Developing an Acetylene Sampler to Enable Quantitative Assessment of Long-term Abiotic Transformation Rates of Chlorinated Solvents

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Chlorinated solvents are the most commonly detected and persistent contaminants in the underground environment. At contaminated sites, it is difficult to quantify the efficacy of abiotic dechlorination in the field due to the co-occurrence of microbial dechlorination and other processes that lead to contaminant attenuation. As a result, significant uncertainty exists regarding the long-term persistence of chlorinated solvents at complex sites. The objective of this study is to develop an in situ reactive sampling probe to capture a key product of abiotic dechlorination of tetra- and tri-chloroethylene (PCE and TCE), namely, acetylene, in order to assess their abiotic reduction rates. The probe is based on copper-catalyzed 1,3-dipolar cycloaddition between terminal alkyne and azide groups, also known as CuAAC click chemistry. This reaction is highly specific and produces a stable triazole product at a quantitative yield, thereby permitting a sampling scheme to capture acetylene arising in the underground environment for quantitation. In this study, an in-situ reactive probe consisting of an azide-based molecule and copper catalyst immobilized in polydimethylsiloxane (PDMS) media was designed to capture acetylene production in the TCE microcosm reactors. We also investigated the effects of various Cu catalysts, temperature, pH, groundwater solutes, and low molecular-weight hydrocarbons on the yield of the triazole product. Our results demonstrated that the azide-based molecular probes can provide sensitive and specific sensing of acetylene in aqueous media, with potential applications in groundwater monitoring and remediation. The design of the probe ensures that the passive sampler captures acetylene without interfering with the degradation of TCE or other chlorinated ethene contaminants in the surrounding environment. This reactive probe will advance our understanding of the effectiveness of engineering treatment for chlorinated ethenes and provide an unequivocal line of evidence for the occurrence of abiotic degradation in the field.

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