# Characterization of the Microbially-Driven Fenton Degradation of Chlorinated Compounds Using a Modeling Approach

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**Background/Objectives.** The microbially-driven Fenton degradation of TCE and PCE as well as other contaminants such as 1,4-dioxane represents a promising bioremediation strategy for the degradation of chlorinated and non-chlorinated organic solvents in contaminated subsurface environments. In this bioremediation process, peroxide is produced via microbial aerobic respiration during an aerobic phase, whereas Fe(II) is produced via microbial Fe(III) reduction of solid iron oxide substrates during an anaerobic period without the need for continual addition of peroxide and Fe(II) to drive hydroxyl radical production. Previous batch liquid cultures of the facultative anaerobe *Shewanella oneidensis* amended initially with Fe(III) citrate, lactate, and contaminants and exposed to alternate aerobic and anaerobic conditions by purging air and dinitrogen gas have demonstrated complete degradation of TCE, PCE, and 1,4-dioxane either as single contaminant or commingled contaminants. The objective of this study was to characterize the network of microbially-driven Fenton reactions and simultaneous degradation of these contaminants using a modeling approach.

**Approach/Activities.** A mathematical model representing the network of possible reactions involved in these batch reactor experiments was developed to diagnose our understanding of the processes taking place when *S. oneidensis* is exposed to redox oscillations. The reactions involved include Fenton-driven iron chemistry, Fe(III) hydrolysis, termination reactions of reactive oxygen species (ROS), microbial respiration of Fe(III) citrate and Fe(III) oxide minerals with lactate as electron donor during the anaerobic phase, microbial respiration of dissolved oxygen with lactate and acetate as electron donor during the aerated phase, and the degradation of the organic contaminants. A total of 6 microbial and 9 chemical reactions regrouping 13 chemical species were combined in a network of rate laws that were solved simultaneously using a Runge-Kutta numerical scheme and mass balance equations.

**Results/Lessons Learned.** These simulations reproduced the redox oscillations rather well for each contaminant incubated independently or commingled. The microbial transformation of lactate and acetate was reproduced by adjusting the kinetic parameters linked to aerobic respiration in the oxic phase and the anaerobic respiration of Fe(III). Fe(III) citrate added to the reactors initially appeared to be completely reduced in the first 24 hours. However, the evolution of Fe(II) after the first anaerobic-aerobic cycle suggested that Fe(II) produced during the first anaerobic phase was oxidized to a different form of Fe(III) during the oxygenation phase. The model results also revealed that the kinetics of production and consumption of ROS during the oxic phase was much smaller than predicted from the literature, suggesting that side reactions involving ROS even in simple batch liquid cultures may play an important role in the degradation of chlorinated contaminants.