A modeling approach integrating microbial activity, mass transfer, and geochemical processes to interpret biological assays: An example for PCE degradation in a multi-phase batch setup

The rate at which organic contaminants can be degraded in aquatic environments is not only dependent upon specific degrading bacteria, but also upon the composition of the microbial community, mass transfer of the contaminant, and abiotic processes that occur in the environment. In this study, we present three-phase batch experiments of tetrachloroethene (PCE) degradation by a consortium of organohalide-respiring bacteria, cultivated alone or in communities with iron- and/or sulfate-reducers. We developed a modeling approach to quantitatively evaluate the experimental results, comprised of chemical and biomolecular time series data. The model utilizes the IPhreeqc module to couple multi-phase mass transfer between gaseous, organic and aqueous phases with microbial and aquatic geochemical processes described using the geochemical code PHREEQC. The proposed approach is able to capture the contaminant degradation, the microbial population dynamics, the effects of multi-phase kinetic mass transfer and sample removal, and the geochemical reactions occurring in the aqueous phase. The model demonstrates the importance of aqueous speciation and abiotic reactions on the bioavailability of the substrates. The model-based interpretation allowed us to quantify the reaction kinetics of the different bacterial guilds. The model further revealed that the inclusion of sulfate-reducing bacteria lowers the rate of PCE degradation and that this effect is moderated in the presence of iron-reducing bacteria.