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Tracing the fate of sulfamethoxazole and its metabolites in subsurface: conceptualization and modelling

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The degradation of low adsorptive SMX in subsurface porous media is spatially and temporally variable. It depends on various environmental factors such as in situ redox potential, availability of nutrients, local soil characteristics, and temperature. Its degradation is better under anoxic conditions and by co-metabolism processes. In this work, we first develop a conceptual model of degradation of SMX under different redox conditions (denitrification and iron reducing conditions), characterizing the metabolite formation in each condition, and second, we construct a mathematical model that allows reproducing different experiments of SMX degradation reported in the literature. The model was validated using the experimental data from Barbieri et al. (2012), Nödler et al. (2012) and Mohatt et al. (2011). The model reproduces the reversible degradation of SMX under the presence of nitrous acid as an intermediate product of denitrification (it is the conjugate acid of nitrite), as well as, the metabolite formation (4-nitro-SMX and desamino SMX). In those experiments degradation was mediated by the transient formation of a diazonium cation, which was considered responsible of the substitution of the amine radical by a nitro radical, forming the 4-nitro-SMX. On the other hand, both the diazonium compound and the methanol present in the experiment produced a deamination in the SMX, producing desamino-SMX. The formation of these metabolites was unstable and they were retransformed to SMX. Concerning the iron conditions, SMX was degraded due to the oxidation of iron (Fe^{2+}), which was previously oxidized from goethite due to the degradation of a pool of labile organic carbon. As the oxidation of iron occurred on the goethite surface, the best model to reproduce the SMX reduction was a power law rate. Our work is an attempt to properly formulate the degradation process of an emerging compound considering the real degradation mechanisms, rather than using an upscaled black-box approach based only on the reported concentrations in a given experiment.
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