Geophysical Research Abstracts
Vol. 18, EGU2016-4765-1, 2016
EGU General Assembly 2016

A Lagrangian model for soil water dynamics: can we step beyond Richard's equation while preserving capillarity as first order control?

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Water storage in the unsaturated zone is controlled by capillary forces which increase nonlinearly with decreasing pore size, because water acts as a wetting fluid in soil. The standard approach to represent capillary and gravity controlled soil water dynamics is the Darcy-Richards equation in combination with suitable soil water characteristics. This continuum model essentially assumes capillarity controlled diffusive fluxes to dominate soil water dynamics under local thermodynamic equilibrium conditions. Today we know that the assumptions of local equilibrium conditions e.g. and a mainly diffusive flow are often not appropriate, particularly during rainfall events in structured soils. Rapid or preferential flow imply a strong local disequilibrium and imperfect mixing between a fast fraction of soil water, traveling in interconnected coarse pores or non-capillary macropores, and the slower diffusive flow in finer fractions of the pore space. Although various concepts have been proposed to overcome the inability of the Darcy – Richards concept to cope with not-well mixed preferential flow, we still lack an approach that is commonly accepted. Notwithstanding the listed short comings, one should not mistake the limitations of the Richards equation with non-importance of capillary forces in soil. Without capillarity infiltrating rainfall would drain into groundwater bodies, leaving an empty soil as the local equilibrium state - there would be no soil water dynamics at all, probably even no terrestrial vegetation without capillary forces. Better alternatives for the Darcy-Richards approach are thus highly desirable, as long they preserve the grain of "truth" about capillarity as first order control.

Here we propose such an alternative approach to simulate soil moisture dynamics in a stochastic and yet physical way. Soil water is represented by particles of constant mass, which travel according to the Itô form of the Fokker Planck equation. The model concept builds on established soil physics by estimating the drift velocity and the diffusion term based on the soil water characteristics. A naive random walk, which assumes all water particles to move at the same drift velocity and diffusivity, overestimated depletion of soil moisture gradients compared to a Richards' solver within three distinctly different soils. This is because soil water and hence the corresponding water particles in smaller pores size fractions, are, due to the non-linear decrease of soil hydraulic conductivity with decreasing soil moisture, much less mobile. After accounting for this subscale variability of particle mobility, the particle model and a Richards' solver performed highly similar during simulated wetting and drying circles in three distinctly different soils.

Alternatively, we tested a computational less approach, assuming only the 10 or 20% of the fastest particles as mobile, while treating the remaining particles located in smaller pores sizes as immobile. For instance in a sandy soil a mobile fraction of 20% revealed almost identical results as the full mobility model and performed even closer to the Richards solver. In this context we also compared the cases of perfect mixing and no mixing between mobile and immobile water particles between different time steps. The second option was clearly superior with respect to match simulations with the Richards' solver. The particle model is hence a suitable tool to "unmask" a) inherent implications of the Darcy-Richards concept on the fraction of soil water that actually contributes to soil water dynamics and b) the inherent very limited degrees of freedom for mixing between mobile and immobile water fractions.

A main asset of the particle based approach is that the assumption of local equilibrium equation during infiltration may be easily released. We tested this idea in a straight forward manner, by treating infiltrating event water particles as second particle type which travel initially, mainly gravity driven, in the largest pore fraction at maximum drift, and yet experience a slow diffusive mixing with the pre-event water particles within a characteristic mixing time. Simulations with the particle model in the non-equilibrium mode were a) rather sensitive to the coefficient describing mixing of event water particles and b) clearly outperformed the Richards model with respect to match observed soil dynamics in a real world benchmark. The proposed non-linear random walk of water particles is, hence, an easy to implement alternative for simulating soil moisture dynamics in the unsaturated, which preserves the influence of capillarity and makes use of established soil physics. The approach is particularly promising to deal with preferential flow and transport of solutes and to explore transit time distributions.