td>
<td>Yes</td>
<td>Alluvial sand and gravel with silt and clay layers</td>
</tr>
<tr>
<td></td>
<td>California</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>12</td>
<td>Nichols Engineering</td>
<td>Organics</td>
<td>Possible</td>
<td>Weathered and fractured shale</td>
</tr>
<tr>
<td></td>
<td>New Jersey</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>13</td>
<td>Olin Corporation</td>
<td>Organics</td>
<td>No</td>
<td>Unconsolidated glacio-fluvial sediment</td>
</tr>
<tr>
<td></td>
<td>Kentucky</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>14</td>
<td>Ponders Corner</td>
<td>L-Sorption</td>
<td>No</td>
<td>Unconsolidated glacio-fluvial sediments</td>
</tr>
<tr>
<td></td>
<td>Washington</td>
<td>Organics</td>
<td></td>
<td></td>
</tr>
<tr>
<td>15</td>
<td>Savannah River Plant</td>
<td>L-Sorption</td>
<td>No</td>
<td>Coastal plain sand, silt, and clay layers</td>
</tr>
<tr>
<td></td>
<td>South Carolina</td>
<td>Organics</td>
<td></td>
<td></td>
</tr>
<tr>
<td>16</td>
<td>Site A</td>
<td>Organics</td>
<td>No</td>
<td>Limestone and sand</td>
</tr>
<tr>
<td></td>
<td>Florida</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>17</td>
<td>Utah Power and Light</td>
<td>Organics</td>
<td>Yes</td>
<td>Alluvium and fractured basalt</td>
</tr>
<tr>
<td></td>
<td>Idaho</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>18</td>
<td>Veronica Well Field</td>
<td>Organics</td>
<td>Yes</td>
<td>Glacial sand, gravel, and clay</td>
</tr>
<tr>
<td></td>
<td>Michigan</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>19</td>
<td>Villie Mercier</td>
<td>H/L-Sorption</td>
<td>Yes</td>
<td>Unconsolidated glacial sediments and fractured rock</td>
</tr>
<tr>
<td></td>
<td>Quebec, Canada</td>
<td>Organics</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

*H=High and L=Low
3. Thirty-seven pump-and-treat remediation systems (in operation for an average of seven years) were evaluated in the Santa Clara Valley, California area. The groundwater was primarily contaminated with Trichloroethane (TCA), Trichloroethene (TCE), and Dichloroethane (DCE) as a result of leaky underground solvent storage tanks associated with the semiconductor industry. The first pump-and-treat system in the Santa Clara Valley came to operation at the San Jose Fairchild Semiconductor Plant in July of 1982 (also listed in Table 2.1). Most sites obtained greater than a 90% reduction in maximum concentrations for one or more of the three contaminants. While only one of the 37 sites obtained maximum contaminant levels for all contaminants, six of the sites reached maximum contaminant levels for at least one of the contaminants. While pump-and-treat successfully reduced contaminant concentrations, site remediation potential is limited (Bartow and Davenport, 1995).

4. Redevelopment of a housing estate located in the Dutch City of Tilburg uncovered a source of TCE from a former textile factory spill occurrence, which contaminated the underlying aquifer to a depth of at least 12.0 m. TCE contaminated soils in excess of 100mg/kg were obtained from the site. Over a seven year period, the installed pump-and-treat remediation system removed 4,391 kg of TCE. Approximately 1500 kg were extracted in the first year but the rates varied between 300 and 600 kg in years following. (Dyer, Zutphen, and Hetterschijt, 2001).
2.1.2. Technology Evaluation

Pump-and-treat can be a successful means of containment, but the heterogeneous nature of soils and the tailing and rebounding effects observed in the field have prohibited systems from achieving maximum contaminant levels (MCLs) (U.S. EPA, 1990a). Tailing refers to the progressively slower rate of decline in dissolved contaminant concentration with continued operation and rebounding refers to the rapid increase in contaminant concentration that occurs after pumping has been discontinued (U.S. EPA, 1996).

The presence of NAPL in the subsurface can serve as a continual source of contamination. Immobile NAPL dissolves into the ground water and concentrations can approach the solubility limit when ground water movement is slow. Even though ground water increases during the pumping operation and contaminant concentration initially decreases, the decline in concentration eventually tails off until the rate of dissolution is in equilibrium with the velocity of the pumped ground water. If pumping is discontinued, concentrations rebound and the process is repeated (U.S. EPA, 1996).

Sorption processes (which are a function of the contaminant concentration as well as sorption capacity) slow contaminant removal rates significantly. Additionally, the amount of contaminant sorbed to the soil is often not accounted for when estimating the time required for remediation. Therefore, remediation schemes typically operate longer than expected (Travis and Doty, 1990).

In addition to the technical limitations, pump-and-treat is expensive to design, install, and operate, and must be maintained and operated for decades before accurate
projections for achievement of the current cleanup standards can be made (Hoffman, 1993).

2.2. The Prefabricated Vertical Well (PVW)

The band-shaped PVW (typically 4 mm by 100 mm) includes an inner core and outer filter jacket. The inner core is an extruded polypropylene strip that has longitudinal grooves on both sides to serve as flow channels. The filter jacket is constructed of durable, non-woven, polypropylene geotextile, tightly wrapped around the core, and sewn at the seam. The filter jacket maintains the cross-sectional profile and hydraulic capacity of the core, but it also filters fluids while preventing fine-grained soil from intruding. It is also referred to as a prefabricated vertical drain or wick drain (Figure 1.1). A 4 mm by 100 mm PVW with a circumference equal to 208 mm has an equivalent drain diameter equal to 66 mm.

Nilex Corporation (Denver, Colorado) installs PVW systems using patented mandrel technology. The mandrel is the component of the installation system that delivers the PVW to the subsurface. PVWs are typically arranged in a triangular or square grid pattern. Using dynamic installation procedures, the mandrel is driven into the subsurface using a vibratory hammer or conventional drop hammer. Using static installation procedures, the mandrel is hydraulically pushed into the soil. A thin steel plate, attached to the PVW prior to installation, anchors the PVW in the soil while the mandrel is retrieved. The installation equipment is simply moved to the next installation location, which is equal to the PVW spacing, and the procedure is repeated for each PVW.

15
PVWs are conventionally used in conjunction with surcharge loads and applied vacuum pressures to accelerate soil consolidation in soft clays during soil and site improvement initiatives. Subsequent to the application of a surcharge load, pore pressures immediately increase, but cannot immediately dissipate due to the low soil permeability. The difference in pore pressure between the clay soil and the PVW induces water movement from the soil to the PVW. Similarly, the difference between existing pore water pressures in the soil media and negative pore pressures in a PVW when a vacuum is applied subsequently induces water movement from the soil to the PVW. The design and application of PVW pre-consolidation systems is beyond the scope of this literature review, but the reader is referred to (Hansbo, 1983) and (Kjellman, 1948), among others.

2.3. Well Injection Depth Extraction (WIDE)

2.3.1. Technology Overview

The Well Injection Depth Extraction (WIDE) system (first proposed by Gabr et al., 1995) is an enhanced pump-and-treat remediation system that utilizes geosynthetic prefabricated vertical wells (PVWs) for in-situ remediation of contaminated, fine-grained soils. An impermeable barrier sleeve can also be attached to the PVW to enable depth-specific extraction and injection capability. WIDE system PVWs are installed in a grid formation at a typical PVW spacing equal to 1.0 m. Preliminary pilot scale testing is required in the field to properly evaluate the zone of influence, which represents the areal extent of the groundwater captured by the PVW under vacuum-induced hydraulic
gradients. In this application, the zone of influence is designed so that the cylindrical soil columns that represent the zone affected by the vacuum-induced gradient overlap, ensuring that all areas are treated.

The PVWs are clamped to rows of PVC piping positioned at the ground surface and controlled by the main manifold. The manifold design enables WIDE technology to operate under extraction-only, injection-only, or concurrent injection-extraction procedures for full system flexibility and control. The PVC pipe network is engineered to distribute air vacuum from the vacuum extraction unit, receive extracted fluids, and inject flushing solutions from the positive injection system. An above-ground contaminant treatment system is utilized for soluble and gas-phase contaminants. WIDE can be used as a stand-alone technology or in conjunction with other methods to enhance recovery of contaminants.

PVW redundancy and short installation spacing ensure accurate plume detection and coverage, accelerated soil flushing or ground water extraction, and advantageous hydraulic head control. The impermeable barrier sleeve provides a unique depth specific remediation feature that can potentially enhance the process. For example, the barrier sleeve can be attached to the PVW to prevent fluid extraction in areas that are not contaminated. WIDE can operate under extraction-only operations (to simulate a vapor extraction system) or it can operate under concurrent injection-extraction operations (to simulate a vacuum enhanced soil flushing unit) depending upon the target contaminant and primary remediation objective. Additionally, the system can be operated in rotational sections to further increase system efficiency.
2.3.2. Laboratory and Field Testing

Preliminary PVW soil flushing tests were performed using 100 % sand and 80 % sand / 20 % kaolinite test samples to discern flow rate, drawdown, and zone of influence information as a function of vacuum pressure ((Gabr et al., 1995), (Gabr et al., 1996), (Quaranta et al., 1996), (Quaranta et al., 1997)). Contaminant recovery column cells (0.3m in diameter) were used to evaluate the PVW zone of influence as a function of vacuum pressure. Contaminant recovery cells (0.59 m by 0.76 m by 0.59 m) were used to evaluate extraction flow rates and system efficiency. The 100 mm wide PVW was scaled down to a 25.4 mm. The Ottawa sand was uniformly graded (particle sizes ranged from 1.0 mm to 0.1 mm) and 90 % passed the No. 20 sieve. Kaolin particle sized ranged from 0.01 mm to 0.001 mm. The permeability of the sand-kaolin sample was approximately $1 \times 10^{-4}$ cm/s.

Both surcharge and vacuum extraction methods were tested but an applied vacuum pressure proved more efficient. For the 100 % sand sample, the areal extent of the PVW zone of influence was approximately 16 to 21 times the equivalent PVW diameter as the vacuum pressure increased from 2.5 kPa to 20kPa. For the sand-kaolin sample, the zone of influence was approximately six to eight times the equivalent diameter as the vacuum pressure increased from 2.5 kPa to 15 kPa. There was no apparent decrease in the discharge over a period of six weeks.

Additionally, a two day, pilot scale PVW field operation was conducted at a site in Weston, West Virginia, contaminated with benzene, toluene, ethylbenzene, and xylene.
Further research is necessary to determine full-scale WIDE system capabilities and limitations in fine-grained soil as a function of time.

2.4. Remediation Alternatives

The following remediation alternatives can be used as stand-alone methods or in conjunction with other methods to enhance the removal of contaminants:

2.4.1. Soil Vapor Extraction

Similar to WIDE technology, soil vapor extraction technology induces subsurface air movement using a vacuum blower/pump system to draw contaminated fluids from each extraction well. Subsurface air movement brings “clean” air in contact with contaminated soil, NAPL, and soil vapor, but the technology is limited by the air movement efficiency within contaminated subsurface zones. Recovered fluids (air and/or water) are subsequently routed to above-ground treatment systems (Nyer et al., 1996). Similar to PVWs, soil vapor extraction wells can be constructed vertically or horizontally. A schematic of a typical soil vapor extraction system is displayed in Figure 2.2.

2.4.2. Conventional Soil Flushing

In-situ soil flushing without the use of PVWs is mainly used in coarse-grained soils. Injection fluids are frequently enhanced using additives to improve contaminant removal. Surfactants are sometimes used to facilitate the removal of low solubility organics including chlorinated solvents like trichloroethylene (TCE). Injection methods
include subsurface injection wells, shallow infiltration galleries, surface flooding, and aboveground sprayers (Rawe, 1996). The fluids infiltrate the subsurface before mobilizing and removing the contaminants. The mix of injection fluids and contaminants eventually reaches the groundwater, which serves as a means for transport before the extraction wells pump the liquids out. The contaminants are then removed for subsequent treatment.

### Table 2.2. Soil Flushing Effectiveness for Contaminant Groups (Rawe, 1996).

<table>
<thead>
<tr>
<th>Contaminant Group</th>
<th>Effectiveness</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Organic</strong></td>
<td></td>
</tr>
<tr>
<td>Halogenated volatiles</td>
<td>♦</td>
</tr>
<tr>
<td>Halogenated semi-volatiles</td>
<td>•</td>
</tr>
<tr>
<td>Nonhalogenated volatiles</td>
<td>•</td>
</tr>
<tr>
<td>Nonhalogenated semi-volatiles</td>
<td>♦</td>
</tr>
<tr>
<td>PCBs</td>
<td>•</td>
</tr>
<tr>
<td>Pesticides (halogenated)</td>
<td>•</td>
</tr>
<tr>
<td>Dioxins/furans</td>
<td>•</td>
</tr>
<tr>
<td>Organic cyanides</td>
<td>•</td>
</tr>
<tr>
<td>Organic corrosives</td>
<td>•</td>
</tr>
<tr>
<td><strong>Inorganic</strong></td>
<td></td>
</tr>
<tr>
<td>Volatile metals</td>
<td>•</td>
</tr>
<tr>
<td>Nonvolatile metals</td>
<td>♦</td>
</tr>
<tr>
<td>Asbestos</td>
<td>♠</td>
</tr>
<tr>
<td>Radioactive materials</td>
<td>•</td>
</tr>
<tr>
<td>Inorganic corrosives</td>
<td>•</td>
</tr>
<tr>
<td>Inorganic cyanides</td>
<td>•</td>
</tr>
<tr>
<td><strong>Reactive</strong></td>
<td></td>
</tr>
<tr>
<td>Oxidizers</td>
<td>•</td>
</tr>
<tr>
<td>Reducers</td>
<td>•</td>
</tr>
</tbody>
</table>

♦ Demonstrated Effectiveness: Successful treatability test at some scale completed.
• Potential Effectiveness: Expert opinion that technology will work.
♠ No Expected effectiveness: Expert opinion that technology will not work.
This system must be carefully designed to prevent unnecessary spreading of contaminants by way of the pore water. Soil flushing is applicable to most contaminants but is more effective in coarser-grained soils like sand and gravel. Soil flushing may be used in conjunction with other technologies depending on the removal efficiency and acceptable level of contaminant concentration in the soil. The efficiency of the technology is limited by the subsurface hydrology and the rate at which the fluids are injected and infiltrate the media. The following table summarizes the effectiveness of soil flushing on different contaminant groups (Rawe, 1996). Note that halogenated volatiles, which include trichloroethylene, receive high marks for this method according to this source. However, the technology, as is, is not recommended for clayey soils.

2.4.3. Soil Washing

Contaminated soils are excavated and mechanically treated using ex-situ soil washing technology. The soil is processed in a wash solution chemically balanced to remove the contaminants while the wash water is treated and the soil is recycled or disposed of. This method is enhanced if fine-grained soils are separated from coarse-grained soils since contaminants tend to bind chemically and/or physically to clay and silt-size particles.

2.4.4. Bioremediation

Bioremediation can be an in-situ or an ex-situ process that involves the use of microbial activity to break down organic compounds into carbon dioxide and water,
leaving out harmful byproducts (McAdams, 1993). In-situ bioremediation is typically used in conjunction with other in-situ technologies including soil flushing to facilitate the circulation of necessary nutrients and oxygen through the subsurface media. The infiltration water is pre-treated to remove metals that may disrupt or inhibit biological growth. For example, iron dissolved in the ground water may bind phosphates needed for this purpose or cause a more rapid depletion of hydrogen peroxide, which can be used as an oxygen source. For treatment purposes, excess phosphate can be added to complex the iron (Rawe, 1996).

Depending on the site conditions, microorganisms and the proper nutrients for the site-specific conditions are added to enhance microbial activity. Additives to adjust the pH are sometimes added to the air and oxygen injected with the water. The chemicals and additives introduced into the soil media and groundwater are dependent upon the existing soil conditions and contaminants in the soil. In order to promote optimum growth of the indigenous microbial population capable of degrading the contaminants in the soil, the components need careful design. Soluble organic contaminants including some chlorinated aliphatic compounds like trichloroethylene have more success with this technology than others.

The same theory applies to ex-situ bioremediation except the excavated soil is placed in mounds which are kept moist and healthy with nutrients and an air supply to induce the same kind of activity.
2.4.5. **Reactive Walls**

Innovative reactive walls are constructed and placed strategically to capture and/or treat contaminants within a groundwater plume. This technology relies on the natural hydraulic gradient to carry contaminated fluids through the reactive wall for groundwater treatment. The intention of this technology is to reduce and/or eliminate mechanically operating remediation systems that require long-term operational and maintenance costs (Nyer et al., 1996). A schematic of a reactive wall cross-section (a) and plan-view (b) is displayed in Figure 2.3.

Reactive walls are constructed using native soil, if possible, but often the native soil is replaced or mixed with a more reactive material. Soil mixing, excavation-backfill, and overlapping caisson methods are often used to construct each wall. Contaminant transformation processes, physical contaminant removal, pH or oxidation-reduction potential modification, metals precipitation, contaminant sorption, and the addition of nutrients are the reaction methods currently under evaluation for this technology (Nyer et al., 1996).
Figure 2.1. Pump-and-Treat Technology (U.S EPA, 1990)
Figure 2.2. Soil Vapor Extraction Technology (Nyer et al., 1996)
Figure 2.3. A Profile View (a) and Plan View (b) of Reactive Wall Technology (Nyer et al., 1996)
3. FIELD DEMONSTRATION

3.1. Introduction

The field testing component of this research was conducted to discern global WIDE system performance issues. Fluid extraction capacity (air and water), injection rates, contaminant recovery rates, and groundwater head control were evaluated. The data gained from the full-scale field demonstration will be used to calibrate the finite element analysis model to study system performance, as presented in the third component of this research.

The field demonstration was conducted on a site located in Ashtabula, Ohio, and owned by Reactive Metals Incorporated (RMI). RMI extruded Uranium ingot for Department of Energy (DOE) defense programs and used Trichloroethylene (TCE) as a solvent during equipment maintenance procedures. RMI concurrently operated an unlined wastewater evaporation pond that was used to dispose of spent solutions containing trace amounts of TCE, which ultimately contaminated the soil and groundwater on-site. It is important to note that this research would not have been possible without the cooperative efforts of RMI during the data collection process.

Prior to WIDE system installation and field demonstration testing, a subsurface investigation was conducted in the area of the former evaporation pond to evaluate the soil profile and measure TCE concentrations in the groundwater and on the soil. The samples obtained during this investigation consisted of low to medium plasticity clay (CL) but there was a silt (ML) seam located approximately 1.8 m to 2.4 m below the
ground surface. The water table was located approximately 0.4 m below the ground
surface at the time of this investigation (September of 1998). TCE contamination levels
as high as 300,000 µg/kg were detected on the soil at a depth consistent with the location
of the silt seam. This concentration was approximately four orders of magnitude higher
than the maximum contaminant level (MCL) for TCE on soil (25µg/kg). The majority of
TCE contamination on the soil existed within 9.0 m of the ground surface. TCE
concentrations as high as 475 mg/L were also measured in the ground water in the area of
the former evaporation pond. The highest concentrations were approximately five orders
of magnitude higher than the MCL for TCE in ground water (5µg/L).

A full-scale (21.0 m by 18.3 m) demonstration test pad was divided into four
quadrants and 494 prefabricated vertical wells (PVWs) were installed by Nilex
Corporation (Denver, CO), to a depth of 6.1 m. A PVC piping network was designed and
installed with an above-ground manifold system that operated the test pad in three modes:
injection-only, extraction-only, and concurrent injection-extraction operations. The PVC
piping network and manifold were attached to vacuum extraction system and a positive
injection unit.

Field testing occurred from February 3 to October 22 of 1999. There were
approximately 265 extraction-only and 15 concurrent injection-extraction operational
hours recorded. The majority of field testing was conducted in Quadrant 4 (the area with
the lowest TCE contamination) to validate technology concepts prior to full-scale (1.25
acre) deployment. Therefore, the data presented in the field demonstration component of
this research reflect Quadrant 4 test results only. Vacuum pressure, injected and
extracted fluid volumes, TCE concentrations (gas and soluble-phase), and water table levels were monitored.

3.2. Test Site Description and Background

The test site, owned by Reactive Metals Incorporated (RMI), was located in an industrialized area, northeast of Ashtabula, Ohio. The static water table, which was located approximately 0.4 m below the ground surface during the subsurface investigation, varied seasonally. Groundwater moved in the northwest direction towards the Ashtabula River, a tributary of Lake Erie. An aerial view of the RMI facility can be viewed in Figure 3.1. Lake Erie is located at the top of this figure.

Until November of 1990, RMI had a contract with the Department of Energy (DOE) to extrude Uranium ingot for the DOE defense programs. RMI simultaneously operated an unlined wastewater evaporation pond (approximately 9.1m wide and 1.0 m deep) adjacent to the main extrusion plant for disposal of spent solutions, which included trace quantities of TCE. TCE was used as a solvent for equipment maintenance operations between 1962 and 1966 and containers of TCE were also stored on-site, thereafter. It was estimated that a TCE spill occurred on or before 1972. The soil and groundwater became contaminated as a result of the evaporation pond operations. The soil in the area of the former evaporation pond has since been excavated 1.0 m deep and backfilled with clean topsoil.

In response to the soil and groundwater contamination problem, the U.S. Environmental Protection Agency (EPA) issued RMI a Resource Conservation and Recovery (RCRA) Act Hazardous Waste Management Permit with conditions mandating
soil and groundwater remediation. A feasibility study was conducted in 1988 to evaluate several remediation alternatives. Conventional pump-and-treat as well as passive cut-off infiltration galleries were evaluated but 50 to 200 year remediation periods were estimated for both methods and considered unreasonable. Additionally, the act of excavating and removing radioactive contaminated soil with a shallow water table generated health and safety concerns. Consequently, the DOE identified a need for new and innovative soil and groundwater remediation technology.

North Carolina State University designed and installed a WIDE demonstration system that encompassed the area of the former evaporation pond to evaluate field performance of the Well Injection Depth Extraction (WIDE) system. Prior to system installation, a subsurface investigation was conducted to evaluate subsurface conditions and measure TCE concentrations on the soil and in the groundwater.

3.3. Subsurface Investigation

A subsurface investigation of the test area was performed during July and September of 1998. Five soil borings (T1 – T5) were drilled and nine monitoring wells (500 – 508) were installed both up-gradient and down-gradient of the former evaporation pond. Standard penetration testing was performed and split spoon samples were obtained every 0.6 m for the first 3.6 m of drilling and every 1.5 m, thereafter. The boring locations and groundwater monitoring well locations relative to the test area are displayed in Figure 3.2. The water table was located approximately 0.4 m below the ground surface.

The samples obtained during this investigation consisted of low to medium plasticity clay (CL), but a silt (ML) seam was located approximately 1.8 m to 2.4 m
below the ground surface. The average in-situ moisture content (ASTM D 2216-90), liquid limit and plastic limit (ASTM D 4318), and specific gravity (ASTM D 854) of the clay (CL) were determined to be 16 %, 26 %, 15 %, and 2.75, respectively. Figure 3.3 displays the grain size distribution curve for soil samples obtained at every sampled depth during boring T1. At least 90 % of the soil passes a No. 200 sieve for all depths. With the exception of the 1.8 m - 2.4 m sample, approximately 35 % - 45 % of the soil was finer than 0.002 mm, indicating a large fraction of clay-size particles. Only 12 % of the soil obtained between 1.8 m and 2.4 m was finer than 0.002 mm. The soil profile was consistent across the test area.

Uncorrected standard penetration test N-values are displayed in Figure 3.4 as a function of depth for borings T1 - T5. The increase in blow counts near the 2.4 m depth indicated the presence of a denser material (silt seam). This conclusion was supported by visual classification in the field and the grain size distribution curve in Figure 3.3.

3.4. Subsurface Contamination

There was no documentation regarding the usage and disposal volume of contaminants on-site. Therefore, soil samples were tested for the presence of volatile organic compounds during the subsurface investigation. The groundwater monitoring wells displayed in Figure 3.2 were used to collect fluid samples to measure contaminant concentrations in the soluble-phase. Figure 3.5 displays the TCE concentration on the soil as a function of depth. Contamination levels as high as 300,000 µg/kg were detected in soil samples obtained approximately 2.6 m below the ground surface in boring T3, which was located in the area of the former evaporation pond, at a depth consistent with
the silt seam. The MCL for TCE on soil (equal to 25µg/kg) was negotiated with the Ohio EPA. Maximum concentrations were approximately four orders of magnitude higher than the acceptable MCL. The MCL was exceeded in all five borings but concentrations were highest at a depth that was consistent with the silt seam.

Figure 3.6 displays TCE concentration contours in the ground water. Ground water concentrations as high as 475 mg/L (475,000 ppb on Figure 3.6) were measured in well 505, located in the area of the former evaporation pond. The federally mandated MCL for drinking water was 5µg/L. Maximum concentrations were approximately five orders of magnitude higher than the MCL.

### 3.5. Field Installation

A 21.0 m by 18.3 m test area was positioned over the former evaporation pond and divided into four quadrants that had 21 injection and extraction rows. A total of 494 PVWs were installed over a two day period by Nilex Corporation (Denver, CO), to a depth of 6.1 m. Figure 3.2 displays the demonstration test area dimensions, quadrants, and PVW locations (injection and extraction).

During field installation, Nilex Corporation rented an excavator locally and attached their patented installation equipment to the boom arm of the excavator where the bucket was normally located, as displayed in Figure 3.7. The installation equipment was designed to work in coordination with the mobility of the excavator to ensure accurate placement of each PVW (Figure 3.8). Prior to PVW installation, an impermeable sleeve was sized and positioned to fit the top 1.5 m of the PVW to reduce short circuiting during extraction-only operations. An anchor plate was attached to the end of each PVW and
the mandrel was hydrostatically pushed into the subsurface. Subsequently, the steel mandrel was retracted while the PVW was anchored in the ground. The PVW was cut off and clamped to the PVC piping before the excavator was relocated to repeat the same procedure.

The manifold that controlled the PVC piping network was designed to operate four different quadrants (in any combination) during injection-only, extraction-only, and concurrent injection-extraction operations. The PVC piping network and manifold were attached to a vacuum extraction system (that had an air blower / pump capable of providing a constant flow rate of 28.3 m³/min at a working vacuum pressure equal to 3.35 m of total head) and positive injection unit. The piping manifold was enclosed under a tent to provide heat during inclement weather. The components of the WIDE system are displayed in Figure 3.9.

3.6. Field Performance and Evaluation

Field testing was performed between the dates of February 3 and October 22 of 1999. The majority of field testing was performed in Quadrant 4 (the region of the demonstration test area with the lowest TCE concentrations) to validate technology concepts prior to full-scale (1.25 acre) deployment. Three different operational scenarios were established: alternating row extraction, full quadrant extraction, and concurrent injection-extraction. Quadrant 4 had a total of 132 PVWs arranged in 11 rows; 72 PVWs were utilized during alternating row extraction and 132 PVWs were utilized during full quadrant extraction. The PVW configuration for alternating row and full quadrant extraction is displayed in Figure 3.10. During concurrent injection-extraction operations,
five rows were used to inject fluids (60 PVWs) and six rows were used to extract contaminated ground water (72 PVWs). Approximately 265 extraction-only and 15 concurrent injection-extraction operational hours were recorded during the nine month demonstration. The complete Quadrant 4 test sequence is presented in Chapter 9 (Appendix A).

Vacuum pressure, injected and extracted fluid volumes, soluble and gas-phase TCE concentrations, and water table levels were monitored during the demonstration. Vacuum pressures were measured at the main manifold of the vacuum extraction system. Fluid volumes were measured using flow totalizers. Charcoal tubes were used to measure gas-phase TCE concentrations from in-line air flow. Fluid samples were obtained from the monitoring wells to measure in-situ soluble-phase TCE concentrations and from the holding tank of the extraction system to measure extracted soluble-phase TCE concentrations. Contaminant concentrations were measured by an independent laboratory using a gas chromatograph. Fifty-three TCE concentration samples (soluble and gas-phase) were obtained during the nine month testing interval.

3.6.1. Effect on Air Flow Rate as a Function of Water Table Depth

Water table depth and corresponding air flow rates (Qa) are displayed as a function of time in Figure 3.11, Figure 3.12, and Figure 3.13 for alternating row extraction, full quadrant extraction, and concurrent injection-extraction operations, respectively. These data were representative of all data collected in Quadrant 4 (consecutive testing days were selected as examples to show the successive trends in the
water table depth and air flow rate from one day to the next). The time scale (Reference Day) refers to the number of days subsequent to the first day of field operation (February 3, 1999). The undisturbed water table was located approximately 0.4 m below the ground surface, but the water table location prior to each field test depended on the testing scheme operated the previous day. In other words, if a long-term, full-quadrant extraction test was performed, the water table typically did not rebound completely overnight during system shutdown.

In general, the water table was lowered during extraction-only operations (alternating row extraction and full quadrant extraction). Simultaneously, air infiltrated the system and increased the air flow rates. It was hypothesized that air infiltration occurred as a cone of depression formed around each PVW. As the water table approached the bottom of the PVW sheathing (which extended 1.5 m below the ground surface), the vacuum pressure decreased and the increase in the air flow rate tapered off.

During the alternating row extraction field test on reference day 6 (Figure 3.11), the water table dropped 0.41 m and the airflow rate measured 511,400 L/hr at the end of a 5 hr test interval. During system shutdown, the water table rebounded 0.13 m. On reference day 7, the water level dropped an additional 0.17 m from the previous day and the airflow rate was 582,800 L/hr at the end of a 4.25 hr test. The increase in the air flow rate tapered off as the water table approached the bottom of the PVW sheathing (1.5 m below the ground surface). Additionally, the water table drop rate decreased from 0.082 m/hr on reference day 6 to 0.070 m/hr on reference day 7.
During full quadrant extraction on reference day 120 (Figure 3.12), similar trends were observed. The water table dropped 0.97 m and the corresponding airflow rate was 575,100 L/hr at the end of a 5.75 hr test, but the air flow rate increase tapered off as the water table approached the bottom of the impermeable sheathing. During the first four hours of the reference day 121 field test, the rate of water table drop decreased from 0.168 m/hr on reference day 120 to 0.123 m/hr on reference day 121 and tapered off, thereafter.

The rate of water table drop during full quadrant extraction was approximately twice that observed during alternating row extraction procedures since the number of PVWs nearly doubled (72 PVWs in the alternating row grid versus 132 PVWs in the full quadrant extraction). For example, the water table dropped 0.076 m/hr on reference day 6 (alternating row extraction) and 0.168 m/hr on reference day 120 (full quadrant extraction).

During concurrent injection-extraction operations, the water table remained relatively shallow due to the concurrent injection of fluids. While the groundwater elevation fluctuated as much as 1.13 m during full quadrant extraction (Figure 3.12), the water table location stayed within 0.15 m of the undisturbed water table during concurrent injection-extraction operations on reference days 54 and 56 (Figure 3.13). Consequently, the air flow rates were significantly lower (less than approximately 200,000 L/hr) compared to the rapid increase displayed during extraction-only testing.

Extracted air flow rates measured at the end of each test interval that had corresponding water table depth data (twenty data points included) are displayed in
Figure 3.14. In conclusion, air flow rates increased as the water table depth dropped during extraction-only operations. However, the increase in air flow rate tapered off near 600,000 L/hr as the water table approached the bottom of the PVW sheathing. It was hypothesized that a cone of depression developed around each PVW during extraction-only operations, generating a desaturated zone for air to infiltrate the soil media. Eventually, the air flow rate reached an equilibrium with the system capacity.

System extraction efficiency increased during full quadrant extraction field testing (Figure 3.14) since the number of PVWs nearly doubled. As a result, all full quadrant extraction air flow rate data on Figure 3.14 ranged between 440,000 L/hr and 630,000 L/hr for corresponding water table depths ranging between 1.2 m and 1.7 m (these data exceeded the values measured during alternating row extraction operations). The WIDE system vacuum performance curve is presented in Figure 3.15 ($R^2 =0.997$) as a function of air flow rate.

### 3.6.2. Extracted Air Flow Rate Versus Extracted Water Flow Rates

Extracted water flow rates ($Q_w$) are displayed as a function of the air:water flow rate ratio ($Q_a/Q_w$) in Figure 3.16 ($R^2=0.81$) for alternating row extraction data (42 data points), full quadrant extraction data (34 data points), and concurrent injection-extraction data (10 data points).

The $Q_a/Q_w$ ratios for concurrent injection-extraction operations were consistently equal to or less than 100 while extraction-only data (alternating row and concurrent injection-extraction) spanned $Q_a/Q_w$ ratios over approximately two orders of magnitude.
(from approximately 45 to 9,000) due to transient test conditions. Full quadrant extraction $Q_a/Q_w$ ratios overlap the ratios measured during alternating row extraction operations but achieve a higher range of values (from approximately 300 to 40,000). The number of PVWs was nearly doubled during full quadrant extraction, which increased system extraction efficiency.

Extraction water flow rates ranged from 260-1100 L/hr during concurrent injection-extraction tests, from 50-1000 L/hr during alternating row extraction schemes, and from 10-600 L/hr during full quadrant extraction operations. Concurrent injection-extraction operations consistently achieved the highest extraction water flow rates due to the concurrent injection of fluid, which promoted an immediate groundwater recovery and prevented water table drawdown.

3.6.3. Contaminant Extraction

3.6.3.1. Monitoring Well 502 TCE Concentrations

Thirteen fluid samples were obtained from monitoring well 502, which was located in the center of Quadrant 4 (Figure 3.2) to evaluate changes in the soluble-phase TCE concentration during the alternating row extraction, full quadrant extraction, and concurrent injection-extraction operations. Figure 3.17 displays the TCE $C/Co$ ratio (existing concentration / initial concentration) as a function of reference day. The initial concentration was approximately 2.72 mg/L and the operational reference days for each scheme are listed in Appendix A (Chapter 9).
Prior to the field demonstration, soluble-phase TCE concentrations were as high as 450 mg/L in Quadrant 4 (Figure 3.6). During the first several weeks of field testing, soluble-phase TCE concentrations decreased as contaminated fluids were displaced during extraction-only operations. For example, C/Co decreased from 1.0 (prior to field testing) to 0.38 on reference day 19. Nine alternating row extraction operational days were included within this time interval. A monitoring well measurement was obtained on reference day 65, which was within the concurrent injection-extraction test interval. C/Co increased from 0.38 (reference day 19) to 0.53 (reference day 65). During full quadrant extraction operations, C/Co values varied with time (ranging from approximately 0.37 to 1.12). TCE extraction was limited by diffusion and mass transfer processes that occurred within the soil matrix.

3.6.3.2. Extracted TCE Concentrations

Figure 3.18 displays gas and soluble-phase TCE concentrations measured during alternating row extraction and concurrent injection-extraction operations as a function of the extracted air flow rate. The average (AVG) and standard deviation (SD) for each phase and operational scheme are reported directly on Figure 3.18. The soluble-phase TCE concentrations for alternating row extraction and concurrent injection-extraction are labeled A and B, respectively, on Figure 3.18. The gas-phase TCE concentrations for alternating row extraction and concurrent injection-extraction are labeled C and D, respectively. There was no indication that the concentration data was time dependent during each individual test. TCE concentration data were not measured during full quadrant extraction tests.
The average extracted soluble-phase TCE concentration measured during alternating row extraction operations was 0.088 mg/L (15 data points). The average extracted soluble-phase TCE concentration measured during concurrent injection-extraction operations was 0.057 mg/L (4 data points). The standard deviations were not a representative measure of data repeatability since each data point represented a single field test and the field testing conditions varied throughout the test sequence. For this reason, the soluble-phase TCE concentration standard deviation values are relatively high. For example, the standard deviation for the soluble-phase concurrent injection-extraction TCE concentration (0.025 mg/L) is approximately half the value of the average (0.057 mg/L). Note that the extracted soluble-phase TCE concentrations were measured from random fluid samples collected from the system holding tank subsequent to each field test.

The average soluble-phase TCE concentration measured during concurrent injection-extraction operations was lower than the average concentration measured during alternating row extraction (0.057 mg/L versus 0.088 mg/L, respectively). The uncontaminated fluids injected during concurrent injection-extraction operations may have diluted the existing contamination concentrations in the ground water and decreased extracted concentrations in the soluble phase.

The average gas-phase TCE concentration measured during alternating row extraction operations was 0.012 mg/L (16 data points). The average gas-phase TCE concentration measured during concurrent injection-extraction operations was 0.018 mg/L (4 data points). The standard deviations for the gas-phase TCE concentration values
on Figure 3.18 are approximately one order of magnitude lower than the standard deviations reported for the soluble-phase contaminant concentration. For example, during concurrent injection-extraction operations, the standard deviations for the soluble-phase and gas-phase TCE concentrations were 0.025 mg/L and 0.004 mg/L, respectively. Note that in-flow gas-phase TCE concentrations were collected using charcoal tubes during the field test, which may have been a more precise sampling technique.

Gas-phase TCE was extracted as a result of the mass transfer processes that occurred in the presence of air flow. TCE volatilized from residual soluble-phase and sorbed contaminant in the unsaturated zone, and from the mobile soluble-phase contaminant in the PVWs and PVC collection piping. A mass transfer from a NAPL-phase to the gas-phase in the top 1.0 m of the soil profile was unlikely since the former evaporation pond was backfilled with clean topsoil, prior to the field demonstration.

Soluble-phase TCE concentrations were slightly higher than gas-phase concentrations; however, the volume of transferred air was orders of magnitude higher than the volume of water. According to Figure 3.16, the water flow rate was 100 L/hr for a corresponding air flow rate equal to 400,000 L/hr. For this reason, the majority of TCE contaminant volatilized and was subsequently extracted in the gas-phase. TCE extractions rates are discussed in the following section.

### 3.6.3.3. Extracted TCE Rates

Calculated gas and soluble-phase TCE extraction rates are displayed in Figure 3.19 as a function of the extracted air flow rate during alternating row extraction and concurrent injection-extraction operations. A regression was performed ($R^2=0.85$) on the
gas-phase data (that ranged from approximately 1 g/hr to 6 g/hr), and an average value is reported for the soluble-phase data (0.022 g/hr). Similar to the TCE concentration data presented in the previous section, the standard deviation was not a representative measure of data repeatability since each data point represented a single field test and the field testing conditions varied throughout the test sequence.

Soluble-phase TCE extraction rates were at least two orders of magnitude lower than the gas-phase TCE extraction rates due to the significant volume of air transferred during system operation. The average soluble-phase TCE extraction rate was 0.022 g/hr (0.017 g/hr SD) for both operational schemes. Gas-phase TCE extraction rates increased as the air flow rate increased. At air flow rates less than approximately 200,000 L/hr, the gas-phase TCE extraction rate was approximately 1 g/hr. Gas-phase extraction rates increased to 6 g/hr as the air flow rate approached 600,000 L/hr.

As the water table dropped, air infiltrated the system and increased the air flow rate, which increased gas-phase TCE extraction. As the water table approached the bottom of the impermeable sleeve, vacuum losses compromised system efficiency and prevented further drop in the water table or increase in air flow.

It can be concluded that sorbed and residual contaminant volatilization was minimized during concurrent injection-extraction operations due to the shallow water table conditions. Therefore, approximately 1 g/hr of gas-phase TCE was volatilized from mobile groundwater within PVWs and PVC piping at air flow rates less than 200,000 L/hr. The increase in the gas-phase TCE extraction rate during alternating row extraction
operations was primarily attributed to TCE volatilization from residual and/or sorbed contaminant exposed to air flow.

3.6.3.4. Estimated Field Remediation Times

The soil contamination profile from boring T3 was extracted from Figure 3.5 and displayed in Figure 3.20. The profile was divided into layers to determine the average contaminant concentration per layer and then calculate a conservative estimate of the existing contaminant mass sorbed to the soil in the field (using the worst-case scenario from Figure 3.20), assuming the estimate is valid across the test area.

Table 3.1 summarizes the depth, soil contaminant concentration, volume, and contaminant mass calculated for each layer of the contaminant profile displayed in Figure 3.20. Equation 3.1 was utilized to calculate the mass of TCE for each layer, which was displayed in the last column of Table 3.1.

Table 3.1. Field TCE Mass Calculation Data

<table>
<thead>
<tr>
<th>Layer #</th>
<th>Layer Thickness (m)</th>
<th>$C_{Top}$ (µg/kg)</th>
<th>$C_{Bottom}$ (µg/kg)</th>
<th>$C_{Average}$ (µg/kg)</th>
<th>Layer Volume (m³)</th>
<th>TCE Mass (kg)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.6</td>
<td>800</td>
<td>85,000</td>
<td>42,900</td>
<td>57.6</td>
<td>5.2</td>
</tr>
<tr>
<td>2</td>
<td>0.6</td>
<td>85,000</td>
<td>170,000</td>
<td>127,500</td>
<td>57.6</td>
<td>15.3</td>
</tr>
<tr>
<td>3</td>
<td>0.6</td>
<td>170,000</td>
<td>310,000</td>
<td>240,000</td>
<td>57.6</td>
<td>28.9</td>
</tr>
<tr>
<td>4</td>
<td>2.2</td>
<td>310,000</td>
<td>77,000</td>
<td>193,500</td>
<td>211.4</td>
<td>85.4</td>
</tr>
<tr>
<td>5</td>
<td>1.5</td>
<td>77,000</td>
<td>3,700</td>
<td>40,350</td>
<td>144.1</td>
<td>12.1</td>
</tr>
</tbody>
</table>

Total = 146.9 kg
TCE Mass = \( (C_{\text{Average}}) (\rho_{\text{Soil}}) (V_{\text{Layer}}) \)  \hspace{1cm} \text{Equation (3.1)}

Where:  
- TCE Mass = Contaminant mass calculated for each layer  
- \( C_{\text{Average}} \) = Average of \( C_{\text{Top}} \) and \( C_{\text{Bottom}} \)  
- \( \rho_{\text{Soil}} \) = Total soil density = 2088 kg/m\(^3\)  
- \( V_{\text{Layer}} \) = (Quadrant 4 Area) (Layer Thickness)  
- Quadrant 4 Area = (9.15 m) (10.5 m) = 96.1 m\(^2\)

Assuming the contaminant sorbed to the soil must either be extracted in the soluble or gas-phase before remediation is complete, the initial contaminant mass estimate (Table 3.1) and the contaminant extraction rates presented in Figure 3.19 (soluble and gas-phase) were utilized to solve for the estimated remediation time (T) using Equation 3.2, assuming the system was operated continuously.

\[
\text{TCE Mass}_{\text{Total}} = \left[ (\text{Rate}_{\text{Soluble-Phase}}) (T) \right] + \left[ (\text{Rate}_{\text{Gas-Phase}}) (T) \right]
\]

\hspace{1cm} \text{Equation (3.2)}

Where:  
- \( \text{TCE Mass}_{\text{Total}} \) = Total existing contaminant mass (Table 3.1)  
- \( \text{Rate}_{\text{Soluble-Phase}} \) = Soluble-phase contaminant extraction rate  
- \( \text{Rate}_{\text{Gas-Phase}} \) = Gas-phase contaminant extraction rate  
- \( T \) = Estimated remediation time

During the concurrent injection-extraction field tests, the average soluble-phase and gas-phase contaminant extraction rates were approximately 0.022 g/hr and 1.0 g/hr, respectively (Figure 3.19). Using these extraction rates, it would take approximately 16 years to remediate Quadrant 4. During the extraction-only field tests, the average soluble-phase contaminant extraction rate was also 0.022 g/hr, but the gas-phase contaminant extraction rate varied between 1.0 g/hr and 6.0 g/hr (Figure 3.19). Using these extraction rates, it would take approximately 2.8 to 16 years to remediate Quadrant 4.
3.6.4. WIDE System Performance Summary

During the test sequence, it was evident that TCE extraction efficiency was maximized during extraction-only operations. For this reason, the number of extraction-only operational hours (265 hr) in Quadrant 4 was significantly greater than the number of concurrent injection-extraction operational hours (25 hr). Approximately 99% of TCE recovery occurred in the gas-phase. Over the course of 265 operational hours, 111,213,754 L of air and 43,956 L of water were extracted during alternating row extraction. Over the course of 15 operational hours, 1,764,594 L of air and 7,752 L of water were extracted during concurrent injection-extraction operations. Using measured data (total operational hours, extracted air and water volumes, and average extracted TCE concentrations), system air and water flow rates, TCE extraction rates, and the total TCE mass removed in the gas and soluble-phases were calculated and presented in Table 3.2.

While concurrent injection-extraction operations generate higher extracted water flow rates, soluble-phase TCE extraction was limited by diffusion and desorption processes within the soil matrix (Figure 3.17). Additionally, soluble-phase TCE extraction rates were at least two orders of magnitude lower than gas-phase TCE extraction rates (Figure 3.19). There was a slight decrease in soluble-phase TCE concentration with the injection of clean fluid during concurrent injection-extraction procedures, indicating a possible dilution effect (Figure 3.18). From an expense perspective, higher extracted water volumes require more waste-water treatment, which adds to the total expense of remediation. From these results, it can be concluded that concurrent injection-extraction operations add no additional benefit to WIDE. Further
research is necessary to determine the maximum remediation depth and optimum sheathing length using this method.

Table 3.2. Field Performance Evaluation

<table>
<thead>
<tr>
<th></th>
<th>Alternating Row Extraction</th>
<th>Concurrent Injection-Extraction</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Air</td>
<td>Water</td>
</tr>
<tr>
<td>Operational Time (hr)*</td>
<td>265</td>
<td></td>
</tr>
<tr>
<td>Extracted Volumes (L)*</td>
<td>111,213,754</td>
<td>43,956</td>
</tr>
<tr>
<td>TCE Extraction Concentrations (mg/L)*</td>
<td>0.012</td>
<td>0.088</td>
</tr>
<tr>
<td>Flow Rates (L/hr)**</td>
<td>419,676</td>
<td>166</td>
</tr>
<tr>
<td>TCE Mass Removed (g)**</td>
<td>1334.6</td>
<td>3.9</td>
</tr>
<tr>
<td>TCE Extraction Rates (g/hr)**</td>
<td>5.04</td>
<td>0.01</td>
</tr>
</tbody>
</table>

* Measured Data
** Calculated from Measured Data

The values in Table 3.2 summarize WIDE system performance during alternating row extraction and concurrent injection-extraction operations. However, the contaminant extraction rates reported for this testing sequence do not incorporate the tailing and rebounding effects expected over longer periods of time. Further research is necessary to explore long-term system efficiency, but the unique design and flexibility of WIDE offers fundamental advantages over conventional pump-and-treat methods.

The values in Table 3.2 are important to the future design of WIDE systems. Without actual field data (air and water flow rates as well as contaminant removal rates), it is difficult to design the mechanics of the system and anticipate maintenance costs during operation. For example, the calculated air and water flow rates will allow an engineer to more efficiently design the vacuum extraction system and surface piping
network. In addition, contaminant removal rates will allow an engineer to estimate the cost of replenishing the granular activated carbon over the life-cycle of the project.

3.7. Technology Cost

A full-scale (1.25 acre) cost evaluation for the WIDE system was independently conducted at the RMI site and compared to proposed pump-and-treat technology (DOE, 2001). Present value construction, operational, and maintenance costs were considered. Based on the assumptions listed in Table 3.3, estimated present value construction and annual operating/maintenance costs for a full-scale WIDE system totaled $1,532,582, assuming a five year test period (DOE, 2001).

<table>
<thead>
<tr>
<th>Table 3.3. Full-Scale WIDE System Cost Evaluation Assumptions</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Full-Scale Test Area</strong></td>
</tr>
<tr>
<td><strong>Estimated Remediation Time</strong></td>
</tr>
<tr>
<td><strong>Number of PVWs</strong></td>
</tr>
<tr>
<td><strong>PVW Spacing</strong></td>
</tr>
<tr>
<td><strong>PVW Installation Depth</strong></td>
</tr>
<tr>
<td><strong>Number of Grid Zones</strong></td>
</tr>
<tr>
<td><strong>Number of Vacuum Extraction Units</strong></td>
</tr>
<tr>
<td><strong>Contaminant Treatment</strong></td>
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<tr>
<td></td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td><strong>Operational Time</strong></td>
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<tr>
<td></td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td><strong>Number of Technicians</strong></td>
</tr>
</tbody>
</table>

As an alternative, the proposed pump-and-treat system called for excavation and ex-situ vapor stripping treatment of the contaminated soil (2676 m³), and the installation of a 152.0 m long by 9.0 m deep groundwater extraction trench placed above bedrock. Maximum projected groundwater extraction rates equal to 19 L/min were anticipated and
an air stripper would be used for soluble TCE extraction. It was estimated that conventional pump-and-treat technology would need to be operated for at least 87 years, requiring long-term operation and maintenance. The estimated present value life cycle cost for pump-and-treat technology over 87 years of operation was $3,207,777 (two times the cost estimated for WIDE) (DOE, 2001).

3.8. Suggested Design Improvements

Based on the outcome of the field demonstration, two specific system aspects (the length of the impermeable sleeve, and the PVW spacing) could be altered to increase system efficiency and decrease construction costs. The length of the impermeable sheathing acted as a limiting boundary condition during extraction-only field testing. As the water table approached the bottom of the impermeable sheathing, the increase in the air flow rate tapered off and the system vacuum pressure was concurrently compromised. An increase in the length of the impermeable sleeve would help maintain the system vacuum pressure and promote further desaturation and TCE volatilization in the unsaturated zone, PVC piping network, and PVW cavity during extraction-only operational schemes.

An increase in the PVW spacing could potentially decrease short circuiting problems and PVW headlosses, further enhancing the vacuum extraction efficiency and decreasing material and installation costs. Further research is necessary to determine the optimum PVW spacing. Such aspect should be determined using site-specific data.
3.9. Summary of the Field Demonstration Component

The field demonstration component of this research was conducted to discern global WIDE system performance issues. Fluid extraction capacity (air and water), injection rates, contaminant recovery rates, and groundwater head control were evaluated. The data gained from the full-scale field demonstration will be used to calibrate the finite element analysis model to study system performance, as presented in the third component of this research.

The field demonstration was conducted on a site contaminated with TCE. The soil profile consisted of low to medium plasticity clay (CL), but there was a silt (ML) seam located approximately 1.8 m to 2.4 m below the ground surface. The water table was located approximately 0.4 m below the ground surface during the subsurface investigation. TCE contamination levels as high as 300,000 µg/kg and ground water TCE concentrations as high as 475 mg/L were detected prior to field testing.

The 21.0 m by 18.3 m WIDE demonstration test area was divided into four quadrants that encompassed 494 PVWs installed to a depth of 6.1 m. All three operational schemes were utilized during the nine month field demonstration. Vacuum pressure, injected and extracted fluid volumes, TCE concentrations, and water table data were collected.

During extraction-only operations (alternating row extraction and full quadrant extraction), the water table depth was lowered. Simultaneously, air infiltrated the system and increased the air flow rates. As the water table approached the bottom of the PVW sheathing (located approximately 1.5 m below the ground surface), the vacuum pressure
decreased and the air flow rate tapered off near 600,000 L/hr. During concurrent injection-extraction operations. During concurrent injection-extraction operations, the water table level was generally unaffected by the vacuum due to the concurrent injection of fluids. Consequently, the airflow rates were significantly lower (less than 200,000 L/hr), as compared to the rapid increase displayed during extraction-only testing.

The extracted water flow rates for concurrent injection-extraction ranged from 260-1100 L/hr while alternating row extracted flow rates ranged from 50-1000 L/hr and full quadrant extracted water flow rates ranged from 10-600 L/hr. Concurrent injection-extraction operations consistently achieved the highest extracted water flow rates due to the simultaneous injection of fluid, which promoted immediate groundwater recovery and prevented water table drawdown. On the other hand, extracted air flow rates and, therefore, gas-phase TCE extraction were maximized during extraction-only operations. Qa/Qw ratios for concurrent injection-extraction operations were less than 100 while extraction-only data ranged from 45 to 40,000 (spanning approximately three orders of magnitude).

The average soluble-phase TCE concentrations measured during alternating row extraction and concurrent injection-extraction operations were 0.088 mg/L and 0.057 mg/L, respectively. The fluids injected during concurrent injection-extraction operations contained no contaminant concentration and, therefore, may have diluted the existing contamination concentrations in the ground water and decreased extracted concentrations in the soluble phase. Soluble-phase TCE extraction was limited by contaminant diffusion and sorption kinetics (evident by the monitoring well TCE concentration data).
average gas-phase TCE concentrations measured during alternating row extraction and concurrent injection-extraction operations were 0.012mg/L and 0.018mg/L, respectively.

Soluble-phase TCE concentrations were slightly higher than gas-phase concentrations, but soluble-phase TCE extraction rates were at least two orders of magnitude lower than the gas-phase TCE extraction rates due to the significant volume of air transferred during system operation. The average soluble-phase TCE extraction rate was approximately 0.022 g/hr and the gas-phase TCE extraction rate increased from 1 g/hr to 6 g/hr depending upon the air flow rate. Volatilization of the sorbed and residual contaminant in the unsaturated zone was minimized during concurrent injection-extraction operations due to the shallow water table conditions. Therefore, approximately 1 g/hr of gas-phase TCE volatilized from mobile groundwater within PVWs and PVC collection piping during concurrent injection-extraction operations. Any increase in gas-phase TCE extraction beyond the 1 g/hr was attributed to TCE volatilization from immobile contaminated in the unsaturated zone.
Figure 3.1. Aerial View
Figure 3.2. WIDE Demonstration Test Area (Plan-View)
Figure 3.3. Grain Size Distribution Curve for Boring T1 Soil Samples
Figure 3.4. Uncorrected Standard Penetration N Value Profile
Figure 3.5. TCE Soil Contamination Profile
Figure 3.6. TCE Groundwater Contamination Contours (Gabr et al., 2000)

Note: concentrations are reported in ppb (1000ppb = 1mg/L)
Figure 3.7. Nilex Corporation PVW Installation
Figure 3.8. Installation Mandrel and PVW
Figure 3.9. Completed WIDE Demonstration Test Area, Ashtabula, Ohio
Figure 3.10. PVW Configuration for Alternating Extraction Row and Full Quadrant Extraction
Figure 3.11. Water Table Depths (a) and Air Flow Rates (b) as a Function of Time for Alternating Row Extraction Testing.
Figure 3.12. Water Table Depths (a) and Air Flow Rates (b) as a Function of Time for Full Quadrant Extraction Testing
Figure 3.13. Water Table Depths (a) and Air Flow Rates (b) as a Function of Time for Concurrent Injection-Extraction Testing
Figure 3.14. End-of-Test Water Table Depth and Air Flow Rate

- Alternating Row Extraction
- Concurrent Injection-Extraction
- Full Quadrant Extraction
Figure 3.15. Vacuum Pressure as a Function of Air Flow Rate

\[ y = -26.8 + (3.9 \times 10^5)x + (-5.6 \times 10^{-11})x^2 + (4.1 \times 10^{-17})x^3 \]

\[ R^2 = 0.997 \]
Figure 3.16. Extracted Air and Water Flow Rates

- Alternating Row Extraction
- Full Quadrant Extraction
- Concurrent Injection-Extraction

R² = 0.81
Figure 3.17. Monitoring Well 502 TCE Concentrations
Figure 3.18  Extracted TCE Concentrations
**Figure 3.19. Extracted TCE Rates**

![Graph showing TCE extraction rates vs. Qa (L/hr).](image)

Mathematical equation:

\[ y = \frac{6.14}{1 + \exp\left( \frac{(247497 - x)}{96608.2} \right)} \]

Graph showing extraction rates for different methods:
- Gas-Phase, Alternating Row Extraction
- Gas-Phase, Concurrent Injection-Extraction
- Soluble-Phase, Alternating Row Extraction
- Soluble-Phase, Concurrent Injection-Extraction
Figure 3.20 Boring T3 Soil Contamination Profile
4. LABORATORY EXPERIMENTATION

4.1. Introduction

The laboratory experimentation component of this research was conducted to evaluate PVW performance using clay soil obtained from the Ohio field site. The zone of influence and maximum extraction depth were investigated in the laboratory, and the potential effects of PVW geometry and long term testing were identified. This information is important for the design of future WIDE remediation projects (PVW spacing and installation depth), and will provide a baseline of information to utilize in future WIDE system research.

A 10 kPa WIDE experiment with a single PVW centered in the test sample was performed using an acrylic test box (0.97 m by 0.97 m by 1.21 m high) lined with a geocomposite to provide a constant head reservoir surrounding the test sample. A parastolic injection pump was used to transfer fluids from a holding tank to the constant head reservoir and a barrel-mounted venturi vacuum was used to extract air and water through the PVW. Vacuum gages were secured inside the PVW prior to installation to measure the vacuum pressure along the length of the PVW.

The test soil was a low to medium plasticity clay (CL) and it was obtained from the field site located in Ashtabula, Ohio. Even though the laboratory test soil was obtained from the field site to simulate similar soil conditions, the field soil was processed and a clay slurry sample was constructed while water content and unit weights were measured for each layer to ensure quality control and sample consistency. The test
sample included a 0.51 m thick clay layer ($\gamma_{AVG} = 16.76 \text{kN/m}^3$), a 0.12m thick sand seam ($\gamma_{AVG} = 17.80 \text{kN/m}^3$), and a second 0.32 m thick clay layer ($\gamma_{AVG} = 16.43 \text{kN/m}^3$). The sand seam was included to simulate a higher permeability layer, similar to field conditions. The average water content of the clay was approximately 55%.

During the sample fabrication process, three settlement plates were installed to monitor settlement as a function of depth and time, 23 piezometers were installed to measure the pressure head distribution relative to the PVW, 27 tracer tubes were installed to monitor the NaCl concentration during a tracer experiment, and three vacuum gages were used to instrument the PVW.

Each settlement plate consisted of a reference rod attached to a square plate. Settlement data were used to estimate the change in soil permeability (as manifested by volume change) at three different depths using the soil permeability versus void ratio relationship developed during a concurrent consolidation and falling head permeability test (performed independently of the test box experiment).

Piezometers were used to measure the zone of influence and maximum extraction depth from the steady state pressure head distribution. The surface of the water in each piezometer was determined using a multi-meter.

Identical in construction to the piezometers, tracer tubes were used to collect fluid samples during an NaCl tracer experiment designed to investigate flow capabilities at three different depths. A small vacuum pump was used to retrieve (Cl) fluid samples and the (Cl) concentration in the test sample was monitored as a function of depth and time.
4.2. Test Soil Description and Preparation

The test soil was obtained from an uncontaminated area of the field site. A number of laboratory tests were performed on the test soil, in conformance with ASTM standards, to characterize the soil. The average in-situ moisture content (ASTM D 2216-90), liquid limit and plastic limit (ASTM D 4318), and specific gravity (ASTM D 854) were determined to be 16 %, 26 %, 15 %, and 2.75, respectively. The test soil grain size distribution curve is illustrated in Figure 4.1. More than 90 % of the test soil passed the No. 200 sieve (0.075 mm). The soil was classified as a low to medium plasticity clay (CL).

Even though field soil was used for laboratory testing to simulate similar soil conditions, a soil slurry sample was generated in the laboratory to facilitate the fabrication of a large-scale clay sample and ensure a consistent water content and unit weight distribution. To accomplish this, the test soil was processed, prior to sample fabrication, to remove rocks and organic debris. A temporary soil processing structure (3.7 m by 4.9 m by 0.3 m) was used to contain the soil while it was sieved, dried, and pulverized (Figure 4.2). The weight of a Bobcat was used to crush the soil before mixing it with water inside a Schwing pump/mixer (Model BPA450-10) (Figure 4.3) and transferring it to a metal storage container.

A 0.75 hp, gear driven electric mixer with a 1.2 m long shaft and 0.3 m diameter blades was used to regenerate the test soil prior to placement in the test box. The electric mixer was mounted vertically to an I-beam and systematically moved within the storage container by way of an overhead crane (Figure 4.4).
4.3. Consolidation and Falling Head Permeability Testing

A consolidation cell (fitted for permeability testing) was used to conduct a concurrent consolidation and falling head permeability test testing in order to determine the soil permeability as a function of void ratio at a 52% water content. The high initial water content facilitated the soil transfer process. The consolidation test (ASTM D2435) was performed using load increments equal to 23.9 kN/m$^2$, 47.9 kN/m$^2$, 95.8 kN/m$^2$, and 191.5 kN/m$^2$. Subsequent to each load increment, a falling head permeability test was performed on the same test specimen to establish a permeability value for each void ratio at the end of primary consolidation. Soil permeability is displayed as a function of void ratio in Figure 4.5 ($R^2=0.96$).

4.4. Experimental Configuration

A 10 kPa WIDE test with a single PVW installed in the center of the test sample was performed using a 0.016 m thick, acrylic test box (0.97 m by 0.97 m by 1.21 m high), a parastolic injection pump, and a barrel-mounted venturi vacuum. The watertight test box was lined with a geocomposite consisting of a geotextile fabric on each side of a geonet layer. The primary function of the geotextile was filtration while the geonet provided the void space necessary to maintain a constant head reservoir boundary around the test sample, and a consistent hydraulic gradient to the test sample. A parastolic injection pump transferred fluids from a 757 L holding tank to the constant head reservoir. The barrel-mounted venturi vacuum extracted air and water through the PVW and was powered by a 15 hp, electric air compressor pump, housed within the laboratory. A Mebra drain wick system (provided by Nilex Corporation) was used during the
laboratory and field testing and the components of the laboratory configuration are illustrated in Figure 4.6.

### Table 4.1. Mebra Wick Drain Specifications

<table>
<thead>
<tr>
<th>Physical Properties</th>
<th>Test Method</th>
<th>Units</th>
<th>MD-88</th>
</tr>
</thead>
<tbody>
<tr>
<td>Drain Material</td>
<td></td>
<td></td>
<td>Polypropylene</td>
</tr>
<tr>
<td>Filter Material</td>
<td></td>
<td></td>
<td>Polypropylene</td>
</tr>
<tr>
<td>Weight</td>
<td>ASTM-D 1777</td>
<td>g/m</td>
<td>85</td>
</tr>
<tr>
<td>Width</td>
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<td></td>
<td>100</td>
</tr>
<tr>
<td>Thickness</td>
<td>ASTM-D 5199</td>
<td>mm</td>
<td>4.34</td>
</tr>
<tr>
<td>Mass of Filter</td>
<td>ASTM-D1777</td>
<td>g/m²</td>
<td>154</td>
</tr>
<tr>
<td>Equivalent Diameter</td>
<td>mm</td>
<td></td>
<td>65</td>
</tr>
<tr>
<td><strong>Mechanical Properties</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Core Grab Tensile Strength</td>
<td>ASTM-D 638</td>
<td>kN</td>
<td>0.996</td>
</tr>
<tr>
<td>Filter Grab Tensile Strength</td>
<td>ASTM-D 4632</td>
<td>kN</td>
<td>0.710</td>
</tr>
<tr>
<td>Filter Grab Elongation</td>
<td>ASTM- D 4632</td>
<td>%</td>
<td>90</td>
</tr>
<tr>
<td>Filter Strength @ 10 % Elongation</td>
<td>ASTM-D 4632</td>
<td>kN</td>
<td>0.230</td>
</tr>
<tr>
<td>Tear Resistance</td>
<td>ASTM-D-4533</td>
<td>kN</td>
<td>0.390</td>
</tr>
<tr>
<td>Puncture Strength</td>
<td>ASTM-D 4833</td>
<td>kN</td>
<td>0.267</td>
</tr>
<tr>
<td>Discharge Capacity @ 10 kN/m²</td>
<td>ASTM-D 4716</td>
<td>m³/s</td>
<td>180x10⁻⁶</td>
</tr>
<tr>
<td>Discharge Capacity @ 300 kN/m²</td>
<td>ASTM-D 4716</td>
<td>m³/s</td>
<td>140x10⁻⁶</td>
</tr>
<tr>
<td>Pore Size Opening</td>
<td>NEN 5168</td>
<td>mm</td>
<td>0.075</td>
</tr>
<tr>
<td>AOS</td>
<td>ASTM-D 4751</td>
<td>mm</td>
<td>0.110</td>
</tr>
<tr>
<td>Flux</td>
<td>ASTM-D 4751</td>
<td>l/min/m²</td>
<td>120/140</td>
</tr>
<tr>
<td>Filter Permeability</td>
<td>ASTM-D 4491</td>
<td>mm/s</td>
<td>0.171</td>
</tr>
<tr>
<td>Permittivity</td>
<td>ASTM-D 491</td>
<td>l/s</td>
<td>0.45</td>
</tr>
</tbody>
</table>

#### 4.5. Test Sample Fabrication and Quality Control

Due to the consistency of the clay, the transfer process from the metal storage container to the test box proved difficult. Initially, a 9 hp, engine driven trash pump with 0.076 m intake and discharge hoses was used. However, the heat generated by the motor decreased the water content of the slurry, which made transfer difficult and soil water inconsistent. As an alternative method, lifting straps were wrapped around the metal storage container, which was subsequently raised above the test box using an overhead
crane. The plug from a 0.10 m diameter flange attached to the bottom of the metal storage container was removed and the clay slurry was transferred from the metal storage container to the test box by way of gravity (illustrated in Figure 4.7).

Unit weight and water content measurements were obtained for each clay layer to ensure consistent values for quality control purposes. The test sample consisted of two clay layers and one 0.12 m thick sand seam (manually placed), as depicted in Figure 4.8. The sand seam was included to provide a high permeability avenue, similar to the silt seam located in the field. The profile percentage occupied by the sand seam in the laboratory (13 %) was equivalent to the profile percentage occupied by the silt seam in the field and the total unit weight was equal to 17.8 kN/m$^3$.

Due to the large initial volume of soil slurry in the metal storage container, it was difficult to impede the transfer of the soil slurry immediately following the removal of the flanged plug. The plug was re-attached when the rapid inflow rate slowed enough to permit it. For this reason, the volume of clay slurry transferred to the first clay layer (0.51 m) was greater than the volume transferred to the second clay layer (0.32 m).

Prior to this test, several preliminary slurry samples were fabricated in the test box for the purpose of developing a procedure to evaluate the density and water content distribution. A Shelby tube was initially used to retrieve in-place soil samples to measure the average water content and unit weight per clay layer during the sample fabrication process. However, the diameter of a standard Shelby tube was too large to retrieve an intact sample due to the soil consistency at a 52 % water content sample. Therefore, two alternative methods were utilized to measure unit weight.
In the first method, sections of copper plumbing pipe (0.16 m in length and 0.016 m in diameter) were pushed into each clay layer to retrieve an in-place soil sample, similar to the Shelby tube method (but on a different scale). The reduction in pipe diameter enabled successful soil retrieval and an accurate measure of weight, volume, unit weight, and water content. As an alternative method, a crane scale was used to measure the weight of soil transferred per clay layer, the volume of soil was determined from the dimensions in the test box, and the overall unit weight was calculated.

Unit weight and water content data are displayed in Table 4.2. The average unit weight of the two clay layers using the crane scale method was 16.90 kN/m$^3$ (0.58 kN/m$^3$ standard deviation) while the average unit weight using the copper pipe method was 16.28 kN/m$^3$ (0.22 kN/m$^3$ standard deviation). The average unit weight from the crane scale method (16.90 kN/m$^3$) minus one standard deviation (0.58 kN/m$^3$) was approximately equal to the average unit weight using the copper pipe method (16.28 kN/m$^3$). Therefore, the average unit weights for the bottom and top clay layers were 16.76 kN/m$^3$ and 16.43 kN/m$^3$, respectively, using the average of both methods. The average water content using copper pipe samples was 54.9 % (0.99 % standard deviation), which was approximately 3 % higher than the target water content. The soil conditions were deemed consistent between clay layers and reliable using either method.

4.6. Instrumentation Installation and Testing Procedures

In order to monitor settlement as a function of time and depth, three settlement plates (S1, S2, and S3) were installed at different depths (Figure 4.8) during the sample fabrication procedure. A hole was drilled and tapped in the center of a 0.20m square
piece of plastic before attaching a threaded reference rod. The length of each rod was
dependent upon placement depth. Immediately after the test sample was constructed, the
initial elevation of each reference rod was measured from the top of the test box and the
elevations were monitored as a function of time.

Table 4.2. Water Content and Unit Weight Measurements for Clay Layers

<table>
<thead>
<tr>
<th>Soil Layer</th>
<th>Copper Tube Method</th>
<th>Crane Scale Method</th>
<th>Water Content (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Clay 1 (0.52m)</td>
<td>16.44</td>
<td>17.31</td>
<td>55.6</td>
</tr>
<tr>
<td>Clay 1 (0.52m)</td>
<td>15.95</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Clay 1 (0.52m)</td>
<td>16.33</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Clay 1 (0.52m)</td>
<td>16.07</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Clay 1 (0.52m)</td>
<td>AVG = 16.2</td>
<td>SD = 0.23</td>
<td></td>
</tr>
<tr>
<td>Clay 2 (0.32m)</td>
<td>16.28</td>
<td>16.49</td>
<td>54.2</td>
</tr>
<tr>
<td>Clay 2 (0.32m)</td>
<td>16.10</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Clay 2 (0.32m)</td>
<td>16.46</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Clay 2 (0.32m)</td>
<td>16.58</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Clay 2 (0.32m)</td>
<td>AVG = 16.36</td>
<td>SD = 0.21</td>
<td></td>
</tr>
<tr>
<td>AVG</td>
<td>16.28</td>
<td>16.90</td>
<td>54.9</td>
</tr>
<tr>
<td>SD</td>
<td>0.22</td>
<td>0.58</td>
<td>0.99</td>
</tr>
</tbody>
</table>

Three rows of piezometers (23 total) were installed during the sample fabrication
procedure in one quadrant of the test box to determine the pressure head distribution 0.15
m from the bottom of the sample (Figure 4.8). A plan-view of the piezometer locations is
displayed in Figure 4.9. The piezometers (Figure 4.10) were constructed by drilling 1.6
mm diameter holes (approximately 4 holes per centimeter) in the bottom 0.05 m of a
rigid, plastic tube 4.8 mm in diameter. The holes were wrapped with the same geotextile
used for the PVW and a metal rod was inserted inside each piezometer tube to increase
the stiffness while each piezometer was manually inserted into the test sample.
A multi-meter was used to determine the water location in each piezometer with reference to a datum so that a pressure head distribution could be determined. One of two multi-meter leads were placed inside the constant head reservoir surrounding the soil sample and the second lead was slowly inserted inside the piezometer tube until the water surface inside the piezometer caused the multi-meter to display an electric current reading, indicating a closed circuit condition. The length of the lead was then measured relative to a reference elevation.

For quality control purposes, data repeatability was independently verified using a section of piezometer tubing secured to the inside of a graduated cylinder filled with water. One of two leads was placed outside of the tubing in the water reservoir and the second lead was lowered inside the piezometer tube until the multi-meter displayed an electric current reading. From visual inspection, the meter reacted to the water surface instantaneously. Nine measurements, ranging from 0.1238 m to 0.1254 m, were obtained to quantify user error. The mean and standard deviation were 0.1247 m and 0.00083 m, respectively.

Nine tracer tube nests (each having a tracer tube located 0.15m, 0.41m, and 0.57m from the sample bottom) were installed in one quadrant of the test box in order to collect fluid samples during the tracer test. The construction of a tracer tube was identical to that of a piezometer. The location (plan-view) of each tracer tube nest is displayed in Figure 4.9. After steady state flow conditions were achieved using tap water as the injection fluid, an NaCl tracer was injected into the system using the same method. Flexible tubing (3.2 mm diameter) that was attached to a small vacuum pump was inserted inside
each tracer tube to retrieve a liquid tracer sample. Samples were contained in 20 mL vials while the (Cl) concentration and pH were measured.

Prior to PVW installation, three vacuum gages were connected to reinforced tubing and inserted inside the PVW. The three tubes were located 0.23 m, 0.46 m, and 0.67 m from the bottom of the PVW. The instrumented PVW is displayed in Figure 4.11. Initially, an aluminum mandrel was fabricated to simulate field installation of the PVW in the laboratory. However, retrieval of the mandrel was difficult. Alternatively, a metal yard stick (approximately 0.05 m wide) was inserted inside the geotextile jacket to stiffen the PVW and subsequently pushed through the center of the test sample to the full depth. The metal yard stick was retrieved with minimal disturbance to the PVW and adjacent soil.

Similar to field installation procedures, an impermeable sleeve was attached to the PVW. The sleeve extended from the venturi vacuum into the slurry sample to ensure a closed system. In addition, a layer of bentonite (approximately 0.03m thick) was placed on top of the test sample to minimize air infiltration. The PVW was clamped to the vacuum unit inlet and water was injected into the constant head reservoir surrounding the test sample to saturate the test sample. The instrumented test sample is illustrated in Figure 4.12.
4.7. Experimental Results

4.7.1. Settlement and Permeability

Settlement plates S1, S2, and S3 (Figure 4.8) measured settlement during the 10 kPa test at three different depths, as presented in Figure 4.13. Approximately 0.076 m, 0.124 m, and 0.176 m of cumulative settlement was measured using settlement plates S1, S2, and S3, respectively, and the equivalent settlement from the soil located directly below each respective settlement plate was equal to 0.076 m, 0.048 m, and 0.052 m, respectively.

The initial void ratio of the clay was equal to 1.36, which corresponded to an initial soil permeability equal to $8.0 \times 10^{-7} \text{ cm/s}$ (Figure 4.5). Subsequent to laboratory testing, the void ratio decreased to 0.69, 1.17, and 0.49 for the soil volumes located directly under settlement plates S1, S2, and S3, respectively, and the corresponding permeability values were approximately $4.0 \times 10^{-8} \text{ cm/s}$, $1.5 \times 10^{-7} \text{ cm/s}$, and $1.7 \times 10^{-8} \text{ cm/s}$, respectively.

The vacuum-induced gradient accelerated settlement towards the top of the test sample, and the overburden soil weight accelerated settlement at the bottom of the test sample. Settlement values measured during laboratory experimentation were high due to the initial water content of the test sample. The initial water content of the laboratory sample was approximately 55% compared to the 16% in-situ water content in the field. Therefore, settlement values of this magnitude would not occur in the field.
4.7.2. Mass Balance

Flow rates were measured to monitor soil flushing efficiency and ensure a mass balance (defined by Equation 4.1) during laboratory testing. The mass of water into the system was equal to the parastolic injection pump rate less the volume of water collected from the overflow valve. The mass of water exiting the system was a combination of measured outflow collected inside the barrel-mounted venturi vacuum and water vapor, which was estimated using psychrometric charts.

\[(M_{\text{in(parastolic pump)}} - M_{\text{overflow}}) = (M_{\text{out(barrel liquid)}}) + (M_{\text{out (water vapor)}}) \quad \text{Equation (4.1)}\]

Measured inflow and outflow rates are displayed in Figure 4.14 as a function of time. The flow rates decreased with time and eventually reached steady state conditions. Prior to the decrease, flow rates were indicative of ranges valid in sandy soils. Therefore, the majority of pore water initially moved through the 0.12 m sand seam. Since measured inflow and outflow rates decreased significantly with time while settlement occurred, it can be concluded that fine-grained particles contaminated the sand seam and decreased the flow potential. As permeability decreased, liquid-phase outflow approached zero and the majority of water was extracted as vapor during steady state conditions, similar to field testing results.

The psychrometric chart used to estimate the water vapor extracted is presented in Figure 4.15 (Shallcross, 1997). The rate of water vapor extracted was equal to the difference between inflow and outflow in Figure 4.14. The temperature, relative humidity, and air-water flow rates necessary to calculate the water vapor extraction rate were measured during laboratory experimentation using a temperature-humidity gage and
a Magnelhelic Gage (Model No. W48KCF, Dwyer Industries, Inc.) that measured the air-water flow rate through the PVW. An example calculation is provided in Appendix B (Chapter 10).

4.7.3. Piezometers

Three rows of piezometers (Figure 4.9) were used to evaluate the zone of influence and the maximum extraction depth. The total hydraulic head calculated from each piezometer measurement during steady state conditions is displayed as a function of lateral distance from the PVW in Figure 4.16, Figure 4.17, and Figure 4.18 for piezometer rows P1 - P10, P13 - P19, and P20 - P29, respectively. The total hydraulic head measured in the piezometers located 0.05 m from the PVW (P9, P19, and P29) was approximately 0.58 m, 0.65 m, and 0.32 m, respectively. The maximum extraction depth (drawdown) measured from piezometer P29 was approximately twice the value measured at the same radial distance from the PVW in piezometers P9 and P19 due to the location of the piezometer relative to the PVW (Figure 4.9). Piezometer P29 was located nearest to the center of the 100 mm wide PVW dimension.

The zone of influence is the diameter of the cylindrical column captured by the PVW under vacuum induced hydraulic gradient. The radius of influence (one half of the zone of influence) for piezometer rows P1-P10, P13-P19, and P20-P29 was found to be approximately 0.30 m, 0.35 m, and 0.40 m, respectively, according to Figures 4.16 through Figure 4.18. Similar to the extraction depth values, the radius of influence was a maximum in the piezometer row closest to the center of the 100 mm PVW dimension. These results suggest that the PVW geometry affected the zone of influence and
extraction efficiency. The piezometers closest to the center of the wide 100 mm PVW dimension benefited from full flow potential due to the increase in PVW surface area relative to surface area of the PVW side corresponding to the 4 mm dimension.

Additionally, an increase, rather than decrease, in the total hydraulic head occurred in piezometer P10 relative to P9 (Figure 4.16). This piezometer was also adjacent to the narrow 4 mm PVW dimension. Due to the band-shaped geometry, it was hypothesized that the flow volume was restricted in the area near the narrow dimension of the PVW, which caused the increase in the corresponding pressure head and existing exit gradient during laboratory experimentation.

A contour plot of the total hydraulic heads was developed in Figure 4.19. A mirror image of the quadrant results was generated to better illustrate the equipotential lines during steady state conditions. The areas of increased exit gradient (choke zones) were identified.

4.7.4. **Vacuum Pressure Inside the PVW**

Vacuum pressure was measured along the length of the PVW. During steady state conditions, the vacuum pressures measured 0.23 m, 0.46 m, and 0.67 m from the bottom of test sample were approximately 6.8 kPa, 8.5 kPa, and 10 kPa, respectively (Figure 4.20). Approximately 7 kPa/m of vacuum was lost between gages. There was no measured loss in vacuum pressure between the top vacuum gage and the venturi vacuum unit. A vacuum gage with greater precision may have measured minor headlosses along the PVW. The decrease in vacuum pressure (due to air filtration) would be less apparent at a higher vacuum level.
4.7.5. **Tracer Testing**

An NaCl tracer was utilized in the tracer test experiment designed to identify the direction and preferential areas of flow. Nine tracer tube nests (three tracer tubes per nest) were installed in one quadrant of the soil sample (Figure 4.9) to monitor the (Cl) concentration in each tube as a function of time and depth. Prior to tracer testing, baseline (Cl) concentrations were measured and the fluid regeneration time was investigated. Water was extracted from each tracer tube during laboratory testing and the subsequent increase in soluble-phase concentration was monitored over time. Tracer tube fluid elevations rebounded within 48 hours in clay and immediately in sand, as a result of the increased soil permeability.

The initial (Cl) concentration \( C_0 \) was equal to 1750 mg/L. Tracer samples were collected during 1200 operational hours until steady state (Cl) concentrations were achieved. Figure 4.21 depicts average (Cl) concentrations (less baseline concentrations) as a function of cumulative test time. It took approximately 400 - 600 hours to achieve steady state concentrations. For data trend clarity, regression lines were included for the 0.15 m \( (R^2 = 0.86) \), 0.41 m \( (R^2 = 0.92) \), and 0.57 m \( (R^2 = 0.94) \) data set.

Over the course of 1200 operational hours, the tracer tubes located 0.41 m and 0.57 m from the sample bottom recovered between 90 % and 100 % of the initial (Cl) concentration during steady state flow conditions, but the (Cl) concentrations measured in the tracer tubes located 0.57 m from the sample bottom were generally higher. Alternatively, the tracer tubes located 0.15 m from the sample bottom only recovered 40 % of the initial (Cl) concentration.
The decrease in measured concentration was a result of the vacuum pressure decrease with depth (Figure 4.20). A decreased vacuum pressure caused the hydraulic gradient as well as the pore water velocity to decrease along the length of the PVW. If the soil permeability had been a factor, the NaCl concentrations measured in the high permeability sand seam (0.57 m from the sample bottom) would not have been approximately equal to the concentrations measured in the low permeability clay (0.41 m from the sample bottom.

4.7.6. PVW Issues

Subsequent to testing, the PVW was retrieved and the geotextile stripped from the core for post-test quality control. Minimal soil clogging was evident in the PVW channels. Soil either piped through the bottom of the PVW seal or through the geotextile directly. Due to the small cross-sectional flow area, channel clogging can significantly reduce the flow capacity of a PVW especially during long-term testing in the field. During PVW installation in the field, a PVW was wrapped around the handle of an anchor plate without sealing bottom, which could pose a problem at higher vacuum pressures over long periods of time.

Circular portions of the PVW geotextile were trimmed to determine the permeability of the fabric following several months of vacuum induced flow through the PVW. The 0.076 m diameter specimens were placed in a permeability cell to conduct falling head permeability tests and the results were compared to the results of permeability tests conducted with a clean fabric sample. There were no solids present in the effluent water during permeability testing. For the soil-embedded fabric specimens,
permeability values ranged from $2.49 \times 10^{-5}$ cm/s to $2.78 \times 10^{-5}$ cm/s. The average permeability and standard deviation were $2.65 \times 10^{-5}$ cm/s and $1.26 \times 10^{-6}$ cm/s, respectively. The permeability for the clean fabric specimen ranged from $2.75 \times 10^{-5}$ cm/s to $3.88 \times 10^{-5}$ cm/s. The average permeability and standard deviation was $3.01 \times 10^{-5}$ cm/s and $3.42 \times 10^{-6}$ cm/s. It can be concluded that there was a 14% permeability decrease in the geotextile fabric over, which is well within the variability of the measured property.

4.8. Summary of the Laboratory Experimentation Component

The laboratory experimentation component of this research was conducted to investigate individual PVW performance during a 10 kPa laboratory test using soil obtained from the field site. The zone of influence and maximum extraction depth were investigated in the laboratory, and the potential effects of PVW geometry and long term testing were addressed. The information from this research is important to the future design of WIDE remediation projects and will provide a baseline of information to utilize for future WIDE system research.

The laboratory test soil was a low to medium plasticity clay (CL) and it was obtained from the field site located in Ashtabula, Ohio. Laboratory experimentation was performed in an acrylic test box lined with a geocomposite to provide a constant head reservoir boundary around the test sample. A clay slurry sample was constructed to ensure sample consistency. The profile included a 0.51 m thick clay layer ($\gamma_{AVG} = 16.76$ kN/m$^3$), a 0.12 m thick sand seam ($\gamma_{AVG} = 17.80$ kN/m$^3$), and a 0.32 m thick clay layer

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(γ_{AVG} = 16.43 kN/m³). The sand seam provided a higher permeability channel, similar to the silt seam described during the field demonstration.

A parastolic injection pump was used to transfer fluids from a holding tank to the constant head reservoir and a barrel-mounted, venturi vacuum was used to extract air and water through the PVW. Three settlement plates, 23 piezometers, 27 tracer tubes, and one PVW were installed during sample fabrication to monitor settlement, the pressure head distribution, and (Cl) tracer concentration over the duration of the test. Vacuum gages measured the vacuum pressure inside the PVW as a function of depth.

Settlement was monitored to estimate the soil permeability change as a function of time due to the initial consistency of the test sample. Approximately 0.076 m, 0.048 m, and 0.052 m of settlement was measured from settlement plates S1, S2, and S3, respectively, which decreased the soil permeability value at the middle of each clay layer directly under each corresponding settlement plate from $8.0 \times 10^{-7}$ cm/s to $4.0 \times 10^{-8}$ cm/s, $1.5 \times 10^{-7}$ cm/s, and $1.7 \times 10^{-8}$ cm/s. Settlement has not been measured in a field situation. However, vacuum induced settlement in the field would be significantly less due to the initial water content of the laboratory sample (55 %) versus the in-situ water content (16 %) and would depend upon the vacuum pressure level.

The zone of influence (equal to two times the minimum radius of influence) of the low to medium plasticity clay (CL) soil during the 10 kPa test was approximately 0.60 m. In this application, the zone of influence is sized to allow the cylindrical soil column that represents the zone affected by the vacuum induced hydraulic gradient to overlap, ensuring that all areas are treated.
The maximum drawdown or extraction depth (approximately 0.45 m) and the largest radius of influence (0.40 m) were both measured in the piezometer located closest to the center of the wide 100 mm PVW dimension. The drawdown measured in piezometer closest to the narrow 4 mm dimension was decreased by a factor of two and the zone of influence was 0.20 m less in this location, which suggests that the band-shaped PVW geometry had an affect on the hydraulics adjacent to the PVW. Flow potential appeared to increase as the adjacent PVW surface area increased. Additionally, pore pressures developed near the narrow 4mm PVW dimension causing a choke zone during testing (Figure 4.19).

Vacuum pressures equal to 6.8 kPa, 8.5 kPa, and 10 kPa were measured inside the PVW 0.23 m, 0.46 m, and 0.67 m from the bottom of test sample, respectively. Approximately 7 kPa/m of vacuum was lost between gages but there was no measured loss in vacuum pressure between the top vacuum gage and the venturi vacuum unit. A more precise vacuum gage may have measured small headlosses along the length of the PVW. The decrease in vacuum pressure (due to air filtration) would be less apparent at a higher vacuum level. The applied field vacuum pressure varied between 15 kPa and 26 kPa dependent upon the location of the water table, which governed the volume of air infiltration into the system. The vacuum pressure (in a field or laboratory setting) will significantly affect flow potential. As the vacuum pressure and applied hydraulic gradient decreased, the corresponding flow rate decreased, which affected WIDE system efficiency.
An NaCl tracer was used in a tracer test experiment designed to identify the direction and preferential areas of flow. The initial (Cl) concentration \( C_0 \) was equal to 1750 mg/L and it took approximately 400 - 600 hours to achieve steady state concentrations. Over the course of 1200 operational hours, the (Cl) tracer samples retrieved 0.41 m and 0.57 m from the sample bottom recovered between 90 % and 100 % of the initial (Cl) concentration, but the samples retrieved 0.15 m from the sample bottom only recovered 40 % of the initial (Cl) concentration. The decrease in measured concentration was a result of the vacuum pressure decrease with depth. The vacuum pressure decrease caused the hydraulic gradient as well as the pore water velocity to decrease along the length of the PVW.

Minimal soil clogging was located in the PVW channels subsequent to laboratory testing. Soil either piped through the bottom of the PVW seal or through the geotextile directly. Due to the small cross-sectional flow area, channel clogging can significantly reduce the flow capacity of a PVW especially during long-term testing in the field. During PVW field installation, each PVW was wrapped around the handle of an anchor plate without sealing bottom, which could pose a problem at higher vacuum pressures over long periods of time.
Figure 4.1. Test Soil Grain Size Distribution Curve
Figure 4.2. Temporary Soil Processing Structure
Figure 4.3. Schwing Pump/Mixer (Model BPA450-10)
Figure 4.4. Electric Mixer
Figure 4.5. Test Soil Permeability as a Function of Void Ratio
Figure 4.6. Experimental Configuration
Figure 4.7. Clay Slurry Transfer
Figure 4.8. Test Sample Profile and Instrumentation
Figure 4.9. Instrumentation Layout (Plan-View)
Figure 4.10. Laboratory Piezometers
Figure 4.11. PVW Instrumented with Vacuum Gages
Figure 4.12. Constructed Test Sample and Instrumentation
Figure 4.13. Cumulative Settlement as a Function of Time
Figure 4.14. Measured Inflow and Outflow

Inflow - Measured Outflow = Vapor Phase Outflow

- Inflow ($R^2=0.92$)
- Measured Outflow ($R^2=0.85$)
Figure 4.15. Psychrometric Chart for a Water-Air System at 1 Atmosphere (Shallcross, 1997)
Figure 4.16. Total Hydraulic Head as a Function of Lateral Distance from the PVW Center (Piezometers P1-P10)
Figure 4.17. Total Hydraulic Head as a Function of Lateral Distance from the PVW Center (Piezometers P13-P19)
Figure 4.18. Total Hydraulic Head as a Function of Lateral Distance from the PVW Center (Piezometers P20-P29)
Figure 4.19. Total Hydraulic Head Contours
Figure 4.20. PVW Vacuum Pressure Profile
Figure 4.21. (Cl) Concentration Ratio (C/C₀) as a Function of Time

- 0.15m From Sample Bottom (CLAY)
- 0.41m From Sample Bottom (CLAY)
- 0.57m From Sample Bottom (SAND)

\[ R^2 = 0.94 \]

\[ R^2 = 0.92 \]

\[ R^2 = 0.86 \]

\[ C_0 = 1750 \text{ mg/L} \]
5. MODEL DEVELOPMENT AND CALIBRATION

5.1. Introduction

A three-dimensional finite element analysis was performed using NAPL Simulator (U.S. EPA, 1997), which was approved for use by the EPA. This chapter describes the methods used to develop and calibrate the model test grid using the subsurface conditions and hydraulic data from the field demonstration.

5.2. Contaminant Transport Mechanisms and Fate Processes

The effects of contaminant transport mechanisms and fate processes that occur within the soil matrix contribute to system performance. The following paragraphs introduce basic subsurface flow and contaminant transport concepts utilized in the three-dimensional finite element analysis model.

The water table defines the boundary between the saturated (positive fluid pressures) and the unsaturated zone (negative fluid pressures). A capillary fringe exists directly above the water table and the height of capillary rise is inversely proportional to the pore size of the soil and directly proportional to surface tension. The soil permeability and the volumetric water content are a function of the pressure head in the unsaturated zone. The relationship between the volumetric water content and the pressure head (capillary suction head) in the unsaturated zone is termed the soil-water characteristic curve, it varies with soil type, and it is typically measured by soil scientists in the laboratory using a tensiometer (Bedient, Refai, and Newell, 1999).
Contaminants are transported in the groundwater by way of advection, diffusion, and dispersion. Advection occurs at a rate equal to the seepage velocity (Darcy velocity divided by the effective porosity associated with the pore space through which water can actually flow in the soil media). Diffusion occurs on a molecular-scale and can be the dominant mode of transport in the case of low ground water velocity. Contaminants diffuse from areas of high concentration to areas of low concentration. Dispersion is ultimately a mixing and/or spreading process caused by soil heterogeneities that create variations in the flow velocity and direction. Dispersion can occur in the longitudinal direction (parallel to flow) and in the transverse direction (perpendicular to flow).

All three contaminant phases (soluble, gas, and NAPL-phases) interact with the soil particles and environment. Contaminant sorption is the association of a dissolved or gaseous contaminant with the solid component of the soil. Sorption can significantly retard the movement of contaminants and influence the remediation of a contaminated site. The fraction of organic matter in the solid phase affects the amount of sorption that takes place between an organic contaminant (TCE) and a solid particle in the soil. The adsorption partitioning coefficient is a measure of the contaminant distribution between solid and aqueous phases. Volatilization is the transfer of a contaminant from the soluble or free product NAPL-phase to the gas-phase. Volatilization is dependent upon the contaminant phase, vapor pressure, and specific site and/or test conditions. The distribution between the soluble and gas-phase is described by Henry’s law coefficient. Abiotic processes and biodegradation were not considered during the modeling process.
5.3. **Numerical Model Description**

NAPL Simulator (U.S. EPA, 1997) was used to model the WIDE system in three dimensions using finite element analysis methods. In comparison to finite difference methods, finite element analysis methods can track a sharp front more accurately, limiting the amount of numerical dispersion during the modeling process (Bedient, Rifai, and Newell, 1999). NAPL Simulator is a saturated and unsaturated subsurface flow and contaminant transport model that can handle a single NAPL species in the soluble, gas, and free product NAPL-phases during inter-phase mass transfer processes in heterogeneous soils. Fluids move by way of advection, dispersion, and diffusion. Free product NAPLs migrate in the vertical and lateral direction by way of gravitational and capillary forces, dissolve into the soluble-phase, and volatilize into the gas-phase. Soluble-phase NAPL volatilizes into the gas phase and sorbs onto the solid phase. Gas-phase NAPL sorbs onto the solid phase only. Darcy’s Law is considered valid to quantify water, gas, and NAPL-phase advection while Fick’s Law is considered valid to quantify water and gas-phase diffusion.

During finite element analysis, the three-dimensional domain is discretized into a finite number of rectangular elements with nodes located at the element boundary intersections. All spatially varying parameters are represented by a linear combination of basis functions. Nodal values are interpolated into adjacent elements in a continuous manner. The numerical solution algorithm is based on a Hermite collocation finite element discretization. An accurate solution of a coupled set of non-linear partial differential equations is generated by combining fundamental balance equations with
NAPL-phase dissolution and vaporization and soluble-phase NAPL vaporization is governed by the rate-limited, first-order, kinetic rule. Soluble-phase NAPL adsorption is governed by a linear equilibrium partitioning rule. Time step control is provided by two algorithms based on the number of iterations required for convergence or the maximum Courant number.

Five mass balance equations are coupled with constitutive and thermodynamic conditions to provide a complete subsurface flow and contaminant transport model when proper boundary conditions are imposed. The mass balance equations are represented by five primary variables (water-phase pressure ($P^W$), water-phase saturation ($S^W$), total liquid phase saturation ($S^L$), mass concentration of soluble-phase NAPL ($\rho^W_n$)), and mass concentration of gas-phase NAPL ($\rho^G_n$)). Physical constants include fluid-phase density, viscosity, interfacial tension, dispersion, mass transfer rates, solubility limits, Henry’s law coefficient, organic carbon-based partitioning parameters, porosity, and permeability.

The mass balance law for each fluid constituent, an ordered pair ($\iota, \alpha$) representing a species $\iota$ (water, gas, or NAPL) and a fluid phase $\alpha$ (water, NAPL, or gas) is displayed in Equation 5.1 (U.S. EPA, 1997). The relevant fluid constituents include the water species in the water phase ($w, W$), NAPL species in the water phase ($n, W$), NAPL species in the NAPL phase ($n, N$), NAPL species in the gas phase ($n, G$), and gas species in the gas phase ($g, G$).

$$\frac{\partial (\varepsilon S^\iota_n \rho^\iota_n)}{\partial t} + \nabla \cdot \left[ \varepsilon S^\iota_n \rho^\iota_n \mathbf{v} \right] = \nabla \cdot \left[ \varepsilon S^\iota_n \rho^\iota_n \mathbf{D}^\iota \nabla \left( \frac{\rho^\iota_n}{\rho^\alpha} \right) \right] + \varepsilon S^\iota_n k^\iota_n \rho^\iota_n = \rho^\iota_n Q^\iota + * \rho^\iota_n$$

Equation (5.1)
where: \( \varepsilon \) = porosity of soil medium
\( S_\alpha \) = saturation of the \( \alpha \) phase
\( \rho_\alpha^\iota \) = mass concentration of species \( \iota \) in the \( \alpha \) phase
\( v_\alpha \) = mass average velocity of phase \( \alpha \), a vector
\( D_\alpha \) = the dispersion coefficient for the \( \alpha \) phase, a symmetric 2\(^{nd}\) order tensor
\( Q_\alpha \) = the point source or sink \( \alpha \) phase mass
\( \kappa_\iota^\alpha \) = the decay coefficient for species \( \iota \) in the \( \alpha \) phase
\( \ast \rho_\iota^\alpha \) = the source or sink of mass for a species \( \iota \) in the \( \alpha \) phase due to inter-phase mass exchange (i.e. dissolution, volatilization and adsorption)

The exchange of mass for each constituent in Equation 5.1 is defined in Equation 5.2 through Equation 5.6 (U.S. EPA, 1997).

\[
\ast \rho_w^W = 0 \quad \text{Equation (5.2)}
\]

\[
\ast \rho_n^W = E_n^W - E_{n/W}^G - E_{n/W}^S \quad \text{Equation (5.3)}
\]

\[
\ast \rho_n^V = -(E_n^W + E_n^G) \quad \text{Equation (5.4)}
\]

\[
\ast \rho_n^G = E_n^G + E_{n/W}^G \quad \text{Equation (5.5)}
\]

\[
\ast \rho_g^G = 0 \quad \text{Equation (5.6)}
\]

where: \( E_n^W \) = dissolution mass transfer of the NAPL species from the NAPL phase to the water phase
\( E_{n/W}^G \) = volatilization mass transfer of the NAPL species from the water phase to the gas phase
\( E_n^G \) = volatilization mass transfer of the NAPL species from the NAPL phase to the gas phase
\( E_{n/W}^S \) = adsorption mass transfer of the NAPL species from the water phase to the soil

Equation 5.7 (U.S. EPA, 1997) describes the mass balance equation required for the NAPL species mass adsorbed on the soil:
\[ \frac{\partial ([1 - \varepsilon] \rho^S \omega^S_n) \partial t}{\partial t} + [1 - \varepsilon] \rho^S k^S_n \omega^S_n = E^S_{nw} \]  

\textbf{Equation (5.7)}

where: \( \rho^S = \) density of the soil  
\( \omega^S_n = \) mass fraction of the adsorbed NAPL on the solid

Equation 5.7 is replaced by the linear equilibrium relationship depicted in Equation 5.8 (U.S. EPA, 1997):

\[ \omega^S_n = K_d \rho^W_n \]  

\textbf{Equation (5.8)}

where: \( \omega^S_n = \) mass fraction of the adsorbed NAPL on the solid  
\( K_d = \) distribution coefficient

To ensure global mass conservation, the following constraints on fluid volume, density, and mass exchange were employed:

1) The \( \alpha \) phase saturation must sum to one \((S_W + S_N + S_G = 1)\)

2) The \( \alpha \) phase mass density is the sum of the species mass concentration in the \( \alpha \) phase

3) The sum of mass fluxes of all species \( \iota \) into the \( \alpha \) phase must equal the total mass change in the \( \alpha \) phase

4) The total mass change over all phases must be zero

5) The sum of the reacting mass must be equal to the sum of the produced mass.

A set of fluid-phase mass balance equations are generated by summing Equation 5.1 for each species with the phase, and by incorporating the above definitions and constraints. Equation 5.9 through Equation 5.11 (U.S. EPA, 1997) represent the fluid-phase balance equations for the water-phase, NAPL-phase, and gas-phase, respectively,
and define the temporal and spatial distribution and flow properties throughout the domain.

\[ \frac{\partial (eS_w \rho^w)}{\partial t} + \nabla \cdot [eS_w \rho^w \mathbf{v}^w] = \rho^w Q^w + E_n^w - E_{n/W}^w - E_n^s \quad \text{Equation (5.9)} \]

\[ \frac{\partial (eS_N \rho^N)}{\partial t} + \nabla \cdot [eS_N \rho^N \mathbf{v}^N] = \rho^N Q^N - E_n^w - E_n^G \quad \text{Equation (5.10)} \]

\[ \frac{\partial (eS_G \rho^G)}{\partial t} + \nabla \cdot [eS_G \rho^G \mathbf{v}^G] = \rho^G Q^G + E_n^G + E_{n/W}^G \quad \text{Equation (5.11)} \]

Two additional NAPL species balance equations (Equation 5.1 with \((1, \alpha) = (n, W)\) and \((n, G)\)) define the temporal and spatial distribution of the NAPL species as they are transported within and between their respective phases. Flow-variable, mass transport, and external flux conditions are assigned to boundary nodes to satisfy numerical equations. Boundary nodes left undefined are considered no-flow boundary conditions. In addition, an initial water saturation \((S_W)\), total wetting phase saturation \((S_{TW} = S_W + S_N)\), and NAPL mass concentration in the soluble and gas-phases \((\rho_n^w\) and \(\rho_n^G\), respectively) are required.

### 5.4. Summary of the In-Situ Field Conditions to be Modeled

A model test grid was developed to simulate field testing conditions in Ashtabula, Ohio. The following paragraphs summarize the subsurface conditions and describe the WIDE demonstration system operated over nine months at the field site. The subsurface profile consisted of a low to medium plasticity clay (CL) with the exception of a silt (ML) layer located approximately 1.8 m to 2.4 m below the ground surface. An average
soil permeability equal to $1 \times 10^{-6}$ cm/s was measured from in-situ field permeability tests. The porosity was estimated to be 0.4 and the water table was located approximately 0.4 m below the ground surface at the time of subsurface exploration.

The field site was contaminated as a result of the operation of an unlined evaporation pond that was used to dispose of spent solutions, which included trace quantities of TCE. It was believed that a single TCE spill occurred from a storage container but this information was unconfirmed. The majority of TCE contamination on the soil was detected within the first 6.1 m of the ground surface. Soil contamination levels as high as 300,000 $\mu$g/kg, and water contamination levels as high as 475 mg/L were measured prior to the field demonstration. The MCL for TCE on soil was 25$\mu$g/kg and the MCL for TCE in the groundwater was 5$\mu$g/L.

To demonstrate the capabilities of the WIDE system, 494 PVWs were positioned over a 21.0 m by 18.3 m test area, which was divided into four operational quadrants (Figure 3.2). The PVWs were installed 6.1 m deep in a grid pattern of offset rows that were spaced approximately 0.91 m apart. Each PVW was sheathed with an impermeable sleeve to a depth of 1.5 m. Vacuum pressure, injected and extracted air and water volumes, TCE concentrations in air and water, and the water table locations were monitored during the field demonstration testing. While field testing provided invaluable data for future WIDE system design and operation. The finite element analysis model was used as a tool to evaluate select input parameters, to perform a sensitivity analysis, and to investigate fundamental design issues that could not be varied in a field situation due to time and budget constraints.
5.5. Model Test Grid Development

5.5.1. Dimensions, Boundary Conditions, and Initial Conditions

The model test grid was 6.0 m by 1.0 m by 1.0 m (X:Y:Z). The X-dimension corresponded to the PVW installation depth, and the Y and Z-dimensions corresponded to the PVW spacing. Field subsurface conditions were consistent across the demonstration test area during subsurface exploration. Therefore, the model test grid dimensions were selected to simulate the volume of soil affected by a repeated element of the WIDE quadrant grid displayed in Figure 3.2, and simulation results for the modeled element were assumed valid for each additional element of the WIDE quadrant grid. For example, a 16 PVW grid is displayed in Figure 5.1. The plan-view dimensions of the model test grid in Figure 5.1 were equal to the PVW spacing of a single grid element in a field test quadrant. By symmetry, one quarter of the extraction flow rate for a single PVW was assigned to the nodes at each corner of the model test grid.

Figure 5.2 displays the analysis model test grid in plan and profile-view and includes the orientation, grid dimensions, boundary conditions, soil parameters, and numbers designated to the each node. The origin of the mesh is located at corner A in Figure 5.2 and the nodes are numbered in order of the Y-coordinate first, X-coordinate second, and Z-coordinates third. There were 25 X-coordinate elements (26 nodes) and 10 Y and Z-coordinate elements (11 nodes) totaling 3,146 nodes (286 nodes on each vertical plane and 111 nodes on each horizontal plane).
Gas pressure head values (flow-variable boundary conditions) equal to atmospheric pressure, and soluble-phase TCE concentrations (mass transport boundary conditions) equal to zero, were assigned to each node located on the top boundary of the model test grid (Figure 5.2). As previously described, extraction wells (external flux boundary conditions) were assigned to nodes located in each corner of the model test grid to simulate PVWs with one quarter of the total extraction flow rate due to symmetry (Figure 5.1). To account for the impermeable sheathing installed on each PVW during field installation, extraction wells in the model were only assigned to nodes located 1.5 m and below.

The global dry unit weight, porosity, and clay permeability values were set to 1.8 kN/m$^3$, 0.4, and $1 \times 10^{-6}$ cm/s, respectively. A $1 \times 10^{-5}$ cm/s permeability was assigned to nodes 2.10 m and 2.40 m from the ground surface to simulate the silt seam detected during subsurface exploration in the field. The accuracy of this value was evaluated during the calibration process. The initial water saturation of the model test grid was equal to 1.0 (fully saturated) to reflect the shallow water table in the field.

### 5.5.2. Calibration

Using the dimensions and soil parameters described in Figure 5.2 with a total extracted water flow rate equal to 0.21cc/s (which is a typical field flow rate), the model test grid was hydraulically calibrated using two different assumptions during extraction-only procedures. First, the extraction flow rate was assumed constant with depth, which eliminated the effects of the higher permeability silt seam. Second, the extraction flow
rate was concentrated in the higher permeability silt seam. The calibration approach used for each method is summarized in the following paragraphs.

5.5.2.1. Assumption 1: Constant Flow Rate with Depth

Assuming a constant extraction flow rate with depth for each node, a series of simulations were performed by varying the extraction well flow rate and the clay permeability to determine the corresponding rate of water table drop for comparison with field demonstration values. Three different full quadrant flow rates ($Q_1=20\ \text{L/hr}$, $Q_2=60\ \text{L/hr}$, and $Q_3=100\ \text{L/hr}$) and three different clay permeability values ($K_{\text{clay1}}=1\times10^{-6}\ \text{cm/s}$, $K_{\text{clay2}}=5\times10^{-6}\ \text{cm/s}$, and $K_{\text{clay3}}=1\times10^{-5}\ \text{cm/s}$) were used to generate the first calibration test matrix consisting of nine simulations. A full quadrant consisted of 132 PVWs (identical to Quadrant 4 in Figure 3.2) and the permeability of the silt seam was consistently one order of magnitude higher than the clay permeability.

Figure 5.3(a) displays the water table drop rate (calculated from simulation output) as a function of the model extraction flow rate assigned to each simulation for $K_{\text{clay1}}$, $K_{\text{clay2}}$, and $K_{\text{clay3}}$. According to field demonstration data, the average extracted water flow rate during full quadrant extraction (full quadrant extraction spacing was equal to the model simulated spacing) was approximately 124.0 L/hr and the water table drop rate measured in the field ranged from 0.115 m/hr to 0.169 m/hr. Using these field data, corresponding water table drop rates from the model simulation data on Figure 5.3(a) were equal to 0.148 m/hr for $K_{\text{clay1}}$, 0.155 m/hr for $K_{\text{clay2}}$, and 0.181 m/hr for $K_{\text{clay3}}$. Since the 0.148 m/hr model-measured value was mid-range of the field measured values
(0.115 m/hr to 0.169 m/hr), a clay permeability equal to $1 \times 10^{-6}$ cm/s and a silt seam permeability equal to $1 \times 10^{-5}$ cm/s was selected for all finite element analysis simulations.

5.5.2.2. Assumption 2: Silt Seam Concentrated Flow

For the second assumption, the extraction well flow rate and the percentage of flow rate assigned to silt seam nodes was varied. Since the model simulation results from the first calibration procedure compared well with the results from the field demonstration using a $1 \times 10^{-6}$ cm/s clay permeability and the $1 \times 10^{-5}$ cm/s silt permeability, these values were used during the second calibration procedure. Three different flow rates ($Q_1=48$ L/hr, $Q_2=95$ L/hr, and $Q_3=102$ L/hr) and three different fractional percentages of the total extraction flow rate were assigned to the silt seam nodes in the model test grid ($P_1=50\%$, $P_2=70\%$, and $P_3=90\%$). For example, if the total extracted water flow rate was equal to 48 L/hr ($Q_1$) and the percentage of flow assigned to the silt seam was equal to 50\% ($P_1$), then an extraction flow rate equal to 12 L/hr is assigned to each corner and 50\% of that flow rate is assigned to the nodes located 2.10 m and 2.40 m from the ground surface. The second calibration test matrix also consisted of nine simulations.

Figure 5.3(b) displays the water table drop rate (calculated from simulation output) as a function of the extraction flow rate. The values were identical for all percentages; using a total extraction flow rate equal to 0.21 cc/sec per extraction well, it would take approximately 3,174 hours to exchange one pore volume with a porosity of 0.4 so changes over an eight hour interval were minimal.
Similar to the procedure used during the first calibration, the average extraction flow rate measured in the field (124.0 L/hr) was used to determine the corresponding model-measured water table drop rate on Figure 5.3(b), which was equal to 0.158 m/hr for all three percentages. This value fell within the 0.115 m/hr to 0.169 m/hr range measured during full quadrant extraction in the field. A 90% percentage was selected for use in simulations, assuming a more concentrated flow rate in the silt seam.

5.5.3. Input Selection

A condensed list of the contaminant transport properties for TCE and the parameters required to generate the model test grid developed in this component of the research are listed in Table 5.1 (references are noted at the bottom). A complete list of NAPL Simulator input parameters (by line number) is located in Chapter 11 (Appendix C).

5.5.4. Grid Refinement

Preliminary extraction-only simulations using the model test grid indicated that the water table depth increased as a function of time relative to the ground surface, but a cone of depression was not generated during this process due to short PVW spacing. Since the drop in water table occurred evenly in the lateral direction, nodal saturation values were the same for the Y and Z-coordinates but varied for the X-coordinates during extraction-only simulations. An analysis of three different test grids (Figure 5.4) was performed to determine the optimum X-coordinate grid refinement at the top of the
model test grid, the area most affected by the water table drop. During this analysis, each
test grid (A, B, and C) had the same soil parameters and boundary conditions, but the X-
coordinate element dimensions were varied at the top of the test grid.

Table 5.1. Summary of Test Grid Input Parameters

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Values</th>
</tr>
</thead>
<tbody>
<tr>
<td>Elements (Nodes)</td>
<td>X: 25 Elements (26 Nodes)</td>
</tr>
<tr>
<td></td>
<td>Y: 10 Elements (11 Nodes)</td>
</tr>
<tr>
<td></td>
<td>Z: 10 Elements (11 Nodes)</td>
</tr>
<tr>
<td>Simulation Time</td>
<td>28,800 sec (8 hours)</td>
</tr>
<tr>
<td>Global Soil Permeabilitya</td>
<td>Clay: $1 \times 10^{-6}$ cm/s</td>
</tr>
<tr>
<td></td>
<td>Silt: $1 \times 10^{-5}$ cm/s</td>
</tr>
<tr>
<td>Porositya</td>
<td>0.4</td>
</tr>
<tr>
<td>Dry Densitya</td>
<td>$1.8 \text{ Mg/m}^3$</td>
</tr>
<tr>
<td>Viscosityb</td>
<td>Water: $1.0$ g/m·s @ $20^\circ$C</td>
</tr>
<tr>
<td></td>
<td>TCE: $0.57$ g/m·s @ $20^\circ$C</td>
</tr>
<tr>
<td></td>
<td>Air: $1.81 \times 10^{-2}$ g/m·s @ $20^\circ$C</td>
</tr>
<tr>
<td>Densityb</td>
<td>Water: $1.0$ Mg/m$^3$ @ $20^\circ$C</td>
</tr>
<tr>
<td></td>
<td>TCE: $1.464$ Mg/m$^3$ @ $20^\circ$C</td>
</tr>
<tr>
<td></td>
<td>Air: $1.205 \times 10^{-3}$ Mg/m$^3$ @ $20^\circ$C</td>
</tr>
<tr>
<td>Surface Tensionb</td>
<td>Water: $72$ g/s$^2$ @ $20^\circ$C</td>
</tr>
<tr>
<td></td>
<td>TCE: $29.3$ g/s$^2$ @ $20^\circ$C</td>
</tr>
<tr>
<td>Interfacial Tensionb</td>
<td>TCE-Water: $34.5$ g/s$^2$ @ $20^\circ$C</td>
</tr>
<tr>
<td>Dispersivityc</td>
<td>Longitudinal: $0.01$ m</td>
</tr>
<tr>
<td></td>
<td>Transverse: $0.001$ m</td>
</tr>
<tr>
<td>Molecular Diffusionb</td>
<td>Water: $8.3 \times 10^{-10}$ m$^2$/s</td>
</tr>
<tr>
<td></td>
<td>Gas: $8.11 \times 10^{-6}$ m$^2$/s</td>
</tr>
<tr>
<td>$K_{oc}$b</td>
<td>126</td>
</tr>
<tr>
<td>$f_{oc}$a</td>
<td>0.03</td>
</tr>
<tr>
<td>Mass Transfer Ratec</td>
<td>Soluble $\rightarrow$ Gas TCE: $4 \times 10^{-5}$ s$^{-1}$</td>
</tr>
<tr>
<td>Dimensionless Henry’s Law Constantb</td>
<td>TCE: $0.372$ (25$^\circ$C)</td>
</tr>
</tbody>
</table>

*aField or laboratory measured
*bCohen and Mercer (1993)
*cDaugherty, Franzini, and Finnemore (1985)
*eArmstrong, Find, and McClellan (1994)
Additionally, the van Genuchten (1980) saturation-pressure function is displayed in Equation 6.1 and the corresponding values were determined from pressure-saturation testing performed on the field test soil by an independent laboratory.

\[ h_c = [(S_e)^{1/m} - 1]^{1/\eta} \cdot a^{-1} \]  
\( \text{(Equation 5.12)} \)

Where:  
- \( h_c \) = capillary pressure head  
- \( S_e = (S_w-S_r) / (S_s-S_r) \) = effective water saturation  
- \( S_w \) = Water saturation  
- \( S_r \) = Minimum saturation for the S-P curve = 0.28  
- \( S_s \) = Maximum saturation for the S-P curve = 1.0  
- \( m = 1 - 1/\eta = 0.107 \)  
- \( \eta \) = curve fitting parameter (reflects the pore size distribution) = 1.12  
- \( a = scaling \ parameter \ (related \ to \ the \ displacement \ pressure \ head) = 14 \)

There were 26 X-coordinate nodes and 11 Y and Z-coordinate nodes totaling 3,146 nodes for each model test grid in Figure 5.4. The number of total nodes as well as the number of X-coordinate nodes could not be increased as the grid was refined in the X-direction. The model was unable to function due to available computer technology limitations when the total number of nodes (3,146) was increased significantly. Secondly, the model would not converge if the number of Y and Z-coordinate nodes divided by the number of X-coordinate nodes (\( \text{Nodes}_{(YZ)} / \text{Nodes}_{(X)} \)) was less than 0.4 due to a dimensioning constraint discovered during the modeling process. In other words, the number of X-coordinate nodes could only be increased if the number of Y and Z-coordinate nodes simultaneously increased to maintain the (\( \text{Nodes}_{(YZ)} / \text{Nodes}_{(X)} \)) ratio of 0.4. However, the addition of only six X-coordinate nodes, for example, would require 13 Y and Z-coordinate nodes, which would magnify the number of total nodes from 3,146 to 5,408 (a significant 70% increase). Therefore, grid refinement in the lower
portion of the model test grid (the area least affected by the water table drop) was sacrificed while grid refinement was increased in the top 1.00 m of the model test grid (the area most affected by the water table drop), as displayed in Figure 5.4.

The X-coordinate dimensions in the top 1.00 m of model test grids A, B, and C were 0.24 m, 0.20 m, and 0.10 m, respectively, as displayed in Figure 5.4. Each test grid was simulated for 8 hours using a total extraction flow rate equal to 0.21 cc/sec per well (a typical field flow rate). Figure 5.5 displays the water table depth as a function of time for the three model test grids displayed in Figure 5.4. Grid refinement affected the outcome of the water table location for simulation time intervals less than three hours but it had a minimal effect, thereafter. There was no measured movement in the water table during an extraction-only simulation for two hours using model test grid A (least refined grid) and one hour for model test grid B, but there was a constant and linear increase in the water table depth using model test grid C (the most refined grid). Therefore, model test grid C was used in all finite element analysis simulations.

5.6. Summary of the Model Development and Calibration

NAPL Simulator (U.S. EPA, 1997), approved and distributed by the EPA, was the three-dimensional finite element analysis model used to simulate soluble and gas-phase contaminant transport in saturated and unsaturated soil media. The objective of this chapter was to describe the numerical model and outline the methods used to develop and calibrate this model to hydraulic data measured during the field demonstration for further finite element analysis and evaluation of WIDE.
The model test grid dimensions (6.0 m in the X-direction and 1.0m in the Y and Z-directions) were the equivalent of a single element in a full WIDE system grid and the total extraction flow rate was equal to that of one PVW. The X-dimension corresponded to the PVW installation depth and the Y and Z-dimensions corresponded to the PVW spacing.

One quarter of the total extraction flow rate was assigned to the nodes located 1.50 m and below at each corner of the model test grid to simulate the PVW sheathing installed in the field. An atmospheric gas pressure head and an initial TCE concentration equal to zero was assigned to each node located on the top boundary of the model test grid to satisfy required boundary conditions. The global dry unit weight, porosity, and clay permeability values were 1.8 kN/m$^3$, 0.4, and 1x10$^{-6}$ cm/s, respectively but a 1x10$^{-5}$ cm/s permeability was assigned to nodes corresponding to the location of the silt seam detected during subsurface exploration in the field. The model test grid was initially saturated with water and the soluble phase TCE concentration was equal to the solubility limit (1100 mg/L) during contaminant transport simulation testing. The soil-water characteristic curve was also determined using field soil to more accurately model the relationship between volumetric water content and water potential in the unsaturated zone.

The model test grid was calibrated using measured hydraulic data from the field demonstration assuming (1) the distribution of the extraction flow rate was constant with depth; and (2) assuming the extraction flow rate was concentrated in the higher permeability silt seam. The rate of water table drop measured from model simulation
results using a clay permeability equal to $1 \times 10^{-6}$ cm/s and a silt seam permeability equal to $1 \times 10^{-5}$ cm/s compared well with field demonstration results using both assumptions. Finally, three different test grids were analyzed to determine the optimum X-coordinate grid refinement at the top of the model test grid, in the area most affected by the water table drop.
Figure 5.1. Plan-View of the Model Test Grid and Flow Symmetry
Figure 5.2. Model Test Grid

GLOBAL SOIL PARAMETERS
Permeability=10^{-6} cm/s
Porosity=0.4
Dry Unit Weight=1.8 kN/m³

LEGEND
A- Node 1
B- Node 11
C- Node 276
D- Node 286
E- Node 2861
F- Node 2871
G- Node 3146

- Extraction Well Node
- Atmospheric Gas Pressure
- Zero Contaminant Concentration
- Permeability = 10^{-5} cm/s
Figure 5.3. Model Calibration Assuming (a) Constant Flow Rate With Depth and (b) Concentrated Flow Rate in the Silt Seam
Figure 5.4. Model Test Grids Used for the Refinement Analysis
Figure 5.5. Test Grid Refinement Analysis
6. **FINITE ELEMENT ANALYSIS**

6.1. **Introduction**

TCE is a Dense Non-Aqueous Phase Liquid (DNAPL); therefore, it tends to migrate in the vertical direction due to gravitational and capillary forces. DNAPLs will only enter the soil matrix if the hydrostatic pressures exerted on the free product supercede the entry pressure existing in the soil matrix. DNAPLs will either form pockets of residual free product, or they will continue to migrate vertically until an impermeable boundary is encountered (Bedient, Rifai, and Newell, 1999). As presented by Bedient, Rifai, and Newell (1999), the fate of DNAPL depends upon (1) the presence of secondary pore channels consisting of fractures and heterogeneities within the clay matrix, (2) the type of DNAPL and the length of time the source is available, (3) the saturation of the soil, and (4) the soil permeability. Over time, immobile DNAPL can serve as a continuous source of contamination, which can significantly affect long term remediation operations.

Free product is difficult to detect and measure in the field. Without sufficient information regarding the volume and length of a given spill, and without knowing the intricate clay matrix configuration (location of fractures and heterogeneities that could significantly affect contaminant transport), it would be difficult to replicate field conditions using a finite element analysis model to accurately predict long term remediation times.
A finite element analysis was performed using NAPL Simulator to investigate contaminant partitioning tendencies as a function of time and operational scheme. Soluble and gas-phase contaminant transport was investigated in saturated and unsaturated soil media. A reference case that simulated field conditions was developed to establish a baseline input parameter set and model test grid configuration. The finite element analysis included three major components: (1) a parametric evaluation, (2) a system performance evaluation, and (3) a sensitivity analysis.

A parametric evaluation was performed to establish the input variables that significantly affect contaminant transport. The baseline input parameter set and model test grid were utilized, but select input parameters individually varied during a series of 8 hr extraction-only simulations. The 8 hr time period was selected since it was comparable to operational times employed during the field demonstration.

System performance and contaminant partitioning tendencies were evaluated as a function of time and operational scheme. Extraction-only and a concurrent injection-extraction simulations were performed over a 24 hr interval. Changes to the soluble-phase, gas-phase, and sorbed contaminant mass were evaluated as a function of time for each operation.

A sensitivity analysis (consisting of 36 simulations) was performed to evaluate the effect of key parameters on contaminant transport following an 8 hr operational time period. Input parameters including the PVW spacing, extraction water flow rate, and mass transfer coefficient were varied. The rate of change in the soluble-phase, gas-phase, and sorbed contaminant mass at the end of each simulation was determined.
6.2. Field Testing Versus Finite Element Analysis Modeling

NAPL Simulator (a three-dimensional, finite element analysis model) was used to simulate soluble and gas-phase contaminant transport in three-dimensional saturated and unsaturated soil media. Field measured hydraulic data and soil parameters were used to develop and calibrate the finite element analysis model as closely as possible to field conditions. However, it is important to note the key differences between the finite element analysis model and field testing so that model and field results can be evaluated appropriately:

1. During the field demonstration, changes in the air flow rate were orders of magnitude higher than changes in water flow rates (Figure 3.16), but in the model, extracted fluid volumes were replaced with the same volume of air during each simulation to maintain a mass balance.

2. Fluid extraction rates varied during extraction-only field operations but the model system extraction flow rate was constant with time. If air flow rate increased during a model simulation, the water flow rate would proportionally decrease to maintain the same total system extraction flow rate.

3. Air flow rates immediately increased during extraction-only field testing, which significantly affected gas-phase contaminant extraction. However, gas-phase contaminant mass was not extracted from the model test grid until the water table dropped below the depth of the simulated impermeable sheathing.
4. Mobile soluble-phase contaminant mass volatilized within the PVW cavity and PVC piping during the field demonstration, but the model was unable to simulate this mechanism of mass transfer.

5. The three-dimensional model test grid domain was discretized into a finite number of rectangular elements ranging from 0.10m to 0.50m in dimension. However, clay soil typically has microscopic flow channels, fractures, and heterogeneities that control the transport of fluids in the subsurface.

6. The band shaped PVW has small geosynthetic flow channels. Suspect hydraulic irregularities or ‘choke points’ were encountered during the laboratory component of this research, but the model was unable to simulate the same irregularities caused by the geometry of the PVW.

7. While the contaminant is in constant equilibrium with the pore volume fluids during the finite element analysis, field contaminants experience a constant sorption and desorption process within the soil matrix in order to reach an equilibrium condition. The on-going sorption processes that occur in the field typically cause a tailing and rebounding effect that is not observed in the finite element analysis model.

### 6.3. Reference Case

A reference case was developed to establish a baseline input parameter set and model test grid configuration. The following sections describe the baseline input parameter set, the model test grid configuration, and the contaminant mass balance equation.
6.3.1. Baseline Input Parameter Set and Model Test Grid Configuration

The model test grid (3,146 nodes) was 6.0 m deep and the PVW spacing was equal to 1.0 m (Figure 5.2). The analysis grid was designed to simulate the volume of soil affected by a single element in a WIDE system (previously depicted in Figure 5.1). The total extraction water flow rate (0.76 L/hr) assigned to the model was equal to the flow rate corresponding to a single PVW in the field, but was divided equally between the four corners of the model test grid (see Figure 5.1). To account for the impermeable sheathing installed on each PVW in the field, extraction well flow rates were assigned to nodes located 1.50 m and below. Gas pressure head boundary conditions (equal to atmospheric pressure) and a soluble-phase TCE concentration boundary conditions (equal to zero) were assigned to each node located on the top boundary of the model test grid (see Figure 5.2).

In order to simulate field conditions as closely as possible, global input parameters included a dry unit weight equal to 1.8 kN/m$^3$, a porosity equal to 0.4, a clay (CL) permeability equal to $1 \times 10^{-6}$ cm/s, and a fraction of organic carbon in the soil equal to 0.03. These values were based on soil characterization studies conducted in the field and in the laboratory. A $1 \times 10^{-5}$ cm/s permeability was assigned to nodes 2.10 m and 2.40 m from the ground surface to simulate the silt seam detected during subsurface exploration in the field. Initially, the soil media was fully saturated ($S_W = 1.0$) to reflect the shallow water table in the field and the soluble-phase TCE concentration was equal to the solubility limit (1100 mg/L) at every node. All simulations took place over an eight hour test interval to simulate a full operational day, as was the case in the field.
Common TCE contaminant transport properties are listed in Table 6.1 (references are noted at the bottom). A complete list of NAPL Simulator (U.S. EPA, 1997) input parameters are located in Chapter 11 (Appendix C).

**Table 6.1. TCE Contaminant Transport Model Input Parameters**

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
</table>
| Viscosity\(^a\)     | Water: 1.0 g/m-s @ 20°C  
                     | TCE: 0.57 g/m-s @ 20°C  
                     | Air\(^c\): 1.81x10\(^{-2}\) g/m-s @ 20°C |
| Density\(^a\)       | Water: 1.0 Mg/m\(^3\) @ 20°C  
                     | TCE: 1.46 Mg/m\(^3\) @ 20°C  
                     | Air\(^b\): 1.205x10\(^{-3}\) Mg/m\(^3\) @ 20°C |
| Surface Tension\(^a\) | Water: 72 g/s\(^2\) @ 20°C  
                       | TCE: 29.3 g/s\(^2\) @ 20°C |
| Interfacial Tension\(^a\) | TCE-Water: 34.5 g/s\(^2\) @ 20°C |
| Dispersivity\(^c\)  | Longitudinal: 0.01 m  
                     | Transverse: 0.001 m |
| Molecular Diffusion\(^a\) | Water: 8.3x10\(^{-10}\) m\(^2\)/s  
                      | Gas: 8.11x10\(^{-6}\) m\(^2\)/s |
| K\(_{oc}\)\(^a\)    | 126 |
| Mass Transfer Rate\(^c\) | Soluble ➔ Gas TCE: 4x10\(^{-5}\) s\(^{-1}\) |
| Dimensionless Henry’s Law Constant\(^a\) | TCE: 0.372 (25°C) |

\(^a\)Cohen and Mercer (1993)  
\(^b\)Daugherty, Franzini, and Finnemore (1985)  
\(^c\)Armstrong, Find, and McClellan (1994)

Additionally, the van Genuchten (1980) saturation-pressure function is displayed in Equation 6.1 and the corresponding values were determined from pressure-saturation testing performed on the field test soil by an independent laboratory:

\[ h_c = [(S_e)^{-1/m} - 1]^{1/\eta} * (\alpha)^{-1} \]  

**Equation (6.1)**

Where:  
\( h_c = \) capillary pressure head  
\( S_e = (S_w-S_t) / (S_s-S_t) = \) effective water saturation  
\( S_w = \) Water saturation  
\( S_t = \) Minimum saturation for the S-P curve = 0.28  
\( S_s = \) Maximum saturation for the S-P curve = 1.0  
\( m = 1 - 1/\eta = 0.107 \)  
\( \eta = \) curve fitting parameter (reflects the pore size distribution) = 1.12  
\( \alpha = \) scaling parameter (related to the displacement pressure head) = 14
6.3.2. Mass Balance

The volume of water removed from the system was replaced by the same volume of air. Using the system extraction water flow rate equal to 0.756 L/hr, approximately 6049 g of water was removed and 7.3 g of air replaced the water removed during the eight hour extraction-only reference case. This is equivalent to 6.05 L of water ($\rho_{\text{water}} = 1000$ g/L) and 6.08 L of air ($\rho_{\text{air}} = 1.205$ g/L).

The total system contaminant mass consisted of a soluble, gas, and sorbed phase and can be described by Equation 6.2.

$$\Delta M_{\text{Total}} = (\Delta M_{\text{Soluble-Phase}}) + (\Delta M_{\text{Gas-Phase}}) + (\Delta M_{\text{Sorbed}})$$  \hspace{1cm} \text{Equation (6.2)}

Where:

- $\Delta M_{\text{Total}}$ = Change in the total system contaminant mass
- $\Delta M_{\text{Soluble-Phase}}$ = Change in the soluble-phase contaminant mass
- $\Delta M_{\text{Gas-Phase}}$ = Change in the gas-phase contaminant mass
- $\Delta M_{\text{Sorbed}}$ = Change in contaminant mass sorbed to the soil solids

The initial soluble-phase mass was equal to the initial concentration in the ground water times the pore volume (porosity = 0.4). The contaminant mass sorbed to the solids was calculated using Equation 6.3 (Guarnanncia, 1997).

$$M_{\text{sorbed}} = (K_d) \left( \frac{C_{\text{w}}}{C_{\text{s}}} \right) (M_{\text{solids}})$$  \hspace{1cm} \text{Equation (6.3)}

Where:

- $M_{\text{sorbed}}$ = Contaminant mass sorbed to the soil solids
- $K_d$ = Contaminant partitioning coefficient = $C_s/C_w$
- $C_s = M_{\text{sorbed}} / M_{\text{solids}}$
- $C_w = M_{\text{water}} / V_{\text{water}}$
- $M_{\text{solids}}$ = Mass of soil solids = Soil Dry Density * Total Soil Volume
- $M_{\text{water}}$ = Mass of water existing in the system
- $V_{\text{water}}$ = Volume of the water existing in the system
6.4. Parametric Evaluation

Using the reference case and corresponding baseline input parameter set, ten input parameters were individually varied to determine their effect on the contaminant transport results. Additionally, simulation output were used to determine if the contaminant transport convergence limits were precise enough to handle the small incremental changes in contaminant mass as a function of time. Table 6.2 summarizes the results from this evaluation. The input parameters and corresponding values selected for this evaluation were summarized in the first and second columns. The rate of change in soluble-phase and gas-phase contaminant mass was reported in the last two columns of Table 6.2.

6.4.1. Extraction Flow Rate

While the extraction flow rate nearly doubled (increased from 0.40 L/hr to 0.76 L/hr), the rate of change in the soluble and gas-phase contaminant mass changed proportionally. For example, the soluble-phase contaminant mass decreased approximately -0.42 g/hr at a flow rate equal to 0.81 L/hr. The rate of decrease doubled to approximately -0.80 g/hr at a flow rate equal to 0.76 L/hr (an approximate 94% increase in the rate of contaminant mass decrease). The rate of change in gas-phase contaminant mass also increased from 0.15 g/hr to 0.29 g/hr, as reported on Table 6.2.

A larger volume of contaminated water was removed during the 8 hr simulation as the extraction water flow rate increased. The volume of water was replaced by the same volume of air, which generated an unsaturated zone suitable for contaminant
volatilization. Therefore, the decrease in soluble-phase contaminant mass and increase in
gas-phase contaminant mass was directly proportional to the extraction flow rate.

### Table 6.2. Parametric Evaluation Results

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>$\Delta M_{\text{Soluble-Phase Per Hour}}$ (g/hr)</th>
<th>$\Delta M_{\text{Gas-Phase Per Hour}}$ (g/hr)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Extracted Flow Rate (L/hr)</td>
<td>0.40</td>
<td>-0.417</td>
<td>0.149</td>
</tr>
<tr>
<td></td>
<td>*0.76</td>
<td>-0.809</td>
<td>0.291</td>
</tr>
<tr>
<td>PVW Spacing (m)</td>
<td>0.70</td>
<td>-0.800</td>
<td>0.291</td>
</tr>
<tr>
<td></td>
<td>*1.00</td>
<td>-0.809</td>
<td>0.291</td>
</tr>
<tr>
<td>Mass Transfer Rate: Soluble $\rightarrow$ Gas-Phase (s$^{-1}$)</td>
<td>4x10$^{-8}$</td>
<td>-0.790</td>
<td>0.018</td>
</tr>
<tr>
<td></td>
<td>4x10$^{-7}$</td>
<td>-0.797</td>
<td>0.128</td>
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<tr>
<td></td>
<td>4x10$^{-6}$</td>
<td>-0.804</td>
<td>0.266</td>
</tr>
<tr>
<td></td>
<td>*4x10$^{-5}$</td>
<td>-0.809</td>
<td>0.291</td>
</tr>
<tr>
<td></td>
<td>4x10$^{-4}$</td>
<td>-0.892</td>
<td>0.292</td>
</tr>
<tr>
<td>Water / Air Molecular Diffusion Coefficient (m$^2$/s)</td>
<td>*8.3x10$^{-10}$ / 8.3x10$^{-6}$</td>
<td>-0.809</td>
<td>0.291</td>
</tr>
<tr>
<td></td>
<td>8.3x10$^{-9}$ / 8.3x10$^{-5}$</td>
<td>-0.809</td>
<td>0.292</td>
</tr>
<tr>
<td></td>
<td>8.3x10$^{-8}$ / 8.3x10$^{-4}$</td>
<td>-0.817</td>
<td>0.292</td>
</tr>
<tr>
<td>Percentage of Organic Carbon (%)</td>
<td>0.1</td>
<td>-1.046</td>
<td>0.291</td>
</tr>
<tr>
<td></td>
<td>0.5</td>
<td>-0.892</td>
<td>0.291</td>
</tr>
<tr>
<td></td>
<td>1</td>
<td>-0.847</td>
<td>0.291</td>
</tr>
<tr>
<td></td>
<td>*3</td>
<td>-0.809</td>
<td>0.291</td>
</tr>
<tr>
<td></td>
<td>5</td>
<td>-0.800</td>
<td>0.292</td>
</tr>
<tr>
<td>Silt Seam Permeability (m/s)</td>
<td>*1x10$^{-7}$</td>
<td>-0.809</td>
<td>0.291</td>
</tr>
<tr>
<td></td>
<td>1x10$^{-5}$</td>
<td>-0.809</td>
<td>0.291</td>
</tr>
<tr>
<td></td>
<td>**1x10$^{-6}$</td>
<td>-1.732</td>
<td>0.620</td>
</tr>
<tr>
<td>Silt Seam Thickness (m)</td>
<td>0.30</td>
<td>-0.809</td>
<td>0.291</td>
</tr>
<tr>
<td></td>
<td>*0.60</td>
<td>-0.809</td>
<td>0.291</td>
</tr>
<tr>
<td></td>
<td>0.90</td>
<td>-0.809</td>
<td>0.291</td>
</tr>
<tr>
<td>Silt Seam X-Coordinates (m)</td>
<td>0.90,1.10, 1.30</td>
<td>-0.808</td>
<td>0.291</td>
</tr>
<tr>
<td></td>
<td>*2.10,2.40</td>
<td>-0.809</td>
<td>0.291</td>
</tr>
<tr>
<td></td>
<td>4.30,4.70</td>
<td>-0.809</td>
<td>0.291</td>
</tr>
<tr>
<td>Impermeable Sheathing Depth Fraction</td>
<td>*0.25</td>
<td>-0.809</td>
<td>0.291</td>
</tr>
<tr>
<td></td>
<td>0.50</td>
<td>-0.811</td>
<td>0.287</td>
</tr>
<tr>
<td></td>
<td>0.75</td>
<td>-0.812</td>
<td>0.289</td>
</tr>
<tr>
<td>Maximum Time Step (s)</td>
<td>300</td>
<td>-0.806</td>
<td>0.290</td>
</tr>
<tr>
<td></td>
<td>900</td>
<td>-0.808</td>
<td>0.291</td>
</tr>
<tr>
<td></td>
<td>*2000</td>
<td>-0.809</td>
<td>0.291</td>
</tr>
<tr>
<td></td>
<td>4000</td>
<td>-0.809</td>
<td>0.291</td>
</tr>
</tbody>
</table>

* Input Parameters for the Reference Case

** Extracted Flow Rate and Permeability Both Increased by a Factor of 10 in the Silt Seam
6.4.2. PVW Spacing

There was no significant change in the soluble or gas-phase contaminant mass as the PVW spacing increased from 0.70 m to 1.00 m (Table 6.2). During the 8 hr interval, the water table was located above the bottom of the impermeable sheathing so the extraction air flow rate remained zero and contaminant extraction was solely dependent upon the volume of contaminated fluids extracted from the system. Regardless of PVW spacing, the same volume of contaminated water was extracted during each 8 hr simulation and replaced by an equivalent volume of air (for an identical flow rate). Consequently, the rate of change in the soluble-phase contaminant mass was unaffected and gas-phase contaminant mass increased accordingly in the unsaturated zone generated during this process.

6.4.3. Mass Transfer Rate Coefficient

As the mass transfer rate increased from $4 \times 10^{-8}$ s$^{-1}$ and $4 \times 10^{-4}$ s$^{-1}$, the soluble-phase contaminant mass rate of change varied from -0.79 g/hr to -0.81 g/hr (a difference of 0.02 g/hr) and the rate of change in the gas-phase contaminant mass varied from 0.02 g/hr to 0.29 g/hr (a difference of 0.27 g/hr). The increase in gas-phase contaminant mass tapered off as the mass transfer rate approached the baseline value ($4 \times 10^{-5}$ s$^{-1}$); the unsaturated zone reached the contaminant saturation level.

The increase in gas-phase contaminant mass (0.27 g/hr) exceeded the decrease in soluble-phase contaminant mass (0.02 g/hr) by at least one order of magnitude. Since the change in the soluble-phase contaminant mass was not equal to the change in gas-phase
contaminant mass, the increase in gas-phase contaminant mass was attributed to sorbed contaminant mass volatilization.

6.4.4. Diffusion Coefficient

Diffusion causes the contaminant to move from an area of higher concentration to an area of lower concentration. It can be the dominant mode of transport in cases of low hydraulic conductivity soils. It also contributes to the dispersion impact on transport. There was an insignificant affect on contaminant transport results since the system was initially saturated and the entire model test grid started out with the same soluble-phase concentration.

6.4.5. Organic Carbon Content

The rate of change in the soluble-phase contaminant mass varied from approximately –1.05 g/hr to –0.80 g/hr (a 24 % difference) as the organic carbon content increased from 0.1 % to 5 %. Sorption processes occur in the presence of organic matter. As a result, there was an increase in the sorption process as the fraction of organic matter increased to 5 %. The effect of the organic carbon content can be described by Equation 6.3. The field measured value of organic carbon content (equal to 3 %) was utilized in all other model simulations, to better simulate field conditions.

6.4.6. Silt Seam Properties and Impermeable Sheathing Depth

Even thought the silt seam baseline permeability value (1x10^{-5} cm/sec) was increased by two orders of magnitude, there was no significant difference in the contaminant transport results. Ground water velocity is directly proportional to soil
permeability and hydraulic gradient. Since the flow rate used during the finite element analysis remained unchanged while the soil permeability was increased, the model internally calculated an adjusted hydraulic gradient to maintain the same pore water velocity.

To verify this conclusion, a third simulation was performed. The silt seam permeability and the extraction water flow rate corresponding to the nodes in the silt seam were both increased by one order of magnitude. As a result, the soluble and gas-phase contaminant rate of change doubled.

Different values for the silt seam thickness, silt seam location, and the impermeable sheathing depth were tested. Changes in contaminant transport results were less than 1% in all cases. In the field, these parameters serve as boundary conditions and they directly affect field flow rates and contaminant transport efficiency. During the finite element analysis, the flow rate was constant so these parameters had little affect on contaminant transport results. It is also important to note that an 8 hr extraction-only simulation only removes 6.0L (0.25% of the total pore volume).

6.4.7. Maximum Time Step

Time steps that are too large or too small can lead to instabilities as numerical round-off errors dominate the solution (Guarnanccia, 1997). The maximum time step was varied between 300 s and 4000 s to quantify the time step effect. Contaminant transport results varied less than 1% in all cases.
6.4.8. **Contaminant Transport Convergence Criteria**

Additionally, the average time step was multiplied by the rate of change in the soluble-phase contaminant mass for each recorded time interval to obtain the change in soluble-phase contaminant mass per time step. The change in soluble-phase contaminant mass per time step was at least one order of magnitude lower than the change in contaminant mass per time interval. Therefore, the contaminant convergence limits were deemed acceptable.

6.4.9. **Extraction Flow Rate Distribution**

Since the flow rate distribution at each PVW as a function of depth was unknown, two different scenarios were investigated. In the first scenario, the extraction water flow rate was equally distributed with depth. In the second scenario, 90% of the extraction water flow rate was assigned to nodes corresponding to the depth of the simulated silt seam (the 90% value was generated during the model calibration process). For the simulations displayed in Table 6.2, the water flow rate was assumed constant with depth. As an alternative, 19 of the 34 simulations were repeated assuming 90% of the water flow rate was concentrated in the silt seam. Ultimately, the differences in soluble and gas-phase contaminant transport results were less than 1% in all cases so the second assumption was utilized for all remaining simulations.

6.5. **System Performance as a Function of Time**

An extraction-only and a concurrent injection-extraction simulation were both performed over a 24 hr interval to investigate contaminant partitioning tendencies
(soluble-phase, gas-phase, and sorbed contaminant mass) and the primary mode of extraction as a function of time and operational scheme. The reference case input parameter set, model test grid configuration, boundary conditions, and soil parameters were utilized. The soluble and gas-phase data were obtained directly from simulation output. The mass sorbed to the soil was calculated at each node using Equation 6.3. The total change in system mass ($\Delta M_{\text{Total}}$) is the sum of all three components, as displayed in Equation 6.2, and a negative value indicates a loss in contaminant mass. The total extraction water flow rate for both simulations was 0.76 L/hr and the injected water flow rate for the concurrent injection-extraction simulation was 0.73 L/hr. The injected flow rate was slightly lower than the extracted flow rate to ensure model stability and better simulate field conditions. While the water table remained shallow, there was a slight increase in the water table depth during the concurrent injection-extraction operations in the field, which initiated a minimal unsaturated volume.

6.5.1. Concurrent Injection-Extraction Simulation

Figure 6.1(a) displays the cumulative change in the soluble-phase, gas-phase, and sorbed contaminant mass existing within the model test grid, as a function of simulation time, for a 24 hour concurrent injection-extraction simulation. Note that Figure 6.1(a) does not represent the contaminant mass extracted from the system. For example, if gas-phase contaminant mass was extracted at a rate equal to 0.1 g/hr, but sorbed and/or soluble-phase contaminant mass volatilized at the same rate to maintain an equilibrium condition, the change in gas-phase contaminant mass existing within the soil matrix would be approximately zero even though gas-phase contaminant mass was extracted
from the system at a rate equal to 0.1 g/hr (mass transfer processes increased while contaminant extraction decreased gas-phase contaminant mass resulting in a net zero effect).

During concurrent injection-extraction simulations, clean water was injected while contaminated fluids were extracted so the water table remained relatively unchanged, but the system did not remain 100% saturated since the injected water flow rate was slightly less than the extracted flow rate. As a result, there was a slight increase in gas-phase contaminant mass (0.12 g) due to the small unsaturated zone generated during the 24 hour simulation. However, gas-phase contaminant was not extracted from the model test grid during concurrent injection-extraction operations since the water table was located above the bottom of the simulated impermeable sheathing and the extracted air flow rate remained zero during the simulation.

Since the air flow rate was zero, soluble-phase contaminant mass was removed by way of extracted ground water, at a flow rate equal to 0.76 L/hr and a concentration equal to the solubility limit (1100 mg/L). At the same time, a portion of the sorbed contaminant mass dissolved into the soluble-phase to maintain a constant equilibrium between the sorbate and the injected pore water as clean fluids were injected. As a result, there was a minimal net change in the existing soluble-phase contaminant mass (-0.54 g during the 24 hr simulation).

The mass of contaminant mass physically extracted from the soil matrix is displayed in Figure 6.2 as a function of simulation time and contaminant phase for the 24 hr concurrent injection-extraction simulation. In summary, gas-phase contaminant mass
was not extracted during concurrent injection-extraction simulations since the water table remained above the bottom of the impermeable sheathing and the extracted air flow rate remained zero. Contaminants could only be removed in the soluble-phase; a process dependent upon the concentration of the ground water and the extraction water flow rate. Sorbed contaminant mass simultaneously dissolved as uncontaminated fluids were injected to maintain a constant equilibrium between the pore water and sorbate.

6.5.2. Extraction-Only Simulation

Figure 6.1(b) displays the cumulative change in the soluble-phase, gas-phase, and sorbed contaminant mass existing within the model test grid, as a function of simulation time, for a 24 hour extraction-only simulation. Note that Figure 6.1(b) does not represent the contaminant mass extracted from the system.

During the first 12 - 13 hours of the extraction-only simulation, the water table was above the bottom of the impermeable sheathing (located 1.50 m from the ground surface) and the soluble-phase contaminant mass decreased approximately -0.81 g/hr. The decrease in soluble-phase mass was primarily attributed to the displacement of contaminated ground water. Therefore, concurrent changes in gas-phase and sorbed contaminant mass occurred independently (the increase in gas-phase contaminant mass was primarily attributed to sorbed contaminant mass volatilization). Approximately 84 % of the gas-phase contaminant mass increased as a result of sorbed contaminant volatilization and the remaining 16 % volatilized from the soluble-phase.

During the second half of the simulation, the water table dropped below the impermeable sheathing and the extracted air flow rate increased, which simultaneously
decreased the extracted water flow rate. Until this point, the water table dropped evenly across the model test grid. Subsequent to this point, the water table began to form cone of depressions around each extraction well. As a result, zones less affected by the hydraulic gradient began to form near the center of the model test grid. The sorbed contaminant mass located in the less affected areas began to dissolve into the soluble-phase. Rather than continuing to decrease at a rate equal to -0.81 g/hr, the soluble-phase contaminant mass decreased approximately -0.64 g/hr, thereafter, reflecting the changes in the hydraulic conditions. The initial soluble-phase and sorbed contaminant mass curves from the first half of the simulation were projected linearly in Figure 6.1(b) to illustrate the increase in desorption and decrease in the soluble-phase contaminant mass rate of decline subsequent to an increase in extracted air flow rate.

Figure 6.2 displays the cumulative change in the extracted contaminant mass as a function of simulation time and contaminant phase for the extraction-only simulation. In summary, gas-phase contaminant was not extracted as long as the water table was located above the bottom of the impermeable sheathing and the extracted air flow rate was equal to zero. Therefore, additional volatilization and sorption processes took place independently. As the water table dropped below the impermeable sheathing, the extracted air flow rate increased and approximately 1.24 g of gas-phase contaminant mass was extracted.

Consequently, the volume of contaminated water removed from the system decreased but the air volume was less concentrated than the water volume so the total contaminant mass extracted during the second half of the extraction only simulation was
less than the mass removed during the concurrent injection-extraction simulation. Approximately 16.60 g and 1.24 g of soluble-phase and gas-phase contaminant mass were removed during the extraction-only simulation, respectively. Approximately 19.97 g of soluble-phase contaminant mass was removed from the system during the concurrent injection-extraction simulation (a 10% difference in total extracted contaminant mass).

### 6.5.3. Discussion of Time-Dependent Results

Although it appears that the concurrent injection-extraction operation was more efficient than the extraction-only operation in Figure 6.2, it is important to recall the key differences between field demonstration testing and finite element analysis modeling previously addressed in Section 6.2. Consequently, Figure 6.2 does not replicate field behaviors, but Figure 6.1 and Figure 6.2 does provide valuable information regarding contaminant partitioning tendencies as a function of time and system operational scheme.

During the field demonstration component of this research, the extraction of volatile organics (TCE) was more effective during extraction-only operations. Therefore, the PVW spacing, extraction water flow rate, and mass transfer coefficient were varied during the sensitivity analysis in order to (1) determine the rate of change in contaminant mass as a function of select input parameter values, and (2) further investigate the tendency for contaminant mass to partition to the soluble-phase, gas-phase, and sorbed-phase during extraction-only operations only.
6.6.  Sensitivity Analysis

Using the reference case, a sensitivity analysis was performed to evaluate contaminant transport results at the end of an 8 hr simulation for select input parameters. Three extraction water flow rates (Q1=0.36 L/hr, Q2=0.72 L/hr, Q3=1.08 L/hr), three PVW spacing dimensions (S1=0.90 m, S2=1.10 m, S3=1.30 m), and four mass transfer rate coefficients (M1=1x10^{-7} s^{-1}, M2=5x10^{-7} s^{-1}, M3=1x10^{-6} s^{-1}, M4=1x10^{-5} s^{-1}) were evaluated (36 total simulations). The rate of change in the soluble-phase, gas-phase, and sorbed contaminant mass was determined at the end of each simulation.

Table 6.3 displays the complete test matrix and corresponding rate changes as a function of soluble-phase, gas-phase, total system, and sorbed contaminant mass. The soluble and gas-phase data were obtained directly from simulation output. The mass sorbed to the soil was calculated at each node using Equation 6.3 and the corresponding nodal volume, and the total change in system mass is the sum of all three components (Equation 6.2). A negative number in Table 6.3 indicates a loss in mass while a positive number represents a gain in mass for each respective phase.

6.6.1. Soluble-Phase Contaminant Mass Rate of Change

The rate of change in the soluble-phase contaminant mass at the end of each 8 hr simulation is displayed in Figure 6.3 as a function of the extraction water flow rate. Data from all 36 simulations were included in this figure and a single regression analysis was performed on all data (R^2=1.0). The rate of change in the soluble-phase contaminant mass varied from approximately -0.35 g/hr to -1.15 g/hr (for all variations of the PVW spacing and mass transfer rate) as the extraction water flow rate increased from 0.36 L/hr
Table 6.3. Sensitivity Analysis Test Matrix

<table>
<thead>
<tr>
<th>36 Simulations</th>
<th>(\Delta M_{\text{Soluble-Phase Per 8 hr}}) (g/hr)</th>
<th>(\Delta M_{\text{Gas-Phase Per 8 hr}}) (g/hr)</th>
<th>(\Delta M_{\text{Total Per 8 hr}}) (g/hr)</th>
<th>(\Delta M_{\text{Sorbed Per 8 hr}}) (g/hr)</th>
</tr>
</thead>
<tbody>
<tr>
<td>S1</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>M1</td>
<td>Q1 -0.369</td>
<td>0.021</td>
<td>-0.417</td>
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<tr>
<td></td>
<td>Q2 -0.758</td>
<td>0.042</td>
<td>-0.785</td>
<td>-0.069</td>
</tr>
<tr>
<td></td>
<td>Q3 -1.143</td>
<td>0.057</td>
<td>-1.155</td>
<td>-0.069</td>
</tr>
<tr>
<td>M2</td>
<td>Q1 -0.372</td>
<td>0.070</td>
<td>-0.370</td>
<td>-0.069</td>
</tr>
<tr>
<td></td>
<td>Q2 -0.763</td>
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<td>-0.688</td>
<td>-0.069</td>
</tr>
<tr>
<td></td>
<td>Q3 -1.152</td>
<td>0.201</td>
<td>-1.019</td>
<td>-0.069</td>
</tr>
<tr>
<td>M3</td>
<td>Q1 -0.373</td>
<td>0.097</td>
<td>-0.344</td>
<td>-0.069</td>
</tr>
<tr>
<td></td>
<td>Q2 -0.767</td>
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<td>-0.772</td>
<td>-0.206</td>
</tr>
<tr>
<td></td>
<td>Q3 -1.156</td>
<td>0.285</td>
<td>-1.147</td>
<td>-0.275</td>
</tr>
<tr>
<td>M4</td>
<td>Q1 -0.375</td>
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<td>-0.381</td>
<td>-0.138</td>
</tr>
<tr>
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<td>Q2 -0.770</td>
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<td>-0.707</td>
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</tr>
<tr>
<td></td>
<td>Q3 -1.158</td>
<td>0.402</td>
<td>-1.100</td>
<td>-0.344</td>
</tr>
<tr>
<td>S2</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>M1</td>
<td>Q1 -0.363</td>
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</tr>
<tr>
<td></td>
<td>Q2 -0.746</td>
<td>0.041</td>
<td>-0.808</td>
<td>-0.103</td>
</tr>
<tr>
<td></td>
<td>Q3 -1.138</td>
<td>0.063</td>
<td>-1.178</td>
<td>-0.103</td>
</tr>
<tr>
<td>M2</td>
<td>Q1 -0.365</td>
<td>0.068</td>
<td>-0.400</td>
<td>-0.103</td>
</tr>
<tr>
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<td>Q2 -0.751</td>
<td>0.141</td>
<td>-0.713</td>
<td>-0.103</td>
</tr>
<tr>
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<td>Q3 -1.147</td>
<td>0.216</td>
<td>-1.034</td>
<td>-0.103</td>
</tr>
<tr>
<td>M3</td>
<td>Q1 -0.366</td>
<td>0.093</td>
<td>-0.376</td>
<td>-0.103</td>
</tr>
<tr>
<td></td>
<td>Q2 -0.754</td>
<td>0.196</td>
<td>-0.660</td>
<td>-0.103</td>
</tr>
<tr>
<td></td>
<td>Q3 -1.152</td>
<td>0.300</td>
<td>-1.159</td>
<td>-0.307</td>
</tr>
<tr>
<td>M4</td>
<td>Q1 -0.369</td>
<td>0.126</td>
<td>-0.447</td>
<td>-0.205</td>
</tr>
<tr>
<td></td>
<td>Q2 -0.758</td>
<td>0.269</td>
<td>-0.694</td>
<td>-0.206</td>
</tr>
<tr>
<td></td>
<td>Q3 -1.158</td>
<td>0.406</td>
<td>-1.060</td>
<td>-0.308</td>
</tr>
<tr>
<td>S3</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>M1</td>
<td>Q1 -0.347</td>
<td>0.023</td>
<td>-0.468</td>
<td>-0.144</td>
</tr>
<tr>
<td></td>
<td>Q2 -0.735</td>
<td>0.041</td>
<td>-0.838</td>
<td>-0.144</td>
</tr>
<tr>
<td></td>
<td>Q3 -1.118</td>
<td>0.059</td>
<td>-1.203</td>
<td>-0.144</td>
</tr>
<tr>
<td>M2</td>
<td>Q1 -0.349</td>
<td>0.072</td>
<td>-0.420</td>
<td>-0.144</td>
</tr>
<tr>
<td></td>
<td>Q2 -0.740</td>
<td>0.139</td>
<td>-0.745</td>
<td>-0.144</td>
</tr>
<tr>
<td></td>
<td>Q3 -1.126</td>
<td>0.206</td>
<td>-1.064</td>
<td>-0.144</td>
</tr>
<tr>
<td>M3</td>
<td>Q1 -0.350</td>
<td>0.096</td>
<td>-0.398</td>
<td>-0.144</td>
</tr>
<tr>
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<td>Q2 -0.743</td>
<td>0.194</td>
<td>-0.692</td>
<td>-0.144</td>
</tr>
<tr>
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<td>Q3 -1.131</td>
<td>0.292</td>
<td>-0.982</td>
<td>-0.144</td>
</tr>
<tr>
<td>M4</td>
<td>Q1 -0.353</td>
<td>0.125</td>
<td>-0.372</td>
<td>-0.144</td>
</tr>
<tr>
<td></td>
<td>Q2 -0.747</td>
<td>0.266</td>
<td>-0.768</td>
<td>-0.287</td>
</tr>
<tr>
<td></td>
<td>Q3 -1.137</td>
<td>0.403</td>
<td>-1.022</td>
<td>-0.287</td>
</tr>
</tbody>
</table>
to 1.08 L/hr. It became evident that the PVW spacing and the mass transfer rate had no affect on changes in the soluble-phase contaminant mass during each 8 hr extraction-only simulation.

During each simulation, the water table was located above the bottom of the simulated impermeable sheathing, air flow rate was consequently equal to zero, and the contaminant mass was, therefore, removed in the soluble-phase as contaminated ground water displaced. For example, the rate of change in the soluble-phase contaminant mass at the end of an 8 hr interval would be approximately equal to 0.88 g/hr for a corresponding initial soluble-phase contaminant concentration equal to 1100 mg/L and flow rate equal to 0.80 L/hr. The corresponding rate of change in Figure 6.3 was approximately equal to this value. Therefore, it was concluded that the changes in gas-phase and sorbed contaminant mass occurred independently of changes in the soluble-phase contaminant mass. Sorbed contaminant mass volatilized, which increased the gas-phase contaminant mass (this aspect was also addressed in Section 6.5.2).

6.6.2. Gas-Phase Contaminant Mass Rate of Change

The rate of change in gas-phase contaminant mass at the end of each 8 hr simulation is displayed in Figure 6.4 as a function of the mass transfer rate. Data from all 36 simulations were included and a regression analysis was performed for each extraction water flow rate ($R^2=0.99$). During the extraction-only simulation, the increase in gas-phase contaminant mass was dependent upon the extraction water flow rate as well as the mass transfer rate. For example, the rate of change of gas-phase contaminant increased by a factor of 7.0 (from approximately 0.06 g/hr to 0.42 g/hr) as the mass transfer rate
increased from $1 \times 10^{-7}$ s$^{-1}$ to $1 \times 10^{-5}$ s$^{-1}$ for an extraction water flow rate equal to 1.08 L/hr (Q3). For the same range of mass transfer rates, the rate of change of gas-phase contaminant increased from approximately 0.02 g/hr to 0.13 g/hr at an extraction water flow rate equal to 0.36 L/hr (Q1).

An increase in the extraction water flow rate displaced a larger volume of water, which was replaced by the same volume of air in each case. The increase in air volume generated an unsaturated zone suitable for volatilization. Sorbed contaminant mass volatilized, which increased the gas-phase contaminant mass, but the volatilization process was enhanced as the mass transfer rate increased from $1 \times 10^{-7}$ s$^{-1}$ to $1 \times 10^{-5}$ s$^{-1}$. PVW spacing had no affect on changes in the gas-phase contaminant mass since the same fluid volume was displaced regardless of the model test grid dimensions (displaced volumes were controlled by the flow rate).

### 6.6.3. Total Contaminant Mass Rate of Change

While soluble and gas-phase contaminant mass data were obtained directly from simulation output, sorbed contaminant mass was manually calculated for each node using Equation 6.3. Sorbed contaminant mass changes are displayed in Table 6.3 for all 36 simulations. The rate of change in the total system contaminant mass at the end of each 8 hr simulation was then calculated using Equation 6.2. Figure 6.5 displays the rate of change in the total system contaminant mass, at the end of each 8 hr simulation, as a function of the extraction water flow rate. A regression analysis was performed on all data ($R^2 = 0.96$).
Similar to the soluble-phase relationship displayed in Figure 6.3, the rate of change in the total system contaminant mass varied as the extraction water flow rate increased. For example, the rate of change in the total system contaminant mass varied from approximately -0.40 g/hr to -1.10 g/hr for extraction water flow rates equal to 0.36 L/hr and 1.08 L/hr, respectively. Since the data in Figure 6.5 incorporates gas-phase contaminant mass (dependent upon the mass transfer rate as well as the extraction flow rate), data variability increased. The $R^2$ value decreased from 1.0 in Figure 6.3 to 0.96 in Figure 6.5.

### 6.7. Summary of the Finite Element Analysis

NAPL Simulator (a three-dimensional finite element analysis model) was used to simulate soluble and gas-phase contaminant transport in saturated and unsaturated soil media. While the finite element analysis model cannot be used to replicate WIDE system performance in the field, the model was utilized to (1) investigate contaminant partitioning tendencies as a function of time and operational scheme, and (2) validate system performance issues observed during the field demonstration. Using the reference case, a parametric evaluation was initially performed to establish the input variables that significantly affect contaminant transport. Second, system performance and contaminant partitioning tendencies were evaluated as a function of time for two different operational schemes. Finally, a sensitivity analysis was performed to evaluate contaminant partitioning tendencies as a function of the PVW spacing, extraction water flow rate, and mass transfer coefficient.
During the 24 hour concurrent injection-extraction simulation, the increase in gas-phase contaminant mass was minimal due to the shallow water table. The system was unable to extract gas-phase contaminant mass since the water table was located above the bottom of the simulated impermeable sheathing and the air flow rate remained zero. Soluble-phase contaminant mass was extracted from the system at rate equal to 0.76 L/hr and a concentration equal to the solubility limit (1100 mg/L) during the 24 hr simulation, but the net change in the existing soluble-phase contaminant mass within the model test grid only changed -0.54 g since uncontaminated fluids were injected, causing sorbed contaminant mass to dissolve into the soluble-phase to maintain contaminant equilibrium.

During the 24hr extraction-only simulation, sorbed contaminant mass volatilized and represented approximately 84 % of the increase gas-phase contaminant mass. The remaining 16 % volatilized from the soluble-phase contaminant mass. During the first 12 – 13 hours, soluble-phase contaminant mass was extracted at full concentration as contaminated fluids were displaced at a rate equal to 0.76L/hr. During the second half of the simulation, the water table dropped below the bottom of the impermeable sheathing and the extracted air flow rate began to increase. The extracted water flow rate simultaneously decreased to maintain the same total extraction flow rate, which affected the rate of change in the soluble-phase contaminant mass (-0.81 g/hr during the first half of the simulation and -0.64 g/hr subsequent to the increase in extracted air flow rate). Additionally, a change in hydraulic conditions caused additional sorbed contaminant mass to dissolve into the soluble-phase.

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Approximately 16.60 g and 1.24 g of soluble-phase and gas-phase contaminant mass were removed during the extraction-only simulation, respectively. Approximately 19.97 g of soluble-phase contaminant mass was removed from the system during the concurrent injection-extraction simulation (a 10 % difference in total extracted contaminant mass).

During the sensitivity analysis, the rate of change in the soluble-phase contaminant mass was directly proportional to the extraction water flow rate. For example, the soluble-phase contaminant mass rate of change varied from –0.35 g/hr to –1.15 g/hr as the extraction water flow rate increased from 0.36 L/hr to 1.08 L/hr. Since the initial concentration remained unchanged and the same volume of water was displaced regardless of the model test grid dimensions, the PVW spacing had no affect on contaminant transport results. The increase in gas-phase contaminant mass and decrease in sorbed contaminant mass occurred independently of the soluble-phase contaminant mass changes. Therefore, the mass transfer coefficient had no effect on the change in the soluble-phase contaminant mass.

The increase in gas-phase contaminant mass was dependent upon the extraction water flow rate as well as the mass transfer coefficient. For example, the rate of change of gas-phase contaminant mass increased from approximately 0.06 g/hr to 0.42 g/hr as the mass transfer rate varied from $1 \times 10^{-7}$ s$^{-1}$ to $1 \times 10^{-5}$ s$^{-1}$) for an extraction water flow rate equal to 1.08 L/hr. For the same change in mass transfer rate, the rate of change of gas-phase contaminant increased from approximately 0.02 g/hr to 0.13 g/hr for an extraction water flow rate equal to 0.36L/hr.
Similar to the soluble-phase relationship, the rate of change in the total system contaminant mass varied as the extraction water flow rate increased. For example, the rate of change in the total system contaminant mass varied from approximately -0.40 g/hr to -1.10 g/hr for extraction water flow rates equal to 0.36 L/hr and 1.08 L/hr, respectively.
Figure 6.1. Cumulative Change in Contaminant Mass as a Function of Time for a Concurrent Injection-Extraction Simulation (a) and Extraction-Only Simulation (b)
Figure 6.2. System Extracted Contaminant Mass
Figure 6.3. Soluble-Phase Contaminant Mass Rate of Change as a Function of Extraction Water Flow Rate
Figure 6.4. Gas-Phase Contaminant Mass Rate of Change as a Function of Mass Transfer Coefficient.
Figure 6.5. Total System Contaminant Mass Rate of Change as a Function of Extraction Water Flow Rate.
7. RESEARCH SUMMARY AND CONCLUSIONS

7.1. Summary

This research consisted of three components: the field demonstration, laboratory experimentation, and finite element analysis. Global WIDE system performance parameters were investigated during the field demonstration, the effect of PVW geometry and the zone of influence was examined during laboratory experimentation, and contaminant partitioning tendencies were determined, as a function of time and operational scheme, using a three-dimensional finite element analysis.

The field demonstration was conducted at a site located in Ashtabula, Ohio. With the exception of a silt seam located approximately 1.8 m to 2.4 m below the ground surface, the subsurface consisted of Clay (CL) (the permeability of the Clay was approximately equal to $1 \times 10^{-6}$ cm/s). TCE contamination levels as high as 300,000 $\mu$g/kg were detected on the soil, and concentrations as high as 475 mg/L were detected in the ground water. A 21.0 m by 18.3 m WIDE demonstration test area was designed and installed over the TCE plume, the test area was divided into four quadrants, and 494 PVWs were installed to a depth of 6.1m. Concurrent injection extraction, alternating row extraction, and full quadrant extraction operations took place over a nine month interval. Vacuum pressure, injected and extracted fluid volumes, TCE concentrations (gas and soluble-phase), and water table levels were monitored during the field demonstration.

A 10kPa laboratory tracer test experiment was conducted on a 1.0 m$^3$ slurry sample with a sand seam. The test box was lined with a geocomposite to provide a
constant head reservoir boundary around the test sample. Three settlement plates, 23 piezometers, and 27 tracer tubes were installed to monitor settlement, pressure head distribution, and tracer concentration, respectively, during the test interval.

NAPL Simulator (a three-dimensional finite element analysis model) was calibrated using hydraulic field data. It was used to simulate soluble and gas-phase contaminant transport in saturated and unsaturated soil media. Using the reference case input parameter set and model test grid configuration, a parametric evaluation was initially performed to establish input variables that significantly affect contaminant transport. System performance and contaminant partitioning tendencies were evaluated as a function of time and operational scheme. Finally, a sensitivity analysis, consisting of 36 simulations, was performed to evaluate contaminant partitioning tendencies as a function of PVW spacing, extraction water flow rate, and mass transfer coefficient.

7.2. Conclusions

1. During extraction-only field testing, the water table was lowered and air simultaneously infiltrated the soil media, which significantly increased air flow rates and decreased the applied vacuum pressure with time. As the water table approached the bottom of the impermeable sheathing, air flow rates began to taper off near 600,000 L/hr, and the water table depth ceased to increase. During concurrent injection-extraction field testing, air flow rates remained less than approximately 200,000 L/hr.

2. The extracted water flow rates ranged from 260 - 1100 L/hr during concurrent injection-extraction operations, from 50 - 1000 L/hr during alternating row
extraction schemes, and from 10 - 600 L/hr during concurrent injection-extraction testing. Concurrent injection-extraction operations consistently achieved the highest extracted water flow rates due to the simultaneous injection of fluid, which promoted immediate groundwater recovery and prevented water table drawdown.

3. Soluble-phase TCE concentrations measured during concurrent injection-extraction operations (0.057 mg/L) were lower than TCE concentrations measured during alternating row extraction (0.088 mg/L). The uncontaminated injection fluid may have diluted existing concentrations and decreased extracted concentration in the soluble phase during concurrent injection-extraction operations.

4. At air flow rates less than approximately 200,000 L/hr, the gas-phase TCE extraction rate was approximately 1 g/hr. Gas-phase extraction rates increased to 6 g/hr as the air flow rate approached 600,000 L/hr. Since the air flow rates were generally less than 200,000 L/hr and the water table remained shallow during concurrent injection-extraction testing, it was concluded that approximately 1 g/hr of TCE was volatilized from mobile groundwater within PVWs and PVC collection piping. The increase in the gas-phase TCE extraction rate beyond 1 g/hr during extraction-only operations was attributed to TCE volatilization from residual and/or sorbed subsurface contaminant exposed to air flow.

5. Approximately 99% of extracted TCE was in the gas-phase during the WIDE field demonstration. WIDE technology proved successful for removal of volatile
organics in fine-grained soils and the system was most efficient during extraction-only operational schemes as long as the working vacuum pressure was maintained.

6. The zone of influence (calculated from the minimum radius of influence) was determined to be 0.60 m during the 10 kPa laboratory experiment.

7. The band-shaped PVW geometry may have had an affect on the flow hydraulics adjacent to the PVW during the laboratory experiment. There was an increase in the total hydraulic head near the narrow 4 mm PVW dimension, indicating an increase in the pore pressure and exit gradient. The band-shaped PVW geometry may have caused a choking effect during the laboratory test. This issue requires further investigation.

8. Over the course of 1200 operational hours, the (Cl) tracer samples measured during the laboratory tracer test retrieved 90 % - 100 % of the initial (Cl) concentration from tracer tubes located 0.41 m and 0.57 m from the sample bottom. Only 40 % of the initial (Cl) concentration was recovered from tracer tubes located 0.15 m from the sample bottom. The vacuum pressure decrease along the length of the PVW caused the hydraulic gradient as well as the pore water velocity to decrease with depth.

9. Soil Clogging was apparent within the PVW flow channels subsequent to the laboratory experimentation, which could pose a problem at higher vacuum pressures over longer periods of time.
10. Results from the finite element analysis indicated that soluble-phase contaminant mass was extracted through contaminated ground water at rate equal to 0.76 L/hr and a concentration equal to the solubility limit (1100 mg/L) while the water table was above the bottom of the simulated impermeable sheathing and the air flow rate was equal to zero.

11. During concurrent injection-extraction simulations, sorbed contaminant mass decreased as it dissolved into the soluble-phase to maintain contaminant equilibrium during the concurrent injection of uncontaminated fluids. As a result, there was no change in the soluble-phase concentration during 24 hour simulation even though soluble-phase contaminant mass was extracted via displaced ground water.

12. Approximately 84 % of the increase in gas-phase contaminant mass was attributed to sorbed contaminant mass volatilization in the unsaturated zone of the model test grid during extraction-only simulations. The remaining 16 % volatilized from the soluble-phase contaminant mass. Even though volatilization processes occurred, gas-phase contaminant mass was not extracted from the system until the air flow rate increased.

13. The rate of change in the soluble-phase contaminant mass during the finite element analysis was directly proportional to the extraction water flow rate. For example, the soluble-phase contaminant mass rate of change varied from -0.35 g/hr to -1.15 g/hr as the extraction water flow rate increased from 0.36 L/hr to 1.08 L/hr. Since the initial concentration and volume of water displaced were
unchanged regardless of PVW spacing, this parameter had no net effect on contaminant transport results in the soluble-phase.

14. The increase in gas-phase contaminant mass was dependent upon the extraction water flow rate as well as the mass transfer coefficient. For example, the rate of change of gas-phase contaminant mass increased from approximately 0.06 g/hr to 0.42 g/hr as the mass transfer rate varied from $1 \times 10^{-7}$ s$^{-1}$ to $1 \times 10^{-5}$ s$^{-1}$ for an extraction water flow rate equal to 1.08 L/hr. For the same range of mass transfer rates, the rate of change of gas-phase contaminant increased from approximately 0.02 g/hr to 0.13 g/hr for an extraction flow rate equal to 0.36 L/hr.

15. The rate of change in total system contaminant mass was primarily dependent upon the extraction water flow rate. For example, rate of decline in total system contaminant mass increased from approximately 0.40 g/hr and 1.10 g/hr as the extraction water flow rate increased from 0.36 L/hr to 1.08 L/hr.

7.3. Contribution to the State of the Art

Based on results from the field demonstration component, the laboratory experimentation component, and the finite element analysis component of this research, the following contributions to the state of the art are advanced:

1. WIDE technology proved successful for the removal of volatile organics in fine-grained soils. System efficiency is maximized during extraction-only operational schemes as long as the system is able to maintain working vacuum pressure.

2. The optimum zone of influence is determined (conservatively) to be 0.6 m during a 10 kPa laboratory experiment performed using Ashtabula glacial till.
3. A possible choking or necking effect was discovered during the laboratory experiment, near the narrow 4 mm dimension of the PVW, as a result of the band-shaped geometry. However, this issue needs further investigation.

4. Nine months of hydraulic and contaminant extraction data collected from the field demonstration will improve future WIDE system design and implementation.

5. The impermeable barrier sleeve can serve as a limiting boundary condition that contributes to the decrease in vacuum pressure during extraction-only field testing, if it is not extended deep enough.

6. System performance curves quantified the correlation between water table depth, air flow rate, and vacuum pressure during the field demonstration.

7. Approximately 99% of the TCE extracted during this field demonstration was in the gas-phase. Contaminant volatilization was found to be the predominant mode of TCE extraction.

8. Approximately 1 g/hr of gas-phase TCE was volatilized from the mobile ground water located in the PVC piping and PVW cavity. Additional gas-phase TCE extraction was attributed to TCE volatilization from immobile contaminant located in the unsaturated soil media.

9. Concurrent injection-extraction testing in the field caused a dilution effect in the extracted soluble-phase TCE concentrations. The average soluble-phase TCE concentration extracted during extraction-only operations was 0.088 mg/L. This concentration decreased to 0.057 mg/L during concurrent injection-extraction operations.
10. Finite element analysis results indicated that the increase in gas-phase contaminant mass in the unsaturated zone was dependent upon the extracted water flow rate as well as the mass transfer rate. Approximately 84% of this increase was attributed to sorbed contaminant mass volatilization. The remaining 16% volatized from soluble-phase contaminant mass.

7.4. Recommendations for Future Research

The following recommendations for future research are advanced:

1. To examine the choking effect that takes place near the narrow 4 mm dimension of the PVW in more detail.

2. To determine PVW vacuum pressure as a function of PVW depth, applied vacuum pressure, and PVW grid location during a field demonstration test.

3. To investigate WIDE system efficiency as a function of soil type during field demonstration testing.

4. To develop an in-situ field test method to measure the zone of influence and maximum extraction depth, prior to full-scale WIDE system deployment.

5. To determine if a smear zone is generated during PVW installation and measure the hydraulic effects of this zone on PVW efficiency.

6. To investigate long-term PVW durability (channel and geotextile Clogging effects).

7. To conduct long-term, extraction-only finite element analysis simulations to investigate contaminant partitioning tendencies and determine the benefit, if any, of de-saturating the soil media.
8. REFERENCES


## 9. APPENDIX A: QUADRANT 4 TEST SEQUENCE

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10. APPENDIX B: WATER VAPOR CALCULATIONS

Measured Data:
Relative Humidity = 24%
Temperature = 18.5°C
Flow Rate$_{vapor+air}$ = 0.566 m$_{vapor+air}$³/min

Calculations:
1. Absolute Humidity = \( \frac{\text{Mass}_{vapor}}{\text{Mass}_{air}} \) = 0.003 kg$_{vapor}$/kg$_{air}$
   - Use the measured temperature (18.5 °C) as the dry bulb temperature on the abscissa axis of the following psychrometric chart (Shallcross, 1997).
   - Interpolating between the 20% and 30% relative humidity curves, find the 24% relative humidity curve and the corresponding absolute humidity value on the ordinate axis.

2. Specific Volume = \( \frac{\text{Volume}_{vapor+air}}{\text{Unit Mass}_{air}} \) = 0.829 m³$_{vapor+air}$/kg$_{air}$
   - Interpolate between the 0.82 m³$_{vapor}$/kg$_{air}$ and 0.84 m³$_{vapor}$/kg$_{air}$ specific volume curves to obtain the corresponding specific volume.

3. Total Density = \( \frac{\text{Mass}_{vapor+air}}{\text{Volume}_{vapor+air}} \) = 1.21 kg$_{vapor+air}$/m³$_{vapor+air}$
   - Mass$_{vapor+air}$ = 0.003 kg$_{vapor}$ + 1.0 kg$_{air}$
   - Volume$_{vapor+air}$ = 0.829 m³$_{vapor+air}$

4. Extraction Rate$_{vapor+air}$ = Flow Rate$_{vapor+air}$ * Total Density = 0.68 kg$_{vapor+air}$/min
   - Flow Rate$_{vapor+air}$ = 0.57 m³$_{vapor+air}$/min
   - Total Density = 1.21 kg$_{vapor+air}$/m³$_{vapor+air}$

5. Extraction Rate$_{vapor}$ = Extration Rate$_{vapor+air}$ * \( \frac{\text{Mass}_{vapor}}{\text{Mass}_{vapor+air}} \) = 0.002 kg$_{vapor}$/min
   - Extraction Rate$_{vapor+air}$ = 0.68 kg$_{vapor+air}$/min
   - Mass$_{vapor}$ = 0.003 kg$_{vapor}$
   - Mass$_{vapor+air}$ = 0.003 kg$_{vapor}$ + 1.0 kg$_{air}$

6. Extraction Rate$_{vapor}$ = 0.002 kg$_{vapor}$/min = 2.03 mL/min
Psychrometric Chart for a Water-Air System at 1 Atmosphere (Shallicross, 1997)
### 11. APPENDIX C: NAPL SIMULATOR MODEL INPUT

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<td>1 ( \text{title} = \text{Variable} )</td>
<td>- ( \text{title} ): Title of simulation (maximum of 68 characters) printed to file ‘echo.out’.</td>
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| 2 \( \text{iphase} = 13 \) | - \( \text{iphase} \): Identifies the phases modeled.  
12 = Water-NAPL (2 flow equations)  
13 = Water-Gas (2 flow equations)  
123 = Water-NAPL-Gas (3 flow equations) |
| 3 \( \text{iscr} = 1 \) | - \( \text{iscr} \): Screen output switch that allows iteration, solution, and time information to be viewed during simulations.  
1 = on  
0 = off |
| 4 \( \text{iherm} = 1 \) | - \( \text{iherm} \): File output switch to print Hermite parameters at each time interval.  
Coefficients are printed for each node and time interval in ‘pa.out’, ‘sw.out’, ‘st.out’, ‘oa.out’, and ‘og.out’.  
1 = on  
0 = off |
| 5 \( \text{mass} = 1 \) | - \( \text{mass} \): Mass balance switch to calculate mass balance after each time step.  
Results are reported in ‘mass.out’, ‘cmass.out’, ‘massw.out’, ‘massn.out’, ‘massg.out’, and ‘masst.out’.  
1 = on  
2 = off |
| 6 \( \text{nex} = \text{Variable} \)  
\( \text{ney} = \text{Variable} \)  
\( \text{nez} = \text{Variable} \) | - \( \text{nex} \): Number of elements in the x dimension.  
- \( \text{ney} \): Number of elements in the y dimension.  
- \( \text{nez} \): Number of elements in the z dimension. |
| 7 \( \text{time} = 0 \) | - \( \text{time} \): Initial reference time used for listing purposes.  
  \( \text{time} = 0 \) (new run)  
  \( \text{time} = \text{end time of previous run} \) (restart run) |
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| 8 $t1pr = \text{Variable}$  
$t\text{mprnt} = \text{Variable}$  
$t\text{max} = \text{Variable}$ | • $t1pr(s)$ Time of first print = $time + t1pr$.  
• $t\text{mprnt}(s)$ Time interval after the first print.  
• $t\text{max}(s)$ Maximum simulation time.  
| 9 $i\text{tincs} = 6*$  
$i\text{itincc} = 10*$  
$t\text{mult} = 1.15*$ | • $i\text{tincs}$ Saturation iterations ($3<i\text{tincs}<15$)  
• $i\text{itincc}$ Contaminant transport iterations ($3<i\text{itincc}<15$)  
• $t\text{mult}$ Increase factor (1 or 1.15)  
Time step controls are based on the iterative solutions of the nonlinear saturation and contaminant transport equations. If the number of iterations required for convergence after each solution interval are less than the values specified for $i\text{tincs}$ and $i\text{itincc}$, the time step is increased by $t\text{mult}$. |
| 10 $i\text{treds} = 8*$  
$i\text{itredec} = 15*$  
$t\text{div} = 1.25*$ | • $i\text{treds}$ Saturation iterations ($i\text{treds} > i\text{tincs}$ and $8<i\text{tincs}<20$)  
• $i\text{itredec}$ Contaminant transport iterations ($i\text{itredec} > i\text{itincc}$ and $8<i\text{itincc}<20$)  
• $t\text{div}$ Reduction factor ($t\text{div} =1.25$)  
Time step controls are based on the iterative solutions of the nonlinear saturation and contaminant transport equations. If the number of iterations required for convergence after each solution interval exceed the values specified for $i\text{treds}$ and $i\text{itredec}$, the time step is reduced by $t\text{div}$. |
| 11 $i\text{thangs} = 15*$  
$i\text{ithangc} = 20*$  
$t\text{divh} = 1.5*$ | • $i\text{thangs}$ Saturation iterations ($i\text{thangs} > i\text{treds}$ and $10<i\text{tincs}<25$)  
• $i\text{ithangc}$ Contaminant transport iterations ($i\text{ithangc} > i\text{itredec}$ and $10<i\text{itincc}<25$)  
• $t\text{divh}$ Reduction factor ($t\text{divh} =1.5$)  
Time step controls are based on the iterative solutions of the nonlinear saturation and contaminant transport equations. If the number of iterations required for convergence after each solution interval exceed the values specified for $i\text{thangs}$ and $i\text{ithangc}$, the time step is reduced by $t\text{divh}$. |
<table>
<thead>
<tr>
<th>Model Input</th>
<th>Input Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>12 itermx = 200*</td>
<td>• <em>itermx</em> Number of iterations permitted to solve any one matrix equation. (<em>itermx</em> \leq 200)</td>
</tr>
</tbody>
</table>
| 13 dslim = 0.1* | • *dslim* An upper limit for the change in effective water saturation and the effective total wetting phase saturation used to define the relative permeability of NAPL phase over a time step.  
*Ds*lim = 1.0 (hysteresis considered)  
*Ds*lim = 0.1 (no hysteresis considered) |
| 14 co = 2* | • *co* Critical Courant number used to define an upper limit on the time step size based on time truncation error.  
Advection-diffusion partial differential equations, such as those which describe phase mass transport, can be characterized by the dimensionless Courant number.  
*co* \leq 2 (2 phases)  
*co* \leq 1 (3 phases) |
| 15 dt0 = 10* | • *dt0* (s) Initial time step used to start the simulation, which is small so that the simulator can propagate boundary and forcing terms which are initially shock-like. |
| 16 tsmmax = 2000*  
*tsmin* = 1* | • *tsmax* (s) Upper limit for the time step.  
• *tsmin* (s) Upper limit for the time step.  
Set to avoid instabilities during convergence.  
The simulation crasheds if the time step falls below *tsmin*. |
| 17 grf_on = 1  
grinc = Variable  
grch = Variable  
gmax = Variable | • *grf_on* Graphical output switch (1 = on, 0 = off)  
• *grinc* (s) Initial time interval  
• *ngrch* Number of time intervals at the *grinc* time interval  
• *fgrch* Time interval multiplier used to change the time interval  
• *gmax* (s) Maximum allowable time interval  
Graphical solutions are viewed in GMS by utilizing *.stf* files generated by the simulator. |
<table>
<thead>
<tr>
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</tr>
</thead>
<tbody>
<tr>
<td>18</td>
<td>( nloop = 0^* )</td>
</tr>
<tr>
<td></td>
<td>• ( nloop ) Number of sequential iteration loops between the pressure equation and the saturation equations during sequential solution. ( nloop = 0 ) (sequential solution) ( nloop &gt; 0 ) (iterative sequential solution)</td>
</tr>
<tr>
<td>19</td>
<td>( erip = 1 \times 10^{-6}^* )</td>
</tr>
<tr>
<td></td>
<td>• ( erip ) GMRES convergence criterion for the pressure equation</td>
</tr>
<tr>
<td>20</td>
<td>( eris = 1 \times 10^{-3}^* ) ( eros = 1 \times 10^{-3}^* )</td>
</tr>
<tr>
<td></td>
<td>Convergence criteria for saturation equations: • ( eris ) (inner iterations) • ( eros ) (outer iterations)</td>
</tr>
<tr>
<td>21</td>
<td>( erit = 1 \times 10^{-5}^* ) ( erot = 1 \times 10^{-3}^* )</td>
</tr>
<tr>
<td></td>
<td>Convergence criteria for contaminant transport equations: • ( erit ) (inner iterations) • ( erot ) (outer iterations)</td>
</tr>
<tr>
<td>22</td>
<td>( idxdy = 1 )</td>
</tr>
<tr>
<td></td>
<td>• ( idxdy ) Mesh definition flag that permits the simulator to generate a uniformly spaced mesh based on the number of elements specified ((nex, ney, nez)) and the maximum dimensions listed in ‘space.in’ or it will generate the exact mesh defined by spacing in ‘space.in’. ( idxdy = 0 ) (uniform mesh) ( idxdy = 1 ) (defined mesh)</td>
</tr>
<tr>
<td>23</td>
<td>( grav = 980.7 )</td>
</tr>
<tr>
<td></td>
<td>• ( grav ) ((cm/s^2)) Magnitude of the gravity vector.</td>
</tr>
<tr>
<td>24</td>
<td>( th_z = 0 ) ( th_y = 0 )</td>
</tr>
<tr>
<td></td>
<td>Grid orientation with respect to the horizontal. • ( th_z ) (deg) Angle to rotate the grid CCW about the z-axis. • ( th_y ) (deg) Angle to rotate the grid CCW about the y-axis.</td>
</tr>
<tr>
<td>25</td>
<td>( permb = \text{Variable} )</td>
</tr>
<tr>
<td></td>
<td>• ( permb ) ((cm^2)) Global intrinsic permeability scalar.</td>
</tr>
<tr>
<td>26</td>
<td>( ndev = \text{Variable} )</td>
</tr>
<tr>
<td></td>
<td>• ( ndev ) Number of node-specific deviations to ( permb ). If ( ndev &gt; 0 ), the simulator opens ‘perm.in’ and reads ( ndev ) lines of input. Each line includes the node number and corresponding ( permb ) value.</td>
</tr>
<tr>
<td>Model Input</td>
<td>Input Description</td>
</tr>
<tr>
<td>-------------</td>
<td>-------------------</td>
</tr>
<tr>
<td>27 $\textit{porb} = 0.4^a$</td>
<td>$\textit{porb}$ Global soil porosity scalar.</td>
</tr>
<tr>
<td>28 $n\text{dev} = 0$</td>
<td>$n\text{dev}$ Number of node-specific deviations to $\textit{porb}$. If $n\text{dev} &gt; 0$, the simulator opens ‘por.in’ and reads $n\text{dev}$ lines of input. Each line includes the node number and corresponding $\textit{porb}$ value.</td>
</tr>
<tr>
<td>29 $\textit{bulkb} = 1.8^a$</td>
<td>$\textit{bulkb}(g/cm^3)$ Global dry bulk density used to model adsorption mass transfer.</td>
</tr>
<tr>
<td>30 $n\text{dev} = 0$</td>
<td>$n\text{dev}$ Number of node-specific deviations to $\textit{bulkb}$. If $n\text{dev} &gt; 0$, the simulator opens ‘bulk.in’ and reads $n\text{dev}$ lines of input. Each line includes the node number and corresponding $\textit{bulkb}$ value.</td>
</tr>
</tbody>
</table>
| 31 $V_w_r = 0.01^b (\text{water, 20}^\circ)$
$v_n_r = 0.005^b(TCE, 20^\circ)$
$V_g_r = 1.81\times10^{-4}^c(\text{air, 20}^\circ)$ | $v_w_r (g/cm-s)$ Pure phase viscosity of water. |
| | $v_n_r (g/cm-s)$ Pure phase viscosity of the NAPL. |
| | $v_g_r (g/cm-s)$ Pure phase viscosity of the gas. |
| 32 $r_w_r = 1.0^b(\text{water, 20}^\circ)$
$r_n_r = 1.464^b(TCE,20^\circ)$
$r_g_r = 1.205\times10^{-3}^c(\text{air, 20}^\circ)$ | $r_w_r (g/cm^3)$ Pure phase density of water. |
| | $r_n_r (g/cm^3)$ Pure phase density of the NAPL. |
| | $r_g_r (g/cm^3)$ Pure phase density of the gas. |
| 33 $\textit{Siggw} = 72^b(\text{water, 20}^\circ)$
$\textit{signw} = 34.5^b(TCE,20^\circ)$
$\textit{siggn} = 29.3^b(TCE,20^\circ)$ | $\textit{siggw} (g/s^2)$ Surface tension (water) |
<p>| | $\textit{signw} (g/s^2)$ Interfacial tension (NAPL and water) |
| | $\textit{siggn} (g/s^2)$ Surface tension (NAPL) |
| 34 $n_phase = 1$ | $n_phase$ Phase pair used to obtain the S-P model fitting parameters to define the capillary pressure scaling relationship. $n_phase = 1$ (gas-water) $n_phase = 2$ (NAPL-water) $n_phase = 3$ (gas-NAPL) |</p>
<table>
<thead>
<tr>
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</table>
| 35 \(swr = 0.28\)  
\(snr = 0.20\)  
\(snwr = 0.20\)  
\(sgr = 0\) | - \(swr\) Global residual saturation (water)  
- \(snr\) Global residual saturation (NAPL-nonwetting)  
- \(snwr\) Global residual saturation (NAPL-wetting)  
- \(sgr\) Global residual saturation (gas) |
| 36 \(ndev = 0\) | - \(ndev\) Number of node-specific deviations to \(swr, snr, snwr, sgr\).  
If \(ndev > 0\), the simulator opens ‘residual.in’ and reads \(ndev\) lines of input. Each line includes the node number and corresponding \(swr, snr, snwr,\) and \(sgr\) values. |
| 37 \(asd = 14\)  
\(asi = 14\)  
\(eta = 1.12\) | Global S-P model curve shape parameters.  
- \(asd\) Pressure scale for drainage.  
- \(asi\) Pressure scale for imbibition.  
- \(eta\) Pore connectivity parameter. |
| 38 \(ndev = 0\) | - \(ndev\) Number of node-specific deviations to \(asd, asi, and eta\).  
If \(ndev > 0\), the simulator opens ‘shape.in’ and reads \(ndev\) lines of input. Each line includes the node number and corresponding \(asd, asi, and eta\) values. |
| 39 \(Perm_b = \) Variable  
\(por_b = 0.4\) | - \(perm_b\) \((cm^2)\) Global intrinsic permeability scalar.  
- \(por_b\) Global soil porosity scalar. |
| 40 \(ndev = 0\) | - \(ndev\) Number of node-specific deviations to \(perm_b and por_b\).  
If \(ndev > 0\), the simulator opens ‘base.in’ and reads \(ndev\) lines of input. Each line includes the node number and corresponding \(perm_b and por_b\) values. |
<table>
<thead>
<tr>
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</tr>
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</table>
| 41 $alfw = 0.5^*$  
$nsew1 = 1.0^*$  
$nsew2 = 1.0^*$ | Parameters used to define the water-phase relative permeability/water-phase saturation functional.  
- $alfw$ Connectivity parameter  
- $nsew1$ Flag to determine the effective water saturation used to define the connectivity term in the water-phase relative permeability functional.  
- $nsew2$ Flag to determine the effective water saturation used to define the integral of the water-phase relative permeability functional. |
| 42 $alfn = 0.5^*$  
$nsen1 = 1.0^*$  
$nsen2 = 3.0^*$  
$nsen3 = 3.0^*$ | Parameters used to define the NAPL-phase relative permeability/water & gas-phase saturation functional.  
- $alfn$ Connectivity parameter  
- $nsen1$ Flag to determine the effective NAPL saturation used to define the NAPL-phase relative permeability functional.  
- $nsen2$ Flag to determine the effective total nonwetting-phase saturation used to define the NAPL-phase relative permeability functional.  
- $nsen3$ Flag to determine the effective total wetting-phase saturation used to define the NAPL-phase relative permeability functional. |
| 43 $alfg = 0.5^*$  
$nseg = 11.0^*$  
$nseg2 = 1.0^*$ | Parameters used to define the gas-phase relative permeability/gas-phase saturation functional.  
- $alfg$ Connectivity parameter  
- $nseg1$ Flag to determine the effective gas saturation used to define the connectivity term in the gas-phase relative permeability functional.  
- $nseg2$ Flag to determine the effective gas saturation used to define the integral of the gas-phase relative permeability functional. |
| 44 $se\_sl = 0.01^*$  
$se\_rl = 0.001^*$ | Both parameters help linearly extrapolate the S-P functionals at effective saturations near one and zero to make them amenable to numerical model implementation. |
<table>
<thead>
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</tr>
</thead>
<tbody>
<tr>
<td>45 $sfact_{kr} = 0.01^*$</td>
<td>• $sfact_{kr}$ Eliminates the effect that small oscillations in the saturation and concentration solutions have on residual saturations.</td>
</tr>
</tbody>
</table>
| 46 $nhyst = 0$ | • $nhyst$ Hysteresis model switch.  
  $1 = \text{on (k-S-P model is used)}$  
  $0 = \text{off (monotonic displacement model is used)}$ |
| 47 $e_r = 1.0^*$ | • $e_r$ Phase entrapment/release definition.  
  Governs how fast the phase becomes entrapped during drainage conditions or how fast it becomes released from entrapment during imbibition.  
  $E_r = 1$ (linear entrapment/release model) |
| 48 $b_a = 0.2^*$ | • $b_a$ Blending parameter which defines how fast the van Genuchten scale parameter changes after a reversal occurs. |
| 49 $sp_{min} = 0.03^*$  
  $sr_{min} = 0.04^*$ | Restriction parameters for S_P curve generation and update.  
  • $sp_{min}$ Minimum span for which a new set of scaling parameters will be calculated ($0.025 > sp_{min} > 0.1$).  
  • $sr_{min}$ Minimum tolerance away from the S-P curve end points above which a scanning curve will be generated after a flow reversal otherwise the computation is suppressed ($sr_{min} > sp_{min}$ and $0.025 > sr_{min} > 0.1$). |
| 50 $factd = 0.001^*$  
  $facti = 0.001^*$ | • $factd$ Tolerance in saturation change to indicate a reversal from drainage to imbibition.  
  • $facti$ Tolerance in saturation change to indicate a reversal from imbibition to drainage. |
| 51 $Pe_w = 2$  
  $Pe_g = 2$ | • $pe_w$ Critical Peclet numbers for the water-phase  
  • $pe_g$ Critical Peclet numbers for the gas-phase  
  The Peclet constraint interrogates grid spacing and ensures the shape conforms to the grid.  
  $pe_w = pe_g = 2$ (on)  
  $pe_w = pe_g = 200$ (off) |
<p>| 52 $pg_{ref} = 1\times10^6$ | • $pg_{ref}$ (g/cm$^2$) Reference gas phase pressure (usually set to atmospheric pressure). |</p>
<table>
<thead>
<tr>
<th>Model Input</th>
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</tr>
</thead>
</table>
| 53  
$ntr\_ow = 1$  
$ntr\_og = 1$ | • $ntr\_ow$ Dissolved NAPL contaminant transport switch.  
• $ntr\_og$ Gaseous NAPL contaminant transport switch.  
1 = on  
0 = off |
| 54  
$\theta = 1*$ | • $\theta$ Projection parameter used to model the coupling between the water and gas-phase contaminant transport equations due to mass transfer of the NAPL species between phases.  
1 = no projection |
| 55  
$along = 1^a$  
$atran = 0.1^a$  
$diff_w = 8.3 \times 10^{-6b}$  
$diff_g = 8.11 \times 10^{-2b}$ | • $along$ (cm) Longitudinal dispersivity  
• $atran$ (cm) Transverse dispersivity  
• $diff_w$ (cm$^2$/s) Molecular diffusion in water  
• $diff_g$ (cm$^2$/s) Molecular diffusion in gas |
| 56  
$p\_oc = 126^b$  
$focb = .03^a$ | • $p\_oc$ Global organic carbon partitioning coefficient  
• $focb$ Fraction of organic carbon |
| 57  
$ndev = 0$ | • $ndev$ Number of node-specific deviations to $focb$.  
If $ndev > 0$, the simulator opens ‘o_c.in’ and reads $ndev$ lines of input. Each line includes the node number and corresponding $focb$ value. |
| 58  
$d\_layer = 0.5^*$ | • $d\_layer$ (cm) Thickness of the boundary layer separating the soil domain from the atmosphere. |
| 59  
$bow\_1 = 0.03^d$ (TCE)  
$bow\_2 = 0.5^*$  
$bow\_3 = 1.0^*$ | • $bow\_1$ (s$^{-1}$) Mass transfer rate coefficient (NAPL-phase dissolving into the water phase).  
• $bow\_2$ Coefficient $\beta_2$ in the equation for mass transfer rate.  
• $bow\_3$ Coefficient $\beta_3$ in the equation for mass transfer rate. |
| 60  
$parow = 0.0011^b$ (TCE) | • $parow$ (g/cm$^3$) NAPL water-phase equilibrium concentration (aqueous solubility). |
| 61  
$bog\_1 = 0.01^f$ (TCE)  
$bog\_2 = 0.5^*$ | • $bog\_1$ (s$^{-1}$) Mass transfer rate coefficient (NAPL-phase vaporizing into the gas phase).  
• $bog\_2$ Coefficient $\beta_2$ in the equation for mass transfer rate. |
<table>
<thead>
<tr>
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</tr>
</thead>
<tbody>
<tr>
<td>62 ( \text{parog} = 0.00537 \text{g/cm}^3 ) (TCE)</td>
<td>( \text{parog} ) (g/cm(^3)) NAPL gas-phase equilibrium concentration (vapor density).</td>
</tr>
<tr>
<td>63 ( \text{bowg}_1 = 4 \times 10^{-5} \text{g/cm}(^3) ) (TCE)</td>
<td>( \text{bowg}_1 ) (s(^{-1})) Mass transfer rate coefficient (dissolved NAPL-phase vaporizing into the gas phase).</td>
</tr>
<tr>
<td>64 ( \text{bowg}_2 = 0.5 )</td>
<td>( \text{Bowg}_2 ) Coefficient ( \beta_2 ) in the equation for mass transfer rate.</td>
</tr>
<tr>
<td>65 ( \text{e-henry} = 0.372 \text{b(TCE, 25\degree C)} )</td>
<td>( \text{e-henry} ) Henry’s law constant (dimensionless).</td>
</tr>
<tr>
<td>66 ( \text{t_half} = 3.11 \times 10^7 \text{s(TCE)} )</td>
<td>( \text{t_half} ) Effective half-life of the NAPL species in the water and gas phases.</td>
</tr>
<tr>
<td>67 ( \text{swinit} = 1 )</td>
<td>( \text{swinit} ) Global fraction of water saturation ( 0 &lt; \text{swinit} &lt; 1.0 ).</td>
</tr>
<tr>
<td>68 ( \text{stinit} = 1 )</td>
<td>( \text{stinit} ) Global fraction of total wetting phase saturation ( 0 &lt; \text{stinit} &lt; 1.0 ).</td>
</tr>
<tr>
<td>69 ( \text{roainit} = 0.0011 )</td>
<td>( \text{roainit} ) (g/cm(^3)) Global initial condition of dissolved contaminant concentration. If ( \text{roainit} &gt; 0 ), set equal to water solubility limit.</td>
</tr>
<tr>
<td>70 ( \text{roginit} = 0 )</td>
<td>( \text{roginit} ) Global initial condition for vapor contaminant concentration. If ( \text{roaginit} &gt; 0 ), set equal to gaseous solubility limit.</td>
</tr>
<tr>
<td>71 ( \text{ncont} = 0 )</td>
<td>( \text{ncont} ) Restart option switch that enables the simulator to read initial conditions from all *.rs files, which contain output from the previous output interval. ( 1 = \text{on} ), ( 0 = \text{off} ).</td>
</tr>
<tr>
<td>72 ( \text{ndev_s} = \text{Variable} )</td>
<td>( \text{ndev_s} ) Number of node-specific deviations to ( \text{swinit} ). If ( \text{ndev_s} &gt; 0 ), the simulator opens ‘sat.in’ and reads ( \text{ndev_s} ) lines of input. Each line includes the node number and corresponding water and total (water + NAPL) saturation values.</td>
</tr>
<tr>
<td>73 ( \text{ndev_roa} = \text{Variable} )</td>
<td>( \text{ndev_roa} ) Number of node-specific deviations to ( \text{roainit} ). If ( \text{ndev_roa} &gt; 0 ), the simulator opens ‘roa.in’ and reads ( \text{ndev_roa} ) lines of input. Each line includes the node number and corresponding dissolved-phase contaminant concentration value.</td>
</tr>
<tr>
<td>Model Input</td>
<td>Input Description</td>
</tr>
<tr>
<td>---------------------</td>
<td>--------------------------------------------------------------------------------------------------------------------------------------------------</td>
</tr>
</tbody>
</table>
| 73 $ndev_{rog} = \text{Variable}$ | • $ndev_{rog}$ Number of node-specific deviations to $roginit$.  
If $ndev_{rog} > 0$, the simulator opens ‘rog.in’ and reads $ndev_{rog}$ lines of input. Each line includes the node number and corresponding gas-phase contaminant concentration value. |
| 74 $nbcroa = \text{Variable}$      | • $nbcroa$ Number of boundary conditions for the mass concentration of NAPL in the water-phase.  
If $nbcroa > 0$, the simulator opens ‘bc_roa.in’ and reads $nbcroa$ lines of input. Each line includes the $nface$, $nod$, and $roa$ values where $nface$ is the mesh face which is normal to the direction from which the condition is applied, $nod$ is the node number, and $roa$ is the concentration. |
| 75 $nbcrog = \text{Variable}$      | • $nbcrog$ Number of boundary conditions for the mass concentration of NAPL in the gas-phase.  
If $nbcrog > 0$, the simulator opens ‘bc_rog.in’ and reads $nbcrog$ lines of input. Each line includes the $nface$, $nod$, and $rog$ values where $nface$ is the mesh face which is normal to the direction from which the condition is applied, $nod$ is the node number, and $roa$ is the concentration. |
| 76 $ncondf = \text{Variable}$      | • $ncondf$ Number of flow-variable boundary conditions different from the default no flow condition.  
If $ncondf > 0$, the simulator opens ‘bc_ow.in’ and reads the data for $ncondf$ boundary nodes. Each boundary node includes the $nface$, $nod$, and $ncode$ values where $nface$ is the mesh face which is normal to the direction from which the condition is applied, $nod$ is the node number, and $ncode$ is condition type, as defined in the documentation. |
<table>
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</thead>
<tbody>
<tr>
<td>77 nwella = Variable</td>
<td>• <strong>nwella</strong> Number of nodes having point sources and/or sinks. If nwella &gt; 0, the simulator opens ‘well.in’ and reads nwella lines of input. Each line includes the nod, q_tot, ff_w, ff_g, roa, and rog values. nod is the node number, q_tot is the flow rate (injection is position, extraction is negative), ff_w is the fractional flow of water injected, ff_g is the fractional flow of gas injected, roa is the concentration of injected dissolved-phase NAPL species, and rog is the concentration of injected gas-phase NAPL species.</td>
</tr>
<tr>
<td>78 timec = Variable</td>
<td>• <strong>timec</strong> Reference time corresponding to the next stress period (set this value to a number higher than the maximum simulation time if there is only one stress period).</td>
</tr>
<tr>
<td>iph_new = 12</td>
<td>• <strong>iph_new</strong> Input parameter iphase (previously defined) for the new stress period</td>
</tr>
<tr>
<td>dtnew = 10</td>
<td>• <strong>dtnew</strong> (s) Time step for the new stress period</td>
</tr>
<tr>
<td>dmax = 2000</td>
<td>• <strong>dmax</strong> (s) Maximum time step for the new stress period</td>
</tr>
<tr>
<td>co_new = 2*</td>
<td>• <strong>co_new</strong> Courant constraint for the new stress period</td>
</tr>
</tbody>
</table>

*Suggested values from NAPL Simulator documentation
*a Measured in the field and/or laboratory using field soil.
bCohen and Mercer (1993)
cDaugherty, Franzini, and Finnemore (1985)
eArmstrong, Find, and McClellan (1994)