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ESTIMATING THE FATE OF AQUATIC CONTAMINANTS USING A FUGACITY BASED MODEL

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ABSTRACT: Interest in environmental contaminants, initially focused on pesticides, has grown since the early 1960's. Recognition of the widespread dispersal of industrial contaminants, especially the PCBs, led to the Toxic Substances Control Act and the Clean Water Act "Priority Pollutant" list. Disinfection by-products in potable water systems added new concerns that have been addressed under the Safe Drinking Water Act. More recently, the finding of pharmaceuticals and personal care products (PPCPs) in effluents and surface waters, particularly by the USGS, has added a new dimension to the aquatic contaminant story. Many legacy pesticides and industrial chemicals have limited water solubilities, leading to relatively high concentrations in biota and sediments. The PPCPs, in contrast, while currently present at very low (ng/L to µg/L) concentrations, appear to be more soluble than the legacy chemicals, and are detected at these low concentrations by modern HPLC/MS instrumentation. Many of these chemicals are bioactive, and some have shown to be endocrine disruptors in certain aquatic species. As a result, increased attention is being given to contaminants, not just to the current PPCPs but also to many of the legacy compounds, which, as a group, have been labeled "emerging contaminants" (ECs) or "re-emerging contaminants." The question arises: "Is there a way to quickly estimate and/or evaluate the possible fate (i.e. the preferred environmental compartment(s) under steady state conditions) of chemicals in the environment?"The response is "yes" as long as there are fundamental physical-chemical data available, such as a compound's aqueous solubility, vapor pressure, octanol-water partition constant (Kow) and various kinetic rate constants (photolysis, sorption, etc.) expressed in first order units. Given sufficient data, a fugacity model (pioneered by Donald Mackay and colleagues) can evaluate the likely fate of a chemical in the environment. The model provides useful initial guidance on environmental fate, especially if sufficient physical-chemical data are available or can be reasonably be estimated for a given compound. Example fugacity model level III calculations and projected steady-state aquatic fate compartments will be demonstrated for contaminant categories such as legacy pesticides, industrial chemicals, disinfection by-products and PPCP compounds.

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