Modeling Microbial Reductive Dechlorination in a Heterogeneous Laboratory Aquifer Cell

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Although microbial reductive dechlorination has proven to be an effective approach for in situ treatment of trichloroethene (TCE), field implementation of this technology is complicated by many factors, including subsurface heterogeneity, electron donor availability, and distribution of microbial populations. While numerous studies have utilized numerical models to assess dechlorination rates in uniform, well-characterized, laboratory (e.g., batch and column) systems, successful application of these rates for predictions of field-scale degradation has been hampered by the presence of natural subsurface variability. Thus, there is an urgent need to improve our understanding of the influence of heterogeneity on “effective” transformation rates and to explore the relationship between effective and laboratory-measured rates.

This work describes the mathematical modeling of a bioremediation experiment conducted in a laboratory -scale aquifer cell that was packed with materials from the Commerce Street Superfund site in Williston, VT, configured to mimic site conditions. Modeling results reveal that application of microcosm (liquid-to-soil volume ratio of 4:1)-derived dechlorination, and microbial growth and decay rates for TCE, cis-1,2-dichloroethene (cis-DCE), and vinyl chloride (VC) reproduced measurements of aquifer cell concentrations. Normalized root mean square errors for predicted and measured effluent concentrations were 18.1%, 23.2%, 51.0%, 36.6% and 16.7% for TCE, cis-DCE, VC, ethene and lactate (electron donor and carbon source), respectively. Additional simulations, comparing predictions for the heterogeneous domain with those for a homogeneous (averaged permeability, porosity, and initial concentrations) domain, demonstrate that an assumption of uniformity resulted in incomplete dechlorination (i.e., “cis-DCE stall”) and underprediction of VC and ethene by factors of 2 and 3. This underprediction of transformation rates contrasts with the literature, which commonly reports model overprediction of observed field-scale dechlorination. These results suggest that ethene formation varied spatially within the domain and was primarily associated with zones with longer residence times, demonstrating the influence of local heterogeneity on dechlorination.

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