

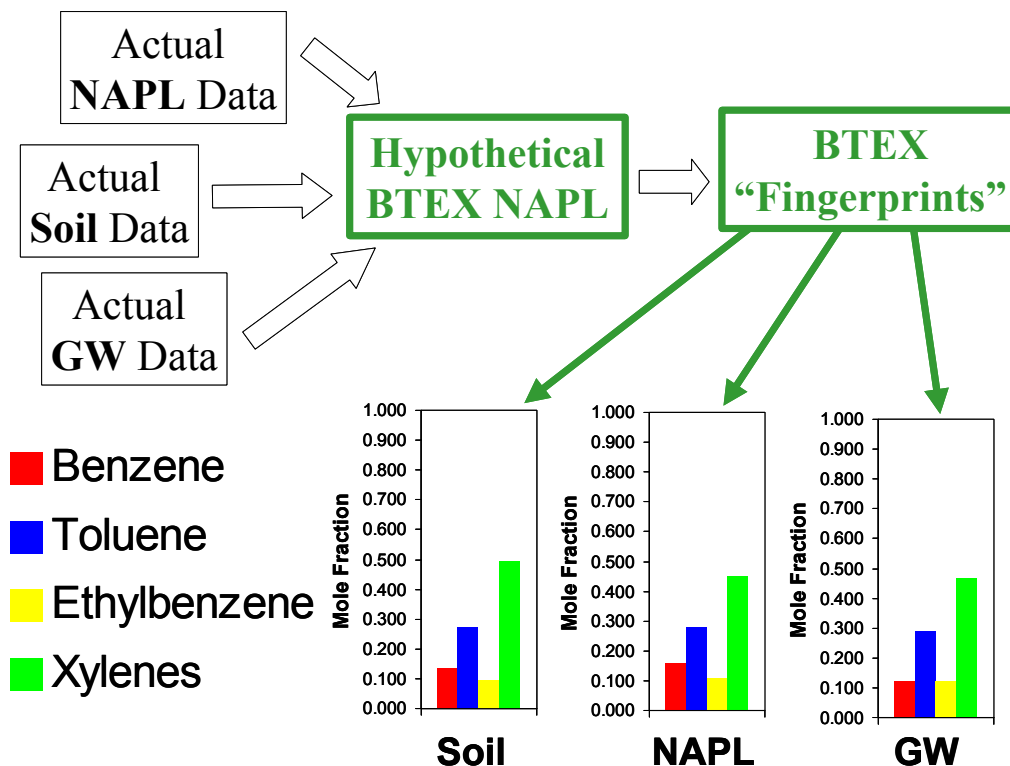
Comparing “Apples” to “Apples” with Ground-water, NAPL, and Soil Data

Subtitle: Conversion of NAPL, Soil, and Ground-water Data to Common Frames of Reference using the Effective NAPL Solubility Relationship

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At sites where non-aqueous phase liquids (NAPL) (*e.g.*, petroleum products) have caused ground-water contamination, it is often necessary to discern the contributions of several NAPL releases. Soil, ground-water, and, possibly, NAPL data are generally available at these sites. However, directly comparing this data to determine source contributions can be difficult since they are from three different phases (soil, ground water, and NAPL), plus dilution has taken place (*i.e.*, the data have different “frames of reference” with respect to phase and dilution). Essentially, with the different frames of references for the soil, ground-water, and NAPL data, we’re comparing “apples” to “oranges”. Luckily, there are data conversions we can make to get all three types of data to a common frame of reference, thus we get to where we can compare “apples” to “apples”.

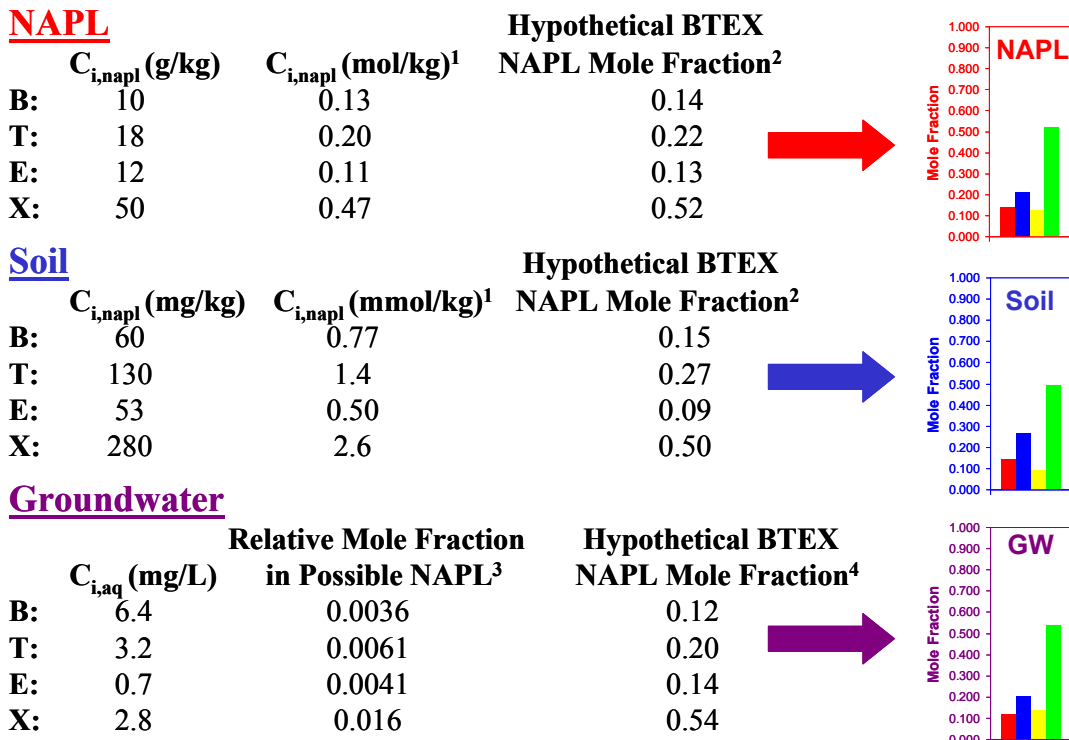
As an example, at most gasoline spill sites we often have benzene, toluene, ethylbenzene, and xylene (BTEX) data for NAPL, soil, and ground-water samples. What we can do is take the actual field data and convert them to BTEX “fingerprints” with common frames of reference, so that they can be directly compared to one another.



NAPL and soil concentration data can be directly converted to relative mole fraction units in a corresponding NAPL phase. Ground-water data can be converted to relative mole fraction units in a corresponding NAPL phase by using the effective NAPL solubility relationship:

$$C_{i, \text{aq}} = X_{i, \text{napl}} C_{i, \text{aq}}^{\circ}$$

$C_{i, \text{aq}}$ is the concentration of the i^{th} component (hydrocarbon) in ground water. $X_{i, \text{napl}}$ is the mole fraction of the i^{th} component in NAPL. $C_{i, \text{aq}}^{\circ}$ is the pure compound solubility of the i^{th} component in water. The NAPL, soil, and ground-water data are now in a common frame of reference with respect to phase (all are converted to a corresponding NAPL phase), however, the extent of dilution is still different for each. To account for dilution, a hypothetical n-component NAPL is created (in this instance, $n = 4$ where benzene, toluene, ethylbenzene, and xylene are the 4 components), and the relative mole fractions are converted to mole fractions in the hypothetical n-component NAPL. The following shows how to convert actual NAPL, soil, and ground-water field data to get BTEX “fingerprints”:



¹ Divide by molecular weight (g/mol or mg/mmol) to get mol/kg or mmol/kg.

² Divide by total BTEX mol/kg or mmol/kg to get mole fraction (mf).

³ Divide by pure compound solubility (mg/L) to get relative mf in possible NAPL.

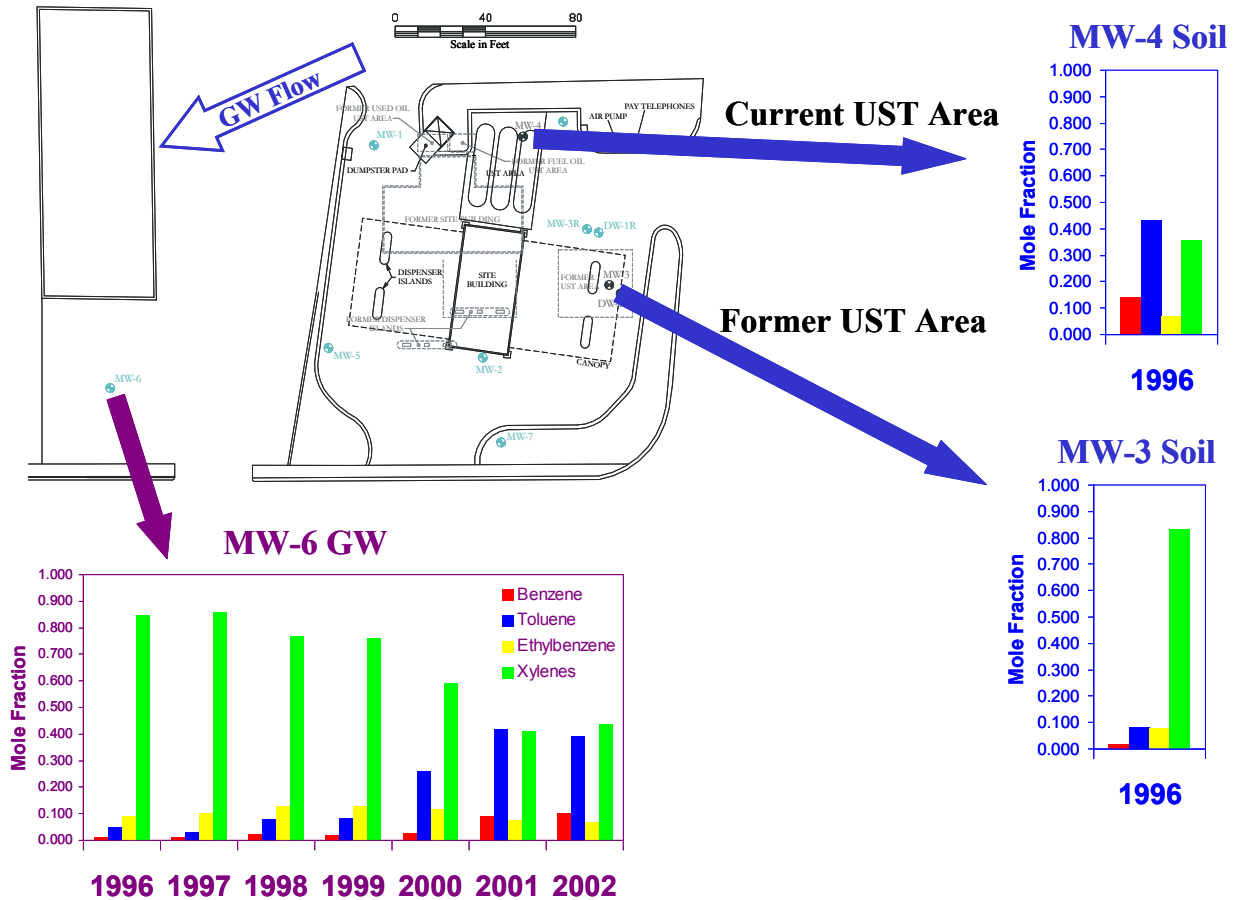
⁴ Divide by total of BTEX relative mf to get mf in hypothetical NAPL.

Component	MW (g/mol or mg/mmol)	$C_{i, \text{aq}}^{\circ}$ (mg/L)
Benzene	78.06	1790
Toluene	92.14	526
Ethylbenzene	106.2	169
Xylenes	106.2	175

Assuming negligible confounding affects of biodegradation (which may be the case near the NAPL source area), the hypothetical n-component NAPL mole fractions for the NAPL, soil, and ground-water data can now serve as ‘fingerprints’ for direct comparison, thus comparing “apples” to “apples.” The following case history helps to illustrate how this data analysis procedure can be used to help resolve a liability issue.

Case History: Demonstration of Multiple Sources

A retail gasoline site was sold and refurbished in 1995. A discharge was suspected in 1996, which led to a site investigation where monitoring wells were installed and soil boring samples were taken. BTEX analysis of the samples was performed. NAPL sheens were periodically observed in some of the monitoring wells, but unfortunately samples of the NAPL sheens were not taken. Subsurface conditions were anoxic and alternate electron acceptor concentrations were low, thus natural attenuation (biodegradation) was occurring slowly. Ground-water samples were taken annually. The situation posed specific liability questions for the current and previous owners, so the hypothetical NAPL data analysis procedure was applied.



BTEX “fingerprints” were obtained for the soil and ground-water samples. MW-6 ground-water BTEX “fingerprints” were representative of soil from the former UST area until 1999. After 2000, however, MW-6 ground-water BTEX “fingerprints” resembled the soil from the current UST area more closely. Thus, contributions from both UST areas were clearly evident in the downgradient MW-6 ground-water data.

Directly comparing NAPL, soil, and ground-water data to determine source contributions can be difficult since they are from three different phases (soil, ground water, and NAPL), plus dilution has taken place. Soil, ground-water, and NAPL data have different frames of reference, so we’re comparing “apples” to “oranges”. Using the data conversions presented all three types of data can be put into a common frame of reference. Thus, we’re able to compare “apples” to “apples,” assuming negligible confounding effects due to biodegradation. A greater understanding can be gained from available field data using this data analysis procedure. The data analysis procedure presented can be applied not only to petroleum spills but also to any NAPL release, thus providing a powerful tool for defensible data interpretation.

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