Modeling of Reductive Dechlorination of Chloethenes by *Desulfitobacterium* and *Dehalococcoides*

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Background/Objectives. Chloroethenes such as tetrachloroethene (PCE) and trichloroethene (TCE) are concerned contaminants in subsurface environments. Biodegradation by dechlorinating microorganisms is a prospective technique for remediating the contaminants. PCE and TCE can be dechlorinated to *cis*-dichloroethene (*cis*-DCE), vinyl chloride (VC) and harmless ethene, and the dechlorinating process is often completed with multiple microbial species. The aim of this study was to simulate the kinetics of sequential reductive dechlorination of PCE to ethene considering dechlorinating microbes characterized with next-generation sequencing.

Approach/Activities. Laboratory biodegradation tests were carried out to determine kinetic parameters. Anaerobic culture solution was used, which had maintained degradability of PCE to ethene over four years. The culture solution and mineral medium were mixed in test bottles at a ratio of 1:5 (v/v), followed by sealing the bottles. The tests were performed with different initial concentrations of PCE: 2, 6 and 30 mg/L, in a dark shaker at 140 rpm at 30°C. The chloroethenes: PCE, TCE, *cis*-DCE, and VC, and ethene in the test bottles were monitored with GC and GC-MS. DNA was extracted from each test solution and dechlorinating microbes were quantified with next-generation sequencing and Q-PCR of V4 variable region of 16S rRNA gene. The reductive dechlorination of chlorinated ethenes was modeled based on Monod kinetics. Monod parameters were determined from the time-course data of chloroethenes and the concentration data of dechlorinating microbes. Non-linear least-squares analysis was performed to regress to the experimental data.

Results/Lessons Learned. The chloroethenes were completely degraded under all tested conditions within 153 days. Next-generation sequencing revealed that *Desulfitobacterium* and *Dehalococcoides* existed in the test solutions. The microbes presumably degraded the chloroethenes based on previous reports. We assumed that *Desulfitobacterium* contributed to dichlorination of PCE and TCE, and *Dehalococcoides* degraded the other chlorinated ethenes. The kinetic model was developed considering these points. Comparative data over the time course of chloroethenes between the experimental and simulated data will be demonstrated.