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Joint numerical microscale simulations of multi-phase flow and NMR relaxation behaviour in porous media

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In addition to the classical experimental approaches to derive flow and transport properties of rocks and soils - in particular for the vadose zone - Computational Fluid Dynamics (CFD) has proven to be a viable complementary tool for analyzing and predicting complex transport systems. In nuclear magnetic resonance (NMR), the measured relaxation signals originate from the pore spaces filled with NMR-active fluid (e.g., water, oil) and gas (e.g. methane) phases. The rate of NMR relaxation - of the wetting phase - is sensitive to the pore size and physicochemical properties of the rock-fluid/-gas interfaces (i.e., surface relaxivity), as well as the concentration of paramagnetic ions in the bulk phases (bulk relaxivity). Thus, the method can be applied to derive hydraulic parameters such as pore size distributions or (relative) permeability. To improve the fundamental understanding of the pore scale processes necessary to translate measured NMR relaxometry signals into soil structural and state properties, numerical simulations of the NMR relaxation (i.e., Bloch equation) and multi-phase flow on a pore scale dimension have been implemented using Lattice Boltzmann methods. To jointly study the transport and NMR behavior of partially saturated soils we carry out sequential CFD simulations using a modified Rothmann-Keller (RK) model for multi phase flow modeling (i.e., de-saturation) and due to its improved efficiency, high accuracy and stability an advection/diffusion model developed by Ginzburg is used to subsequently calculate the NMR relaxation signals at different saturation states. Simulations have been compiled for synthetic as well pore systems derived from micro-CT images of porous ceramics (reference samples) and natural unconsolidated sediments. The simulations have been validated by (1) using analytical and finite element models for simple geometries and (2) corresponding joint pressure-curve and NMR measurements on fully and partially saturated reference and soil samples. In a next step we aim to further advance the model by implementing simulations of Induced Polarization (IP) responses in the time and frequency domain that are complementary to NMR data. Based on these simulations we aim to develop a joint interpretation scheme for combined NMR and (Spectral) IP measurements in order to assess structure, state and thus flow properties of partially saturated soils.