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A micro-macroscale approach coupling processes that shape rhizosphere diffusivity and permeability

Alice Lieu, Alexander Prechtel, Nadja Ray, and Raphael Schulz
Friedrich-Alexander-Universität Erlangen-Nürnberg, Applied Mathematics I, Mathematics, Erlangen, Germany
(alice.lieu@fau.de)

A novel, comprehensive modeling approach extending (Ray et al., 2017, Rupp et al., 2018, Rupp et al., 2019) is used to study the interplay between biogeochemical processes in the rhizosphere. Understanding these local interactions is crucial for the habitat as they influence processes in the root-soil system such as the water and nutrient uptake by the roots. The mechanistic model explicitly represents the pore structure and allows for dynamic structural organization of the rhizosphere at the single root scale.

At this microscale, the movement of interacting entities - nutrients, bacteria and possibly charged chemicals - in the fluid is described by means of the diffusion and Nernst-Planck equations with a Henry transmission condition at the liquid/gas interfaces. A biomass phase can develop from agglomerations of bacteria and stabilising sticky agents may grow or decay at the solid surfaces. To take into account specific properties of the rhizosphere, root cells and an explicit phase of exudated mucilage as well as root hairs are included. In addition to solving the continuous partial differential equations, a discrete cellular automaton method (Tang and Valocchi 2013, Ray et al. 2017, Rupp et al., 2019) is used, enabling structural changes in the solid and mucilage phases at each time step. The partial differential equations are discretised with a local discontinuous Galerkin method which is able to handle discontinuities induced by the evolving geometry.

The microscale model is not amenable to large scale computations because of its high complexity. Upscaling techniques enable the incorporation of information from the rhizosphere scale to the macroscale. We apply these techniques to dynamically evolving microstructures taking the spatiotemporal evolution of the rhizosphere into account. Although the setting is periodic, the underlying geometries can be arbitrarily complex. The resulting hydraulic properties (e.g. diffusion coefficient, permeability) are an important input for existing root-water uptake models, involving e.g., the effect of mucilage.

In this study, we use two- and three-dimensional CT scans of maize root, and show how mucilage concentration as well as its distribution in the pore space result in changes of macroscopic soil hydraulic properties. The access of nutrients in small pores for the root is assessed in simulation studies and its effect on effective diffusivity is evaluated.

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