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# Modeling of redox reaction network and sensitivity analysis for predicting methane production potential by anoxic microsites

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Anaerobic microsites have been recognized as important features of the shallow subsurface, where locally anoxic and potentially methanogenic conditions can be sustained. This leads to significant redox heterogeneities within domains that are otherwise considered oxic at the macroscale. Such heterogeneities are hypothesized to be the result of spatial variation in organic carbon speciation and availability, moisture content as affected by soil hydraulic properties, the presence of active microbial communities and concentrations of trace metals that may inhibit microbial metabolism. To understand the potential generation of significant quantities of methane by anaerobic microsites at the pore scale, and to predict whether this local methane generation can result in net surface production of methane, a mechanistic understanding of those factors in conditions relevant to the field is necessary.

In this modeling study, we explore the impact of the aforementioned factors, namely organic carbon availability, microbial community distribution and presence of trace metals, on Fe and S redox, as an indicator of near-methanogenic conditions and CH4 generation, in fully saturated, synthetic domains. A numerical model is developed in Python to simulate the redox reaction network that leads to the generation of methane. First, the model is formulated as a homogeneous, well-mixed domain in which substrate utilization and microbial growth is simulated within anoxic microsites. Using Monod kinetics parameters reported in the literature, a sensitivity analysis is performed to evaluate carbon availability, trace metal inhibition and microbial community thresholds that produce levels of methane that could lead to net methane emissions. Then, a two-domain model that represents an anoxic microsite within a bulk oxic domain is used to explore the impact of methane oxidation and transport limitations for substrate availability and to qualitatively assess the dynamics of microsite boundaries. These findings will then be compared with X-Ray fluorescence 2D imaging utilized by the novel Laboratory for Observing Anaerobic Microsites in Soils (LOAMS) approach. Upon calibration with bench scale experimental data, the model will support data collection at field investigations of anoxic microsites, and will assist in the development of appropriate upscaled parameterizations for earth systems models at a scale relevant to field scale observations.