Lumping analysis for abiotic transport modeling of an organic pollutant mixture

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Abstract. Environmental contamination often results in the presence of mixtures of compounds in the subsurface. The presence of contaminant mixtures poses challenges for accurate risk assessment and effective risk management, particularly since predicting the fate and transport of a mixture is very difficult. Thus, the primary goal of this study is to model the fate and transport of organic compound mixtures using lumping analysis which describes the fate and transport of multicomponent mixture in terms of a few lumped pseudocompounds that approximates the properties of the detail mixture.

In view of the inherent complexity of heterogeneous natural organic matter (NOM) and mineral systems, well-characterized mineral surfaces and reference NOM were utilized and manipulated to elucidate the role of humic coatings and mineral surfaces in the sorption of compound mixtures to low-carbon aquifer materials. The mixture compounds were comprised of 12 organic compounds including alkyl-substituted benzenes, alkyl-substituted phenols, ketones, and chlorobenzenes.

Batch equilibrium sorption tests evaluating sorption of the individual chemicals and their mixtures to untreated, humic acid-coated, humified via peroxidase-mediated oxidative coupling, iron (aluminum) hydroxide-coated, and iron (aluminum) hydroxide and humic acid-coated natural model sorbents have been conducted. Experimental data reveal that sorption equilibrium to all sorbents except the humified sorbents was attained less than 24 h for both polar and nonpolar compounds, indicating that intraorganic matter diffusion is the rate-limiting sorption regime. While sorption isotherms of nonpolar compounds were linear or near linear except with humified sorbents, those of polar compounds to all sorbents were nonlinear. Although variations in organic carbon partition coefficient (K_{oc}) values for polar compounds were greater than those for nonpolar compounds, the affinity of NOM for all compounds significantly depends on the content and structure of NOM. In addition, mixture effects for nonpolar compounds were minimal except with the humified sorbents.

Statistical methods (cluster analysis and multidimensional scaling) were used to group the compound mixtures, and these groups changed in a logical manner and can be characterized by the properties of the NOM, the mineral composition of sorbents, and the properties of the individual mixture components. Therefore, the lumping approach may help to simplify the complex fate and transport model of mixtures of organic compounds, reduce experimental efforts, and yet provide results that are sufficiently accurate for practical purposes.

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