

Fugacity-Based Modeling of the Environmental Fate and Transport of Emerging Contaminants

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Pharmaceuticals and personal care products (PPCPs) are of emerging environmental concern because of their potential for endocrine disruption at a very low chronic exposure level. Recently, many reports have been published regarding the environmental occurrence of these emerging contaminants in water, soil, sediment and biota in Europe and the United States. Fugacity-based models play an important role in assessment of the fate and transport of PPCP emissions to the environment.

In this talk, an analysis is presented of the environmental fate and emission rates of 30 PPCPs listed in the National Reconnaissance of the United States Geological Survey (USGS) as the most frequently detected organic wastewater contaminants in U.S. streams and rivers. The so-called USGS 30 include pharmaceuticals, antibiotics, organic wastewater metabolites and estrogenic compounds. The mass distributions, loss pathways, and surface water concentrations of the USGS 30 compounds were computed for a county-sized model environment using Level II and Level III steady-state fugacity models.

It was found that the USGS 30 compounds can be categorized into three groups based upon their phase partitioning behavior and the sensitivity of their predicted surface water concentrations to the chemical properties and landscape parameters used as inputs to the model. Moreover, it is observed that many USGS 30 compounds exhibit physicochemical properties that depart significantly from those of traditional chemicals of Superfund interest such as halogenated solvents and persistent organic pollutants (POPs). Hence, conventional treatment strategies such as air stripping or adsorption on activated carbon may be unsuitable for the removal of USGS 30 compounds from wastewater.

Brominated flame retardants (BFRs) comprise another class of emerging contaminants upon which much attention has recently been focused, due to the propensity of BFRs to bioaccumulate, and speculation that these compounds may also act as endocrine disruptors. A transient (Level IV) fugacity model is presented that interprets the fate of hexabromobiphenyl emissions into Lake Huron during the 1970s from the Michigan Chemical Corporation's Pine River manufacturing facility. The Level IV model is also used to project the current emission rates of BDE-47, a tetrabrominated diphenyl ether flame retardant, into the Great Lakes from non-point sources.