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Modelling the transport and retention of nanoparticles in a single partially-saturated pore in soil

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Due to the wide application of nanotechnology in several fields including various consumer products, industrial processes, and biomedical fields, release of nanoparticles into the subsurface is inevitable. Once they enter the soil, they get transported through the vadose zone, where a fraction of the infiltrated particles is retained at grain surfaces (also called solid-water interface, SWI), air-water interface (AWI), and air-water-solid contact region (AWS). These retained particles may get remobilized due to change in water flow and chemistry making the vadose zone a secondary pollution source. Hence to evaluate groundwater pollution, it is necessary to understand the transport mechanisms of these particles in the unsaturated part of subsurface. In this study, a 3D mathematical model is developed to simulate the transport and retention of nanoparticles within a single partially-saturated pore with an angular cross-section. The model accounts for particle deposition at SWI, AWI, and AWS. A novel formulation for particle diffusive transport from AWI to AWS, where particles are assumed to be retained irreversibly by capillary forces is developed. The transport in the pore is modelled using the advection-diffusion equation and the mass exchange with the SWI, AWI and contact region are modelled as first-ordered reactions that depend on the interaction energy of particles with the interfaces. Quantitative relationships for attachment and detachment rate coefficients of nanoparticles towards various interfaces with respect to twelve different pore-scale parameters were developed. It was found that the geometry and flow parameters play a significant role in the retention of particles at various interfaces, and parameters describing the system chemistry have a negligible effect on particle retention. The formulas for attachment and detachment rate coefficients of nanoparticles towards various interfaces developed in this study can be further incorporated into a pore-network model to upscale particle transport to the continuum scale.

Participation

In-Person

References

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