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Microbially enhanced dissolution and reductive dechlorination of PCE by a mixed culture: Model validation and sensitivity analysis

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ABSTRACT

Reductive dechlorination catalyzed by organohalide-respiring bacteria is often considered for remediation of non-aqueous phase liquid (NAPL) source zones due to cost savings, ease of implementation, regulatory acceptance, and sustainability. Despite knowledge of the key dechlorinators, an understanding of the processes and factors that control NAPL dissolution rates and detoxification (i.e., ethene formation) is lacking. A recent column study demonstrated a 5-fold cumulative enhancement in tetrachloroethene (PCE) dissolution and ethene formation (Amos et al., 2009). Spatial and temporal monitoring of key geochemical and microbial (i.e., *Geobacter lovleyi* and *Dehalococcoides mccartyi* strains) parameters in the column generated a data set used herein as the basis for refinement and testing of a multiphase, compositional transport model. The refined model is capable of simulating the reactive transport of multiple chemical constituents produced and consumed by organohalide-respiring bacteria and accounts for substrate limitations and competitive inhibition. Parameter estimation techniques were used to optimize the values of sensitive microbial kinetic parameters, including *maximum utilization rates*, *biomass yield coefficients*, and *endogenous decay rates*. Comparison and calibration of model simulations with the experimental data demonstrate that the model is able to accurately reproduce measured effluent concentrations, while delineating trends in dechlorinator growth and reductive dechlorination kinetics along the column. Sensitivity analyses performed on the optimized model parameters indicate that the rates of PCE and *cis*-1,2-dichloroethene (*cis*-DCE) transformation and *Dehalococcoides* growth govern bioenhanced dissolution, as long as electron donor (i.e., hydrogen flux) is not limiting. Dissolution enhancements were shown to be independent of *cis*-DCE accumulation; however, accumulation of *cis*-DCE, as well as column length and flow rate (i.e., column residence time), strongly influenced the extent of reductive dechlorination. When *cis*-DCE inhibition was neglected, the model over-predicted ethene production ten-fold, while reductions in residence time (i.e., a two-fold decrease in column length or two-fold increase in flow rate) resulted in a more than 70% decline in ethene production. These results suggest that spatial and temporal variations in microbial community composition and activity must be understood to model, predict, and manage bioenhanced NAPL dissolution.

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1. Introduction

Chlorinated solvents (e.g., tetrachloroethene [PCE], trichloroethene [TCE]), are widely used in industrial processes, and at military installations and government facilities, and have often been released as dense non-aqueous phase liquids (DNAPLs). DNAPL dissolution, whether from pools retained above or within low-permeability strata or from residual saturation ganglia trapped in the porous soil or rock matrix, creates a persistent source of groundwater contamination. In the past two decades, numerous remediation technologies have been developed to treat DNAPL source zones; however, the ability of a single technology to completely remove or destroy all DNAPL mass and reduce dissolved-phase contaminant concentrations below drinking water standards is limited. Among potential in situ remediation technologies, microbial reductive dechlorination has emerged as an attractive plume remedy, and an approach to enhance rate-limited contaminant mass transfer at sites where contaminants are sequestered in low permeability zones (e.g., Scheutz et al., 2010) or present in DNAPL source zones (Da Silva et al., 2006; Schaefer et al., 2010; Sleep et al., 2006). In these applications microbial reductive dechlorination may also serve as a source zone polishing step to control residual contaminant concentrations following aggressive physicochemical treatment (Christ et al., 2005; Mravik et al., 2003; Ramsburg et al., 2004). During DNAPL source zone bioremediation, microbial activity serves to lower dissolved-phase contaminant concentrations, thereby increasing the driving force for contaminant dissolution from the nonaqueous to the aqueous phase, a process commonly referred to as bioenhanced dissolution (Adamson et al., 2003; Amos et al., 2008; Cope and Hughes, 2001; Glover et al., 2007; Sleep et al., 2006; Yang and McCarty, 2000, 2002). While dissolution enhancements can lead to short term increases in dissolved phase transformation products (i.e., *cis*-DCE), the overall source longevity and associated cleanup times decrease, potentially resulting in reduced long-term risk.

Results obtained from batch, column, and aquifer cell experiments indicate that the extent of DNAPL dissolution enhancement due to bioactivity can vary widely, from a negligible effect to a more than 20-fold increase (e.g. Amos et al., 2008, 2009; Carr et al., 2000; Cope and Hughes, 2001; Philips et al., 2011; Schaefer et al., 2010; Sleep et al., 2006; Yang and McCarty, 2000). This variability in dissolution enhancement has been attributed to several factors, including differing microbial populations, electron donor limitations, competitive and threshold inhibitions, and competitor populations (e.g., methanogens), as well as changing flow conditions due to gas formation, microbial growth, and experimental design. While bench-scale experiments provide excellent demonstrations of the conditions leading to bioenhanced DNAPL dissolution (e.g., Amos et al., 2009; Schaefer et al., 2010), their use as a design tool for treatment applications in the field is limited. Numerical simulators provide a complementary tool that allows for more efficient assessment of individual parameters and inter-related processes impacting microbial activity, guiding future efforts to understand and optimize in situ bioenhanced dissolution.

Prediction of bioenhanced DNAPL dissolution requires a model that quantifies inter-relationships between dechlorination and mass transfer processes. A number of models capable of simulating organohalide respiration kinetics have been presented in the literature that incorporate electron donor flux (i.e., fermentation) and competition (i.e., methanogenesis) (e.g. Bagley, 1998; Becker, 2006; Becker and Seagren, 2009; Fennell and Gossett, 1998; Haest et al., 2010; Huang and Becker, 2009, 2011; Kouznetsova et al., 2010; Lee et al., 2004; Sabalowsky and Semprini, 2010a,b; Yu and Semprini, 2004; Yu et al., 2005). These models, however, are limited to the simulation of dechlorination in batch reactors or single-phase, aqueous systems. While several models that include both dechlorination and dissolution have been presented (Chambon et al., 2010; Chu et al., 2003; Hammond et al., 2005; Widdowson, 2004), those models have only been applied to simplified systems (e.g., no dissolution) and thus, have not considered the potential influence of a diminishing DNAPL mass on the temporal and spatial evolution of the mobile aqueous phase flow and microbial activity. Although a number of multi-phase, multi-component simulators have been adapted to model organohalide respiration in DNAPL source zones (Abriola et al., 1997; Battisstelli, 2004; Clement et al., 2004; Delshad et al., 1996; Rathfelder et al., 2000; Willis and Shoemaker, 2000), very few studies (Becker and Seagren, 2009; Christ and Abriola, 2006) have explored dissolution enhancements due to microbial activity. Christ and Abriola (2006) adapted a multiphase compositional simulator (e.g., MISER — Michigan Subsurface Environmental Remediation Simulator) to incorporate dynamic interphase mass transfer, non-linear dechlorination kinetics, microbial inhibition, and competition in a framework that is capable of simulating two-dimensional non-uniform source zones. Their comparisons to available data indicated that the model was capable of capturing effluent concentrations consistent with bioenhanced dissolution. However, these data were limited to the PCE-to-*cis*-DCE dechlorination step, and did not provide the information necessary to fully calibrate and validate the model. The resulting simulations were thus hypothetical in nature and provided limited insight into the fundamental factors controlling bioenhanced dissolution efficacy within a source zone, including conditions leading to incomplete or stalled reductive dechlorination, a frequent limitation of bioremediation during field application.

A continuous-flow column experiment (Amos et al., 2009), instrumented to quantify aqueous phase constituent concentrations (e.g., organic acids, PCE, TCE, *cis*-DCE, vinyl chloride [VC], ethene) and the distributions of key dechlorinating populations (i.e., *Geobacter lovleyi* strain SZ [GEOSZ] and *Dehalococcoides mccartyi* [DHC]) along the length of the column, provides a novel, high resolution data set to elucidate factors controlling bioenhanced dissolution and reductive dechlorination within DNAPL source zones and associated down-gradient plume regions. In this work, the experimental results of Amos et al. (2009) are compared to model simulations to: (i) examine the ability of a state-of-the-art mathematical model to simulate spatial and temporal changes in bioenhanced dissolution and reductive dechlorination; (ii) quantify microbial transformation, utilization, and growth rates using parameter estimation techniques; and (iii) identify and assess system parameters most influential in controlling bioenhanced dissolution and reductive dechlorination within a DNAPL source zone. Knowledge gained from the analysis of the relative importance of system parameters to each step of

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