

Modelling isotope fractionation of organic pollutants: beyond carbon isotopes and aquifers

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Key words: Compound-specific stable isotope analysis, Isotope fractionation, Reactive transport modelling, Groundwater pollution, Diffuse pollution

Abstract

Compound-specific stable isotope analysis (CSIA) is increasingly being used for source identification and degradation assessment of various types of organic pollutants in the environment. Reactive transport modelling (RTM) enables simulation of isotope fractionation effects of compounds following biological, chemical, and physical processes. RTM thereby serves as a framework for qualitative and quantitative interpretation of CSIA data. This presentation discusses recent RTM work on 1) chlorine and hydrogen isotope fractionation during sequential reductive dechlorination (Figure 1; [1]); 2) aquitard-aquifer interaction carbon isotope effects; and 3) carbon isotope fractionation of diffuse pesticide pollution on catchment scale (Figure 2; [2]).

Figure 1 illustrates the successful modelling of chlorine and hydrogen CSIA data during biological reductive dechlorination of chlorinated ethenes. Expanding this model with isotope fractionation associated with alternative transformation processes such as oxidation and chemical reduction is expected to lead to better assessment of chlorinated ethene fate at contaminated sites.

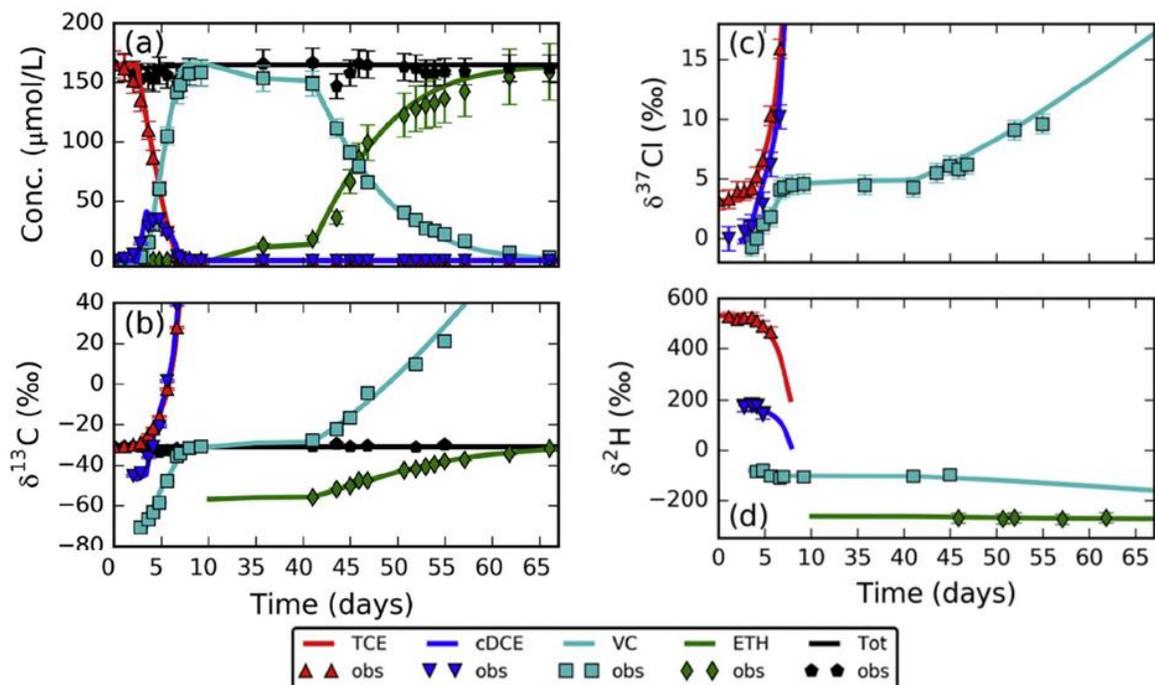


Figure 1: Reductive dechlorination of trichloroethene (TCE) to non-toxic ethene (ETH) via intermediates cis-dichloroethene (cDCE) and vinylchloride (VC) in a microcosm experiment [1]. Measurements (symbols) and simulations (lines) are shown for concentrations (a), and isotope ratios of carbon (b), chlorine (c) and hydrogen (d).

Figure 2 shows the promising results of simulating carbon isotope fractionation of pesticides on catchment scale with a conceptual mathematical model using the transport formulation by travel-time distributions [2]. CSIA data are expected to yield a better assessment of pesticide fate in catchment studies. The model indicated that degradation half-lives increase with soil depth.

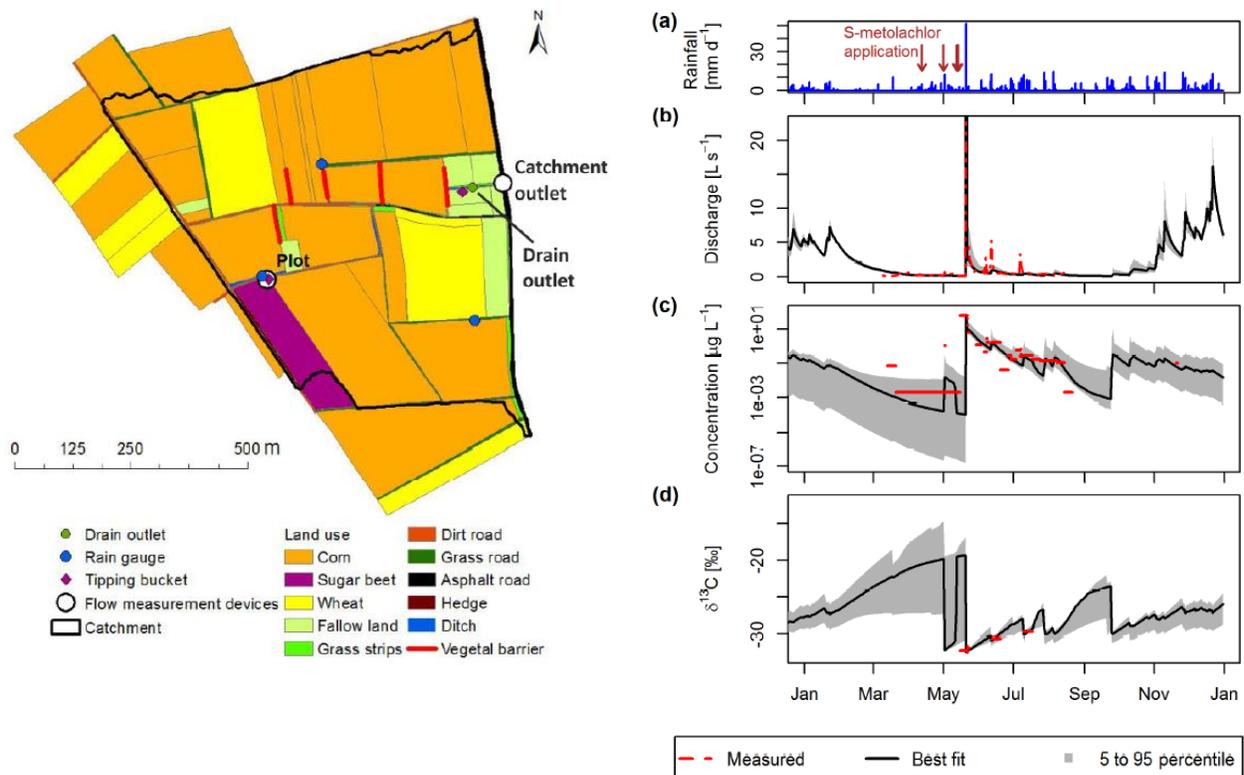


Figure 2: Simulation of carbon isotope fractionation of diffuse pollution on catchment scale [2].

Left: Scheme of the Alteckendorf catchment (France) with landcover and crop types.

Right: Daily precipitation (a), and measured (red lines) and modelled time series for discharge (b), S-metolachlor concentrations (c; note the log-scaling), and $\delta^{13}\text{C}$ values (d) at the catchment outlet in 2012.

The black line indicates the results of the calibration run with the best fit. Shaded areas show the range between the 5th and 95th percentiles of all simulation results.

References

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Open Access: <https://doi.org/10.1016/j.jconhyd.2017.07.003>

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Open Access: <https://doi.org/10.5194/hess-21-5243-2017>