C26 First-Order Exponential Regression of Ethylbenzene/Xylenes Ratios for Estimating Release Date

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After attending this presentation, attendees will understand how to evaluate petroleum hydrocarbon data to estimate release or significant source reduction date, support a new from old release determination, and indicate the potential for free phase conditions.

This presentation will impact the forensic community and/or humanity by adding to the arsenal of petroleum hydrocarbon release site investigation techniques, using typically available or easily obtainable chemical analysis data to investigate site conditions and release timing. This research has direct impact on who is the liable party and what funding is available for contaminant cleanup.

A model is proposed to estimate a "petroleum hydrocarbon release or significant source reduction date range" (RDR) based on groundwater time series data exhibiting anaerobic, first-order exponential biodegradation decay. Groundwater monitoring data for sites with known release or source termination/reduction dates are compared with model predictions.

Gasoline, kerosene, diesel, and heating oil have composition ratios of ethylbenzene to xylenes of approximately 0.17 ± 0.05. Upon a release, typically aerobic bacteria rapidly use the available oxygen and drive the release environment anaerobic. Ethylbenzene and xylenes are C_2 benzene compounds that have nearly identical boiling points, vapor pressures, water solubilities, and carbon-water sorption coefficients. Therefore, the major fate mechanisms of evaporation and water washing and transport mechanism of groundwater velocity retardation treat ethylbenzene and xylenes alike. Anaerobic biodegradation will remove xylenes faster than ethylbenzene and the ratio of ethylbenzene to xylenes (EXR) in groundwater will increase with time.

Petroleum hydrocarbon biodegradation can be reasonably simulated using first-order exponential approximations. The ratios of these hydrocarbons will also follow first-order exponential approximations. Given the 1) difference in ethylbenzene and xylenes biodegradation rates and 2) similar properties and fate and transport will not significantly effect the EXR over time, simulating the EXR using a first-order exponential approximation will eliminate the need to know the initial ethylbenzene and xylenes release concentrations and allow for modeling the observed groundwater data to predict a RDR using a minimum (0.17 - 0.05 = 0.12) and maximum (0.17 + 0.05 = 0.22) initial EXR representing a new release.

Ethylbenzene and xylenes groundwater monitoring data that exhibit anaerobic, first-order exponential biodegradation decay are used to estimate a RDR, or at least indicate the release could not have occurred after the estimated RDR, that were in reasonable agreement with known release and source reduction dates. The field examples suggest that regression analysis of post release data can be used or obtained to provide a reasonable estimate of the RDR, without the need for early time data. Historic EXR data are modeled and projected forward in time to support a new from old release determination. EXR data not showing an increasing trend and remaining near the range anticipated for a new release are associated with an example of intermittent free product conditions suggesting a means to indicate the continuing presence of free phase hydrocarbons and significant source material.

Petroleum, Release, Date

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