Modeling Microbial Oxidation of Vinyl Chloride Under Simulated Field Conditions

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Background/Objectives. Reductive dechlorination of solvents, such as PCE and TCE, often result in the accumulation of vinyl chloride (VC). Complete reductive dechlorination of VC to ethene is possible, but often challenging and costly. Microbial oxidation is a promising alternative or complementary strategy. The existence of vinyl chloride-oxidizing bacteria is well known, and there is evidence from field studies that these organisms play a role in attenuating VC plumes. One study has shown that these organisms can oxidize VC under low dissolved oxygen concentrations, suggesting that this process may be more important than currently appreciated. Microbial VC oxidation appears to be a common natural process that could proceed without intervention, which supports the use of monitored natural attenuation (MNA) as a remedial alternative for VC. However, regulatory acceptance of MNA requires demonstrating a sound basis for success in a reasonable time frame. Such a basis may include using a mathematical model to simulate contaminant degradation processes and rates.

No model currently exists for the estimation of VC-oxidation rates in the field. Kinetic studies have been performed in the lab using pure cultures under a narrow range of conditions, and are thus of limited value for MNA. A recent field study has demonstrated a semi-quantitative relationship between observed bulk VC attenuation rates and the abundance of VC-oxidizing bacteria, as determined through quantitative polymerase chain reaction (qPCR) measurements targeting the VC-oxidation functional genes *etnC* and *etnE*.

The objective of this study is to develop a model of VC oxidation that can be applied as part of a MNA strategy. This model will be unique, as it will utilize VC-oxidation functional genes as a specific measurement of active biomass that can be measured from field samples. It will also include important field parameters such the VC and oxygen concentrations, pH, and temperature.

Approach/Activities. Groundwater has been collected from three VC contaminated sites and used to establish VC-utilizing enrichment cultures. A series of studies will be conducted in which these cultures will be grown under varying conditions (substrate concentration, pH, etc.), and the rates of VC oxidation will be determined. A model will be constructed based on Monod kinetics and incorporating terms for each of the parameters evaluated. The data will be fitted to the model and the kinetic parameters will be estimated using AQUASIM 2.0 software. Sensitivity analysis will be performed and the model will be validated using previously collected field data.

Results/Lessons Learned. We anticipate that these experiments will provide the necessary data to adequately model VC-oxidation under field conditions. This will include estimates of yield, maximum substrate depletion rates, and half velocity constants as well as terms to account for non-substrate parameters such as pH. Several cultures have already been shown to utilize VC as a sole electron donor for sustained growth over a period of 60-130 days. Melting curves, performed as part of qPCR analysis, show that at least two distinct groups of VC-oxidizers were enriched from different sites. These melting curves also confirm that a mixed population of microbes is being sustained in the enrichments. VC toxicity has also been noted in some cultures, with growth occurring at 3.8 µM and inhibition at 32 µM.