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Inverting stop-flow leaching experiments and detection of physical and chemical non-equilibria

Lian Zhou[1], Laurent Lassabatere[2], and Khalil Hanna[1]
[1]Institut des Sciences Chimiques de Rennes UMR 6226, Ecole Nationale Supérieure de Chimie de Rennes, 11, Allée de Beaulieu, CS 50837, 35708 Rennes Cedex 7, France
[2]Univ Lyon, Université Claude Bernard Lyon 1, CNRS, ENTPE, UMR5023 LEHNA, F-69518, Vaulx-en-Velin, France

Flow heterogeneity strongly impacts mass transport. In particular, the presence of water fractionation into mobile and immobile water fractions may affect pollutant sorption to soil particles. Indeed, before sorbing, the pollutants need to diffuse from mobile water to immobile water fractions. In a previous study, we investigated the possibility of stop-flow experiments for the detection of physical and chemical non-equilibria. A sensitivity analysis proved that it was possible to detect the two types of non-equilibria. The effect of parameters related to physical (mobile water fraction and solute exchange rate) and chemical (chemical kinetics) non-equilibria were varied and related impacts on the shape of the breakthrough curves were characterized for stop-flow experiments. However, the feasibility of inverting procedures was not investigated at all. In particular, the estimation of these parameters by fitting the model to real experimental data (with noise) may be feasible but may also bring some uncertainty with biased and non-unique estimates. In this study, using both numerically generated data and experimental data, we characterize the estimate uncertainty and equifinality. This study will help in optimizing the inverting procedure for the design of more robust and less biased estimates and the quantification of physical and chemical non-equilibria parameters.