Simulation of TCE DNAPL Distribution and TCE Anaerobic Reductive Dechlorination in Soil Columns

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A three-dimensional, three-phase finite difference groundwater fate and transport model was used to simulate the processes occurring in five anaerobic experimental columns under different trichloroethene (TCE) contamination scenarios. These scenarios varied in terms of TCE DNAPL presence, TCE aqueous concentration and presence of sulfate. This study was conducted as part of the SABRE (Source Area in situ Bioremediation) project, a collaborative remediation program whose objective is to prove in a scientifically robust manner that enhanced anaerobic bioremediation can result in remediation of TCE DNAPL source areas.

The first part of this study focused on the simulation of TCE DNAPL distribution using the Brooks-Corey capillary pressure-saturation relationship. It was found that the transport of the organic phase was highly sensitive to soil permeability and to capillary pressure–saturation parameters. A homogeneous permeability approach was not sufficient to reproduce either the injected amount of DNAPL or its spatial distribution. For this reason, the effect of heterogeneity was investigated by simulating the DNAPL distribution under two different scenarios: (i) using a random, log-normally distributed permeability field and (ii) using a soil layout in which pathways of higher permeability were incorporated. The random approach underestimated the extent of DNAPL rise in the column, whereas the preferential pathway approach adequately modelled both the DNAPL amount and its distribution.

The second part of this study dealt with the simulation of the sequential reductive dechlorination of TCE to dichloroethene (DCE), vinyl chloride (VC) and ethene (ETH). A simplified first order approach was applied in order to minimize the number of calibrated parameters. The dechlorination rates were calibrated to the experimental TCE concentrations and its dechlorination products, for the following contamination scenarios: (i) in the presence of TCE DNAPL at 0.86% organic saturation, (ii) in the presence of TCE DNAPL at 4.24% organic saturation, (iii) at an average TCE concentration 24% of the solubility limit, (iv) at an average TCE concentration 63% of the solubility limit and (v) at an average TCE concentration 57% of the solubility limit, in the presence of 480mg/L SO$_4^{2-}$. In the cases where DNAPL was present, equilibrium dissolution was assumed and dechlorination was only considered in the aqueous phase.

The maximum TCE dechlorination rates achieved for the five scenarios were 0.14, 0.01, 1.73, 0.22, 0.78 day$^{-1}$ respectively. These rates are in agreement with ones reported in the literature and give useful insight into the effect of each contamination pattern modelled. The impact of the addition of a partitioning electron donor, SRS$^\text{TM}$ and of the
KB-1® dechlorinating culture was reflected in the temporal variations of the dechlorination rates. For contamination scenarios i) and iii), the dechlorination rates increased exponentially with time suggesting a correlation between microbial growth and dechlorination rates. The limitations introduced by the first-order approach used in our study will be addressed by incorporating electron donor and substrate concentration in the kinetics while maintaining the advantage of simplicity. In addition, the effect of heterogeneity on the dechlorination efficiency will be further investigated.