

## Utilizing Dual Carbon and Hydrogen Isotope Analyses to Differentiate between Various Biodegradation Pathways of 1,2-Dichloroethane

**Orfan Shouakar-Stash** (orfan@it2isotopes.com) (Isotope Tracer Technologies Inc., Waterloo, ON, Canada)

Jordi Palau (jordi.palau@ub.edu) (Universitat de Barcelona, Barcelona, Spain)

Daniel Hunkeler (Daniel.Hunkeler@unine.ch) (University of Neuchâtel, Neuchâtel, Switzerland)

Martin Elsner (martin.elsner@helmholtz-muenchen.de) (Helmholtz Zentrum München, Neuherberg, Germany)

Siti Hatijah Mortan (hatijah256@gmail.com) and Ernest Marco-Urrea (Ernest.Marco@uab.cat) (Universitat Autònoma de Barcelona, Bellaterra, Spain),

Monica Rosell (monica.rosell@ub.edu) and Albert Soler (albertsolergil@ub.edu) (Universitat de Barcelona, Barcelona, Spain),

Rong Yu (rongyu@clemson.edu) and David L. Freedman (dfreedm@clemson.edu) (Clemson University, Clemson, SC, USA)

**Background/Objectives.** Chlorinated solvents are one of the most commonly found perilous organic compounds in soil and groundwater in contaminated sites. Compound-specific isotope analysis (CSIA) is an innovative approach that can provide unique information about the source and the fate of organic contaminants in the subsurface. In recent years, researchers showed the potential of utilizing dual element isotope approach to better understand the transformation mechanisms and degradation pathways of these compounds in the field. However, the dual C-H isotope patterns during biodegradation of many predominant groundwater contaminants such 1,2-dichloroethane (1,2-DCA) are still unknown.

**Approach/Activities.** Recent analytical advancements in H-CSIA have opened new possibilities and enabled consultants and researchers to start employing hydrogen isotope data in their case studies along with carbon and chlorine. In this laboratory study, dual C-H isotope fractionation patterns were investigated during *aerobic* and *anaerobic* biodegradation of 1,2-DCA by different microbial strains and enrichment cultures harboring different bacteria.

**Results/Lessons Learned.** The anaerobic dihaloelimination of 1,2-DCA showed secondary  $e^H$  values of  $-60.7 \pm 2.9\%$  and  $-81.5 \pm 9.1\%$  for *Dehalococcoides* and *Dehalogenimonas*-containing cultures, respectively. In contrast, the aerobic hydrolytic dehalogenation ( $S_N2$ ) exhibited a much lower and similar secondary  $e^H$  values for both experiments with *Ancylobacter* and *Xanthobacter* strains ( $-29.2 \pm 2.0$  and  $-31.7 \pm 4.1\%$ , respectively). The highest  $e^H$  value was observed for C-H bond oxidation by *Pseudomonas* strain DCA1 ( $-87 \pm 13\%$ ) which is in agreement with a primary H isotope effect. Combined with carbon, these different hydrogen isotope effects resulted in distinct C-H isotope correlations ( $\Delta\delta^{13}C/\Delta\delta^2H$ ) in a dual isotope plot:  $0.55 \pm 0.01$  and  $0.282 \pm 0.008$  for dihaloelimination,  $1.1 \pm 0.1$  and  $1.3 \pm 0.2$  for hydrolytic dehalogenation, and  $0.035 \pm 0.006$  for C-H bond oxidation. This result illustrates the potential of a dual C-H isotope approach to elucidate biodegradation pathways of 1,2-DCA in the field.