C41 Cosolvency

James S. Smith, PhD, Trillium, Inc., 28 Grace's Drive, Coatesville, PA 19320*

After attending this presentation, attendees will understand that water insoluble organic chemicals are rarely made more soluble in water when co-deposited with a water-soluble solvent(s).

This presentation will impact the forensic community and/or humanity by explaining that higher than expected concentrations of a water-insoluble organic chemical in water should not be attributed to cosolvency without extraordinary proof.

Cosolvency has been used to explain why water-insoluble organic compounds are found at concentrations significantly above their equilibrium water-soluble concentrations in groundwater. This has been especially true for polychlorinated biphenyls (PCBs). For example, assume that PCBs and a chlorinated solvent such as trichloroethene (TCE) were discarded together. Now, in a groundwater sample from the monitoring well, one finds concentrations of PCBs that exceed the water solubility for PCBs. The explanation used for the higher than expected concentrations of PCBs is cosolvency. In other words, it was assumed that higher concentrations of PCBs such as Aroclor 1260 in water were caused by the ability of TCE or another solvent to carry the PCBs into the water solution and hold the PCBs in a soluble form.

However, research and recent publications[1,2,3,4] show that cosolvency rarely occurs and certainly not with TCE and PCBs. What does occur is that the solvent "salts out" or decreases the water solubility of the PCBs. The equilibrium solubility of PCBs is lowered by the presence of a solvent in the groundwater until the solvent reaches percent values. The solvent does not increase the solubility of insoluble materials such as PCBs in the groundwater.

Is that the end of the story? Of course not. In another example, the Stringfellow lagoons above Glen Avon, California, contained cutting oils that migrated through the aquifer. How is that possible? Cosolvency is the answer here. At the Stringfellow site, there were high concentrations of detergents from water-soluble cutting oils which were used to solubilize oil in water. They continued to do their job in the aquifer material. Although these oils were never reported on the laboratory data sheets from analyses of the water being transported through aquifer material from the lagoons toward Glen Avon, they were confirmed to be present based on the total ion chromatograms from the semivolatile organic compounds analyses.

It is obvious that forensic investigations need to consider cosolvency, but the regulatory analytical chemistry tests required for an investigation are not always the tests necessary to demonstrate cosolvency. Cosolvency must be carefully proven scientifically before it is used as an explanation for the forensic investigation.

[1] Coyle, G.T., T.C. Harmon, and I.H. Suffet, "Aqueous Solubility Depression for Hydrophobic Organic Chemicals in the Presence of Partially Miscible Organic Solvents," Environmental Science & Technology, Vol. 31, pp. 384-389, 1997.

[2] Munz, Christoph and Paul V. Roberts, "Effects of Solute Concentration and Cosolvents on the Aqueous Activity Coefficient of Halogenated Hydrocarbons," Environmental Science & Technology, Vol. 20, pp. 830-836, 1986.

[3] Groves, Jr., Frank R, "Effect of Cosolvents on the Solubility of Hydrocarbons in Water," Environmental Science & Technology, Vol. 22, pp. 282-286, 1988.

[4] Ulrich, Glenn, "Fate and Transport of Ethanol-Blended Gasoline in the Environment," Governer's Ethanol Coalition, pp. 15-16, October 1999.

Cosolvency, Water Solubility, Salting Out

** Presenting Author*