



Three-dimensional Solute Transport Modeling in Coupled Soil and Plant Root Systems

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Many environmental and agricultural challenges rely on the proper understanding of water flow and solute transport in soils, for example the carbon cycle, crop growth, irrigation scheduling or fate of pollutants in subsoil. Current modeling approaches typically simulate plant uptake via empirical approaches, which neglect the three-dimensional (3D) root architecture. Yet, nowadays 3D soil-root water and solute models on plant-scale exist, which can be used for assessing the impact of root architecture and root and soil hydraulic resistances on the root uptake pattern and solute transport and water flow in soil. In this thesis, we used a numerical model, which offers the possibility to describe soil and root interaction processes in a mechanistic manner avoiding empirical descriptions of root water uptake as a function of averaged water potential and root length density. Water flow is simulated along water potential gradients in the soil-root continuum and the model accounts for solute movement and root solute uptake. Solute movement in soils is modeled with a particle tracking algorithm. With this model, three research questions are investigated. The first study investigates how root water uptake affects the velocity field, and thus the dispersivity length. The solute breakthrough curves from the three-dimensional results and different simulation setups were fitted with an equivalent one-dimensional flow and transport model. The obtained results of the apparent soil dispersivities show the effect of the plant roots on solute movement, and illustrate the relevance of small scale 3D water and solute fluxes, induced by root water and nutrient uptake. Second, we show how local matric and osmotic potentials affect root water uptake. We analyze the difference between upscaled time and root-zone integrated water potentials, as often measured in experimental studies, and local water potentials at the root-soil interface. In addition, we demonstrate the relation between the shape of local stress function and the global (time-integrated) plant stress response to salinity. The last part explores how water uptake could be deduced from tracer concentration distribution monitored in a soil-plant system by Magnetic Resonance Imaging (MRI). We show the effects of root system architecture, fine roots, and root conductance on solute and compare numerical and measured data. This shows the capabilities and limitations of both, the model prediction and the MRI measurement methodology. Furthermore, it points out the extensive effect of root architecture and its conductance parameters on solute spreading.

This publication was written at the Jülich Supercomputing Centre (JSC) which is an integral part of the Institute for Advanced Simulation (IAS). The IAS combines the Jülich simulation sciences and the supercomputer facility in one organizational unit. It includes those parts of the scientific institutes at Forschungszentrum Jülich which use simulation on supercomputers as their main research methodology.