# Assessment of Site Specific Factors Affecting the Potential Mobility of DNAPL Within the Subsurface


## Victoria M. Bisbing

## Primary Reader: Richard Karr; Secondary Reader: Craig Calabria

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## BACKGROUND

- While conducting a subsurface boring and sampling program drilling through the overburden to weathered bedrock at a hazardous waste site, a Dense-Non Aqueous Phase Liquid (DNAPL) was encountered.
- DNAPL will act as a long term source causing dissolve phase contamination, therefore delineating the extent of the DNAPL Source Zone is a critical component when considering a remedial approach.
- This paper investigates the various factors that impact DNAPL migration at the Site. It also utilizes a series of calculation to determine specific locations where DNAPL may be present.
- The results of the calculations are then compared to observations noted during the investigational work.
- The conclusion reached is a potential DNAPL source zone, which can then be targeted for remediation.

## OBJECTIVES

- Examine specific Site factors and DNAPL properties which influence DNAPL migration at the Site.
- Examine the visual observations against calculated DNAPL potential source zone.
- Determine the extent of the dissolved phase plume as a result of DNAPL present within the subsurface.

## DESIGN/METHODS

- Subsurface investigation work during 2011 and 2012 provided soil chemical and physical properties for the Site. It also provided rock matrix chemical and physical properties as well. Groundwater analytical data was obtained by utilizing groundwater results collected from the site during 2011 and 2012.
- The DNAPL encountered at the Site was analyzed three times to determine the composition of the multi-component DNAPL.
- The composition of each DNAPL was taken into consideration when calculating threshold values which then demonstrate the potential that DNAPL is present within the vicinity.

| Compounds (µg/L) | First Sample Concentration | Second Sample Concentration | Third Sample Concentration |
|---|---|---|---|
| Benzene | 47700 | 36200 | NA |
| Chlorobenzene | 674000 | 434000 | NA |
| 1,2-Dichlorobenzene | 8530000 | 5450000 | NA |
| 1,3-Dichlorobenzene | 3650000 | 2390000 | NA |
| 1,4-Dichlorobenzene | 14700000 | 9460000 | NA |
| Ethylbenzene | 756000 | 518000 | NA |
| Ispropylbenzene | 169000 | 102000 | NA |
| Styrene | 22100000 | 12800000 | NA |
| Toluene | 13400000 | 8230000 | NA |
| 1,2,3-Trichlorobenzene | 14300000 | 10400000 | NA |
| 1,2,4-Trichlorobenzene | 112000000 | 48500000 | NA |
| m,p-Xylene | 340000 | 208000 | NA |
| o-Xylene | 366000 | 219000 | NA |
| Xylene (total) | 706000 | 427000 | NA |
| Aniline | 407000 | 179000 | 2550000 |
| Anthracene | 2550 | ND | NA |
| Benzo(a) anthracene | 4300 | ND | NA |
| 1,1' Biphenyl | 113000 | ND | NA |
| Carbazole | 2680 | ND | NA |
| Chrysene | 4170 | ND | NA |
| Dimethyl phthalate | 1380000 | 11600 | NA |
| Fluroanthene | 6630 | ND | NA |
| 2-Methylnapthalene | 6570 | ND | NA |
| Naphthalene | 21600 | ND | NA |
| Nitrobenzene | 395000000 | 3390000 | 998000000 |
| Phenanthrene | 8400 | ND | NA |
| Pyrene | 7090 | ND | NA |
| 1,2,4,5-Tetrachlorobenzene | 2970000 | 11700 | NA |
| Methylene chloride | ND | 113000 | NA |

ND – Not detected
NA – Not Analysis Requested
Concentrations are in micrograms per liter.

**Table 2. Individual Chemical Properties for each Compound detected in DNAPL**

| Compound | Molecular Weight (g/mol) | Solubility (mg/L) | $K_{oc}$ (ml/g) |
|---|---|---|---|
| Benzene | 78.11 | 1780 | 97 |
| Chlorobenzene | 112.56 | 448 | 318 |
| 1,2-Dichlorobenzene | 147 | 148 | 343 |
| 1,3-Dichlorobenzene | 147 | 118 | 463 |
| 1,4-Dichlorobenzene | 147 | 79 | 594 |
| Ethylbenzene | 106.16 | 150 | 622 |
| Ispropylbenzene | 120.2 | 0 | 1380 |
| Styrene | 104.14 | 162 | 380 |
| Toluene | 92.14 | 500 | 242 |
| 1,2,3-Trichlorobenzene | 181.45 | 0 | 1380 |
| 1,2,4-Trichlorobenzene | 181.46 | 30 | 1080 |
| m,p-Xylene | 106.17 | 156 | 552 |
| o-Xylene | 106.17 | 170 | 552 |
| Xylene (total) | 106.17 | 170 | 363 |
| Aniline | 93.13 | 34000 | 13 |
| Anthracene | 178.22 | 0.073 | 26000 |
| Benzo(a) anthracene | 240.13 | 0.014 | 125719 |
| 1,1' Biphenyl | 154.07 | 7.5 | 1400 |
| Carbazole | 167.21 | 0 | 3390 |
| Chrysene | 228.29 | 0.022 | 420108 |
| Dimethyl phthalate | 194.19 | 0.1 | 41 |
| Fluroanthene | 252.32 | 0.275 | 198000 |
| 2-Methylnapthalene | 142.2 | 25.4 | 8500 |
| Naphthalene | 128.19 | 30 | 1080 |
| Nitrobenzene | 123.11 | 0.0019 | 141 |
| Phenanthrene | 178.22 | 1.29 | 23000 |
| Pyrene | 202.26 | 0.135 | 63400 |
| 1,2,4,5-Tetrachlorobenzene | 215.89 | 0.3 | 5890 |
| Methylene chloride | 84.92 | 13200 | 25 |

## RESULTS

**Table 7 – Exceedance of Threshold Chemical Concentrations Within the Overburden**

| Boring | Exceedance occurs (AC, WC, BC, | Compounds that were exceeded |
|---|---|---|
| B2-11 | AC and BC | Nitrobenzene |
| B3-11 | WC | Nitrobenzene and Aniline |
| B4-11 | AC, WC, BC, WBR | Nitrobenzene |
| B5-11 | WC and WBR | Nitrobenzene |
| B6-11 | AC and WC | Nitrobenzene |
| B7-11 | AC and BC | Nitrobenzene |
| B8-11 | AC, WC, BC, WBR | Nitrobenzene |
| B9-11 | AC and WC | Nitrobenzene |
| B10-11 | AC, WC, BC, WBR | Nitrobenzene |
| B11-11 | AC, WC, BC, WBR | Nitrobenzene |
| B12-11 | AC, WC, BC, WBR | Nitrobenzene |
| B13-11 | AC, WC and WBR | Nitrobenzene |
| B14-11 | AC and WC | Nitrobenzene |
| B15-11 | WC, BC and WBR | Nitrobenzene |
| B16-11 | AC and BC | Nitrobenzene |
| B17-11 | WC and BC | Nitrobenzene |
| B18-11 | BC and WBR | Nitrobenzene |
| B19-11 | WC | Nitrobenzene |
| B22-12 | AC | Nitrobenzene |
| B23-12 | AC | Nitrobenzene |
| B24-12 | AC | Nitrobenzene |
| B25-12 | AC | Nitrobenzene |
| B26-12 | AC and BC | Nitrobenzene |
| B27-11 | WC | Nitrobenzene and Aniline |
| B28-12 | WC | Nitrobenzene |
| B34-12 | AC, WC, BC | 1,2-Dichlorobenzene and 1,4- |

**Table 10.3 – Sample 3 - Threshold Chemical Concentration in Rock Based on Partitioning Relationships**

| Compound | Calculated Kd | Rock Matrix Concentration |
|---|---|---|
| Aniline | 1.04 | 122.5073 |
| Nitrobenzene | 11.28 | 0.021417 |

Note: Kd value is calculed by multiplying each compound's individual $K_{oc}$ by the site specific fractional organic carbon. The value of which could not be obtained through sample analysis. The value chosen is 0.05 which is based upon a typical value used for sandstone. The bulk density of the rock matrix chosen for analysis was 2.7 g/cm³. This was an average of bulk density measurements of samples collected from the site. The porosity value chosen for this analysis is 0.082. The porosity value chosen is an average of measured porosity samples collected from the rock matrix.

The values obtained for each DNAPL sample will be used as a range to compare nitrobenzene and aniline analytical results. The comparison is shown in the table below.

**Table 10.1 - Sample 1 - Threshold Chemical Concentration in Rock Based on Partitioning Relationships**

| Compound | Calculated Kd | Rock Concentration |
|---|---|---|
| Benzene | 4.85 | 1.178933 |
| Chlorobenzene | 15.9 | 9.496953 |
| 1,2-Dichlorobenzene | 17.15 | 32.78918 |
| 1,3-Dichlorobenzene | 23.15 | 15.09324 |
| 1,4-Dichlorobenzene | 29.7 | 52.19537 |
| Ethylbenzene | 31.1 | 7.389942 |
| Isopropylbenzene | 69 | 0 |
| Styrene | 19 | 145.3923 |
| Toluene | 12.1 | 196.0222 |
| 1,2,3-Trichlorobenzene | 69 | 0 |
| 1,2,4-Trichlorobenzene | 54 | 222.3315 |
| m,p-Xylene | 27.6 | 3.06756 |
| o-Xylene | 27.6 | 3.598483 |
| Xylene (total) | 18.15 | 4.567296 |
| Aniline | 0.65 | 22.46641 |
| Anthracene | 1300 | 0.000302 |
| Benzo(a)anthracene | 6285.95 | 0.00035 |
| 1,1' Biphenyl | 70 | 0.085608 |
| Carbazole | 169.5 | 0 |
| Chrysene | 21005.4 | 0.001876 |
| Dimethyl phthalate | 2.05 | 0.000329 |
| Fluroanthene | 9900 | 0.015898 |
| 2-Methylnapthalene | 425 | 0.110847 |
| Naphthalene | 54 | 0.060696 |
| Nitrobenzene | 7.05 | 0.009592 |
| Phenanthrene | 1150 | 0.015539 |
| Pyrene | 3170 | 0.003334 |
| 1,2,4,5- | 294.5 | 0.270134 |

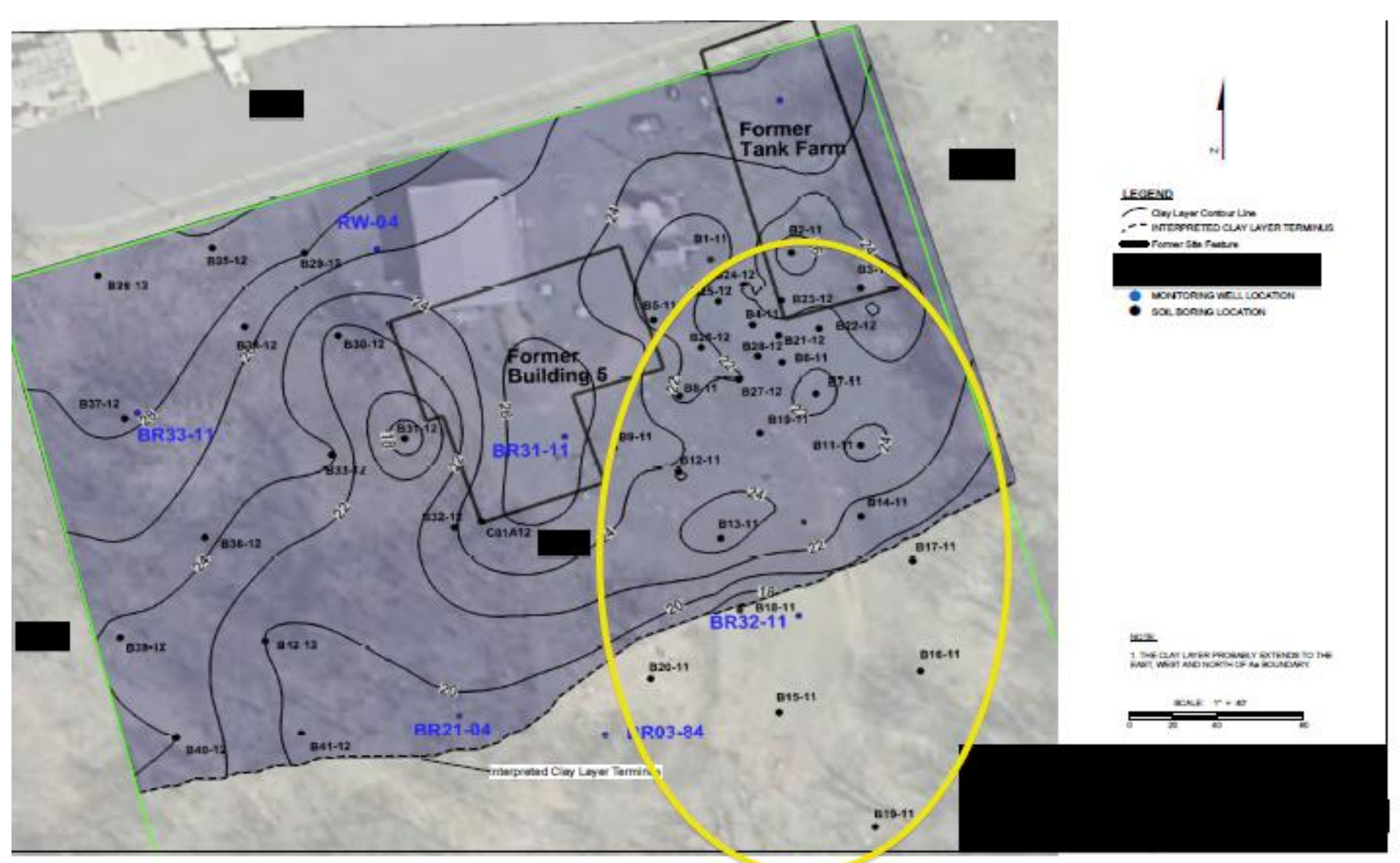
Note: Kd value is calculed by multiplying each compound's individual $K_{oc}$ by the site specific fractional organic carbon. The value of which could not be obtained through sample analysis. The value chosen is 0.05 which is based upon a typical value used for sandstone. The bulk density of the rock matrix chosen for analysis was 2.7 g/cm³. This was an average of bulk density measurements of samples collected from the site. The porosity value chosen for this analysis is 0.082. The porosity value chosen is an average of measured porosity samples collected from the rock matrix.

**Table 10.2 - Sample 2 - Threshold Chemical Concentration in Rock Matrix Based on Partitioning Relationships**

| Compound | Calculated Kd | Rock Matrix Concentration |
|---|---|---|
| Benzene | 7.76 | 5.722781 |
| Chlorobenzene | 25.44 | 39.11488 |
| 1,2-Dichlorobenzene | 27.44 | 134.0003 |
| 1,3-Dichlorobenzene | 37.04 | 63.21431 |
| 1,4-Dichlorobenzene | 47.52 | 214.8492 |
| Ethylbenzene | 49.76 | 32.38746 |
| Isopropylbenzene | 110.4 | 0 |
| Styrene | 30.4 | 538.6257 |
| 1,2,3-Trichlorobenzene | 110.4 | 0 |
| 1,2,4-Trichlorobenzene | 86.4 | 615.8181 |
| m,p-Xylene | 44.16 | 12.00343 |
| o-Xylene | 44.16 | 13.77242 |
| Xylene (total) | 29.04 | 17.66893 |
| Aniline | 1.04 | 63.20045 |
| Dimethyl phthalate | 3.28 | 1.77E-05 |
| Nitrobenzene | 11.28 | 0.000527 |
| 1,2,4,5- | 471.2 | 0.006807 |
| Methylene Chloride | 2 | 319.6763 |

Note: Kd value is calculed by multiplying each compound's individual $K_{oc}$ by the site specific fractional organic carbon. The value of which could not be obtained through sample analysis. The value chosen is 0.05 which is based upon a typical value used for sandstone. The bulk density of the rock matrix chosen for analysis was 2.7 g/cm³. This was an average of bulk density measurements of samples collected from the site. The porosity value chosen for this analysis is 0.082. The porosity value chosen is an average of measured porosity samples collected from the rock matrix.

- Table 7 shown above demonstrates the following soil boring and sample depth at which one or more component of the DNAPL threshold saturation value was exceeded, indicative of the presence of DNAPL within the vicinity.
- Tables 10.1 through 10.3 demonstrate threshold values for the individual components of the DNAPL which would indicate that DNAPL was present in the rock matrix samples.
- The results of the calculations successfully demonstrate a potential source zone area where DNAPL is present within the soil and bedrock matrix. The results also implicate the dissolved phase plume.
- The figure shown below demonstrates the potential source zone within the unconsolidated overburden.

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## SUMMARY

**Objective 1: SUPPORTED**
Understand the mechanics of two phase flow to demonstrate its impact on DNAPL migration at the Site.
**Objective 2: SUPPORTED**
Utilize Site-specific DNAPL data and other values to complete a series of calculations to determine where DNAPL has migrated
**Objective 3: SUPPORTED**
Compare the calculations to visual observations. The calculations confirmed visual observations.

## CONCLUSION & IMPLICATIONS

- Generally, the quantitative data obtained through calculations in this paper, tended to support the qualitative observations made in the field.
- Because the calculations are supportive of the observations, the calculations served to demonstrate a potential DNAPL zone within the overburden and deep bedrock, as well as demonstrating a dissolved phase plume.
- It is necessary to note several shortcomings that arose from the calculations.
  - The site-specific values utilized for bulk density were not site specific. The FOC value for soil was based upon a sample submitted by another consulting firm, several years ago. Inability to determine groundwater flow and velocity.
  - If these values were obtained, a more complete understanding of contaminant transport could be obtained.

## Works Cited


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