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What control reactions in unsaturated soils? On the dynamic effect of small-scale heterogeneity and (spatially variable) diffusion

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Soils are complex systems where different physical, chemical and biological processes occurring simultaneously and interact in a non-linear way. This includes the diffusion process, which is known to be affected by the tortuosity, and therefore the water content. Additionally, the high degree of soil heterogeneity poses significant challenges in studying soil reactivity due to its high impact on mixing. In this study we evaluate the effect of a series of what we could be key controlling factors of effective reaction rates in soils at the plot scale: the degree of heterogeneity, the hydraulic structure, the reaction rate, the initial distribution of reactants, and the heterogeneity in the diffusion coefficient.

We tackle this by explicitly simulating hypothetical biomolecular soil reaction (A+B -> C) for different degrees of heterogeneity, different hydraulic structures, different reaction rates, different initial distribution of the reactants and different representation of diffusion. Results are evaluated in terms of effective reaction rates at the plot scale.

The simulation results reveal that mixing conditions control reactions in unsaturated soils. Non-ideal reactivity due to mixing-limited conditions is not *only* a consequence of the simple presence of heterogeneity or even of its intensity. Instead, it results from (*at least*): the characteristics of heterogeneity, the *Pe* number, the *Da* number, the spatial distribution of the reactants. Interestingly, the spatial variability of the (tortuosity-dependent) diffusion coefficient appears to also have a significant effect on mixing conditions.

By these results, we illustrate the high complexity of reactive systems in unsaturated soils, which makes the use of average macroscopic reaction rates (as in most agriculture, environmental and geoengineering models) at least questionable.