

## ACS Required Short Abstract

### Modeling Biogeochemical Interactions in Co-Contaminant Systems

**Jeanne M. VanBriesen**

Carnegie Mellon University  
Department of Civil and Environmental Engineering  
Porter Hall 119  
Pittsburgh, PA 15213

**Bruce E. Rittmann**

Northwestern University  
Department of Civil Engineering  
2145 Sheridan Road  
Evanston, IL 60208-3109

#### Abstract

Complex interactions among chemical and biological processes affect contaminant fate and transport. Mixtures of contaminants present special challenges to predictive modeling. The recently developed batch biogeochemical model, CCBATCH, explicitly considers the effect of aqueous speciation on biodegradation reactions and the effect of biological reactions on the concentration of chemical species (e.g.,  $\text{H}_2\text{CO}_3$ ,  $\text{NH}_4^+$ ,  $\text{O}_2$ ). Aqueous speciation reactions including complexation and acid/base are modeled by assuming thermodynamic equilibrium. Biological reactions are modeled using a dual-Monod kinetic formulation coupled to stoichiometric representations for substrate removal, cell growth, and cell decay. The coupling of chemical and biological reactions allows systematic investigation of complex interactions that affect behavior of co-contaminants. The capability of CCBATCH to couple aqueous speciation changes to biodegradation reaction kinetics and stoichiometry is demonstrated in mixed metal/chelate systems.

**KeyWords:** biogeochemistry, biodegradation, modeling, coupled processes