

How porous media heterogeneities influence biodegradation of a self-inhibiting substrate

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Many organic substances at high concentration levels have an adverse effect on degradation rates of enzymes metabolizing them. The mechanism is known as substrate self-inhibition and regarded detrimental for the efficiency of bioremediation in porous environments. Structural heterogeneities are considered as another limiting feature that reduces in-situ microorganisms' access to substrate by creating preferential flow paths and thus negatively affecting the even distribution of substrate inside medium. The interplay between these two disadvantageous mechanisms is not yet well-understood. While it was shown by analytical equations that bioavailability limitations can dampen the effect of substrate inhibition at certain concentration levels [1], the potential occurrence of this effect *in situ* has not yet been explored.

To investigate the influence of pore matrix heterogeneities on substrate inhibition, we apply a numerical reactive transport model capable of solving transport processes in the presence of such heterogeneities. To that end, an established reactive pore network model [2] is upgraded and used to model both, transient and steady state reactive transport of a self-inhibiting substrate through media with various, spatially correlated, pore-size distributions. For the first time, we explore on the basis of a core-scale model approach the link between pore-size heterogeneities and substrate inhibition. By performing model simulations at several levels of heterogeneities we obtain an improved characterization of the terms contributing to overall biodegradation of self-inhibiting substrates inside porous media. Our results show that (1) pore-scale heterogeneities can noticeably promote degradation rates of a self-inhibiting substrate within certain levels of concentration, (2) the effect reverses when the concentrations fall to levels essential for microbial growth, and (3) an engineered combination of homogeneous and heterogeneous media can increase the overall efficiency of bioremediation.

[1] Gharasoo *et al.* (2015) *Environ. Sci. Technol.* **49** (9), 5529-37. [2] Gharasoo *et al.* (2012) *Environ. Model. Softw.* **30**, 102-14.