

Arey, J.S., Nelson, R.K., Xu, L., and Reddy, C.M., *Estimating partitioning properties for a complete set of diesel fuel hydrocarbons using comprehensive two-dimensional gas chromatography retention indices*, Analytical Chemistry, 2005; v77, pp. 7172-7182

Comprehensive two-dimensional gas chromatography (GCxGC) provides nearly complete composition data for some complex mixtures such as petroleum hydrocarbons. However, the potential wealth of physical property information contained in the corresponding two-dimensional chromatograms is largely untapped. We developed a simple but robust method to estimate GCxGC retention indices for diesel-range hydrocarbons. By exploiting n-alkanes as reference solutes in both dimensions, calculated retention indices were insensitive to uncertainty in the enthalpy of gas-stationary-phase transfer for a suite of representative diesel components. We used the resulting two-dimensional retention indices to estimate the liquid vapor pressures, aqueous solubilities, air-water partition coefficients, octanol-water partition coefficients, and vaporization enthalpies of a nearly complete set of diesel fuel hydrocarbons. Partitioning properties were typically estimated within a factor of 2; this is not as accurate as some previous estimation or measurement methods. However, these relationships may allow powerful and incisive analysis of phase-transfer processes affecting petroleum hydrocarbon mixtures in the environment. For example, GCxGC retention data might be used to quantitatively deconvolve the effects of water washing and evaporation on environmentally released diesel fuels.