6.4.1 Multiple Solutes

- Solubility is reduced where multiple hydrophobic components are encountered.
- Concentration is lower than if solute is alone.

$S_i^e = X_i \, S_i$

S_i = pure phase solubility, (mg/L) for compound i

X_i = mole fraction of component i in DNAPL

ie Lab analysis of source

Mole fraction = $\frac{\text{Moles of compound } i}{\text{Total moles of soln.}}$

* Mole fraction since solubility controlled by available molecules

S_i^e = effective solubility of i

- Effective solubility is an upper theoretical bound
- Does not account for co-solvency and other non-ideal behaviours

Smithville

Compound	"Free phase" %by wt	Formula Wt (g)	Moles per 100g of cocktail	Mole fraction X_i	Pure phase Solubility (mg/L)	S_i^e
TCE	2%	131.4	$\frac{2}{131}$ = 0.0152	$\frac{.0152}{.677}$ = 2.2%	1060	23
TCB	10	181.45	.055	8.12%	19	1.5
PCB	50	220 (average)	.227	33.5%	.2	.0
Mineral oils	38	100 (guess)	.38	56.1%		
			.677			

.677 = moles per 100g

i.e. $.677 \times 10^{23}$ molecules

1 mg/L = 1 ppm.

Mole of substance = formula wt in g.

Moles of solute per liter of solution = MOLARITY = $\frac{\text{Density}}{\text{Formula wt}}$

Water = $\frac{1000\text{ g/L}}{(16+2)}$ = 55.

Worksheet 7-1: Calculation of Effective Solubility (from Newell and Ross, 1992; after Shiu et al., 1988; and Feenstra et al., 1991)

For a single-component DNAPL, the pure-phase solubility of the organic constituent can be used to estimate the theoretical upper-level concentration of organics in aquifers or for performing dissolution calculations. For DNAPLs comprised of a mixture of chemicals, however, the effective solubility concept should be employed:

$$S^e_i = X_i S_i$$

where

S^e_i = the effective solubility (the theoretical upper-level dissolved-phase concentration of a constituent in groundwater in equilibrium with a mixed DNAPL; in mg/l)

X_i = the mole fraction of component i in the DNAPL mixture (obtained from a lab analysis of a DNAPL sample or estimated from waste characterization data)

S_i = the pure-phase solubility of compound i in mg/l (usually obtained from literature sources)

For example, if a laboratory analysis indicates that the mole fraction of trichloroethylene (TCE) in DNAPL is 0.10, then the effective solubility would be 110 mg/l. This is derived by multiplying the pure phase solubility of TCE by the TCE mole fraction:

$$1100 \text{ mg/l} * 0.10 = 110 \text{ mg/l}$$

Effective solubilities can be calculated for all components in a DNAPL mixture. Nearly insoluble organics in the mixture (such as long-chained alkanes) will reduce the mole fraction and effective solubility of more soluble organics, but will contribute little dissolved-phase organics to groundwater.

Please note that this relationship is approximate and does not account for non-ideal behavior of mixtures, such as co-solvency, etc.