Using Molecular Tools to Predict Rate Constants for Anaerobic Biodegradation of *cis*-DCE and Vinyl Chloride in Groundwater

John T. Wilson (john@scissortailenv.com) and Barbara Wilson (Scissortail Environmental Solutions, LLC, Ada, OK, USA)
Mandy Michalsen (U.S. Army Engineer Research Center, Vicksburg, MS, USA)
Katarzyna Kucharzyk and Fadime Murdoch (Battelle Memorial Institute, Columbus, OH, USA)
Frank Löffler (University of Tennessee and Oak Ridge National Laboratory, Knoxville, TN, USA)

Background/Objectives. It should be relatively straightforward to predict a rate constant for anaerobic biodegradation of *cis*-DCE and vinyl chloride using molecular tools. The transformation is carried out by specific and restricted groups of organisms (strains of *Dehalococcoides*) which can be recognized by the *Dhc* biomarker for their ribosomes. In addition, they use a limited number of reductase enzymes to carry out the transformation (e.g., *tceA, bvcA and vcrA*). There is usually only one copy of each gene in a *Dehalococcoides* cell; however, the number of enzyme molecules in the cell can vary widely. A tool that measured the abundance of the enzyme should provide a better predictor. The qPCR assays for the gene copies are readily available. A targeted proteomic assay for the TceA reductase has recently been developed. This study compares the qPCR assay and the proteomic assay to predict rate constants for anaerobic degradation of cis-DCE and vinyl chloride.

Approach/Activities. The natural attenuation of *cis*-DCE and vinyl chloride has been evaluated at Site 5 at the Naval Air Station North Island near San Diego, California. The field-scale rate constants for attenuation can be extracted from monitoring data acquired in 2007, 2013, 2016 and 2021. First order rate constants for attenuation of *cis*-DCE varied from 5.0 to 8.6 per year. Rate constants for attenuation of vinyl chloride were 6.7 per year in 2013 and 13.6 per year in 2021. The abundance of the *Dhc* qPCR gene biomarker was determined in six wells at the site in 2013. Based on Michaelis-Menten kinetic parameters published by Cupples et al. for the Victoria strain of *Dehalococcoides macartyi* the rate constant for degradation of cis-DCE varied from 1.5 per year to 217 per year, and the rate constant for vinyl chloride degradation varied from 0.8 per year to 256 per year in the six wells. The overall rate constants we calculated as the time averaged distance from the source well to the other individual wells down gradient. The time weighted average rate constant for *cis*-DCE degradation calculated from the abundance of the *Dhc* qPCR biomarker was 84 per year. The time weighted average for vinyl chloride was 98 per year. In 2021 the abundance of the TceA reductase was determined by targeted proteomics. Based on kinetic parameters published by Rowe et al. for the Cornell strain of *Dehalococcoides macartyi,* the predicted rate constant for degradation of *cis*-DCE varied from 0.17 to 22.34 in three wells. The time averaged rate constant of the predicted rate constants was 11.5 per year, compared to a rate constant of 8.6 per year that extracted from the monitoring data.

Results/Lessons Learned. The rate constants predicted from the abundance of the qPCR biomarkers varied widely from one well to another. It will be necessary to collect data from several wells to get a representative prediction. At this field site, rate constants predicted from the abundance of qPCR markers overestimated the field scale rate by an order of magnitude. The rate constant estimated from the abundance of the TceA enzyme fell within the 80% confidence interval of the field-scale rate constant.