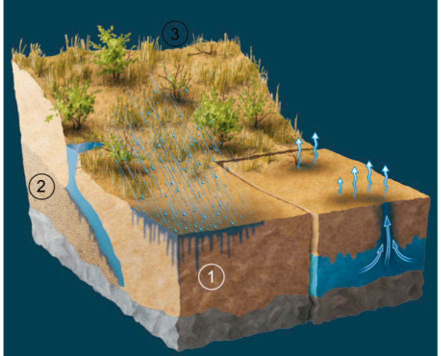
Special Section: MUSIS

P. Lehmann*
I. Neuweiler
J. Vanderborght
H.-J. Vogel



The guest editors introduce the special section MUSIS, **MU**lti **S**cale **I**nterfaces in unsaturated **S**oil, with contributions that originated from the MUSIS workshop on interfacial phenomena. The presence and complexity of various interfaces limit the predictability of flow and transport processes in the vadose zone.

P. Lehmann, Soil and Terrestrial Environmental Physics, ETH Zurich, Zurich, Switzerland; I. Neuweiler, Institute of Fluid Mechanics, Univ. of Hannover, Hannover, Germany; J. Vanderborght, Agrosphere, IBG-3, Forschungszentrum Jülich, Jülich, Germany; H.-J. Vogel, Dep. of Soil Physics, Helmholtz Center for Environmental Research, Halle, Germany. *Corresponding author (peter.lehmann@env.ethz.ch).

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Dynamics of Fluid Interfaces and Flow and Transport across Material Interfaces in Porous Media—Modeling and Observations

Prediction of fluid phase dynamics in the vadose zone is hampered by the presence of different types of sharp interfaces, questioning the validity of standard theory that is based on assumption of continuity of air and water phases, uniform distribution of fluids in a control volume, local equilibrium of phase contents and pressures, and slow process velocities. Complexity of fluid front morphology and burst-like redistribution processes may be accentuated across material contrasts or at the interface between soil and atmosphere. This special section presents eleven contributions highlighting the role of interfaces on water and air distributions and outlining methods to improve prediction of interfacial displacement.

The critical role of the vadose zone for the local, regional, and global water balance and for the transport of nutrients and contaminants is widely acknowledged (Harter and Hopmans, 2004). Water fluxes in the vadose (Latin for "shallow") zone are coupling the hydro-systems "atmosphere" and "groundwater." While flow patterns and water fluxes change rapidly in the atmosphere, conditions in groundwater flow can often be approximated reasonably well as steady state. Therefore the hydrologic response of the vadose zone depends on its proximity to the groundwater table and the soil surface. Accurate predictions of water distribution and fluxes in the vadose zone are important to (i) quantify vapor and energy exchange with atmosphere during evaporation; (ii) assess groundwater recharge rates, infiltration depth, and redistribution of water after heavy rainfall events; and (iii) optimize water management to sustain plant available water. Notwithstanding the importance of reliable predictions, our standard models offer limited predictive capabilities in simulating fluxes, flow pathways, and water distribution. Even common processes such as infiltration front displacements and water redistribution in coarse material after a heavy rainfall (Glass et al., 1989; Kung, 1990; Wang et al., 2003) or dynamics of evaporation from heterogeneous soils (Lehmann and Or, 2009; Shokri et al., 2010) cannot always be predicted accurately with standard models.

The reasons for shortcomings of the standard theory on flow processes in the vadose zone are often related to the presence of a variety of interfaces and their interactions at different scales. The effect of interfaces on flow in the vadose zone is addressed in this special section. As shown in Fig. 1, interfaces can be classified based on their nature as interfaces between liquids (e.g., water and air), material interfaces (including the interface between soil and plant roots), and the soil surface as the interface between subsurface and atmosphere.

Alternatively, interfaces can be specified regarding their length scale, ranging from the air–water meniscus at pore scale to thickness of soil layers and the lateral spacing between patterns of different soil types. While in the vertical direction the extent of the vadose zone is limited by the presence of a usually water-saturated aquifer, length scales in lateral direction are much larger (Harter and Hopmans, 2004), with heterogeneities defined by soil association, vegetation types, and topography at regional or catchment scale (Wagenet, 1998; Western et al., 2001; Vogel and Roth, 2003). In this special section we limit the upper range of scales by the "radius of influence" of a heterogeneity in soil texture or surface topography on lateral water flow that is within the range of a few meters (Lehmann and Or, 2009; van der Ploeg et al., 2012). Because an accurate description of the water distribution in the vadose zone can only be achieved by a more complete understanding of dynamics at the pore scale, the smallest scale addressed in this special section is the pore scale. Before summarizing the contents of the special section, we give a short summary of problems related to the different types of interfacial phenomena, including key publications.

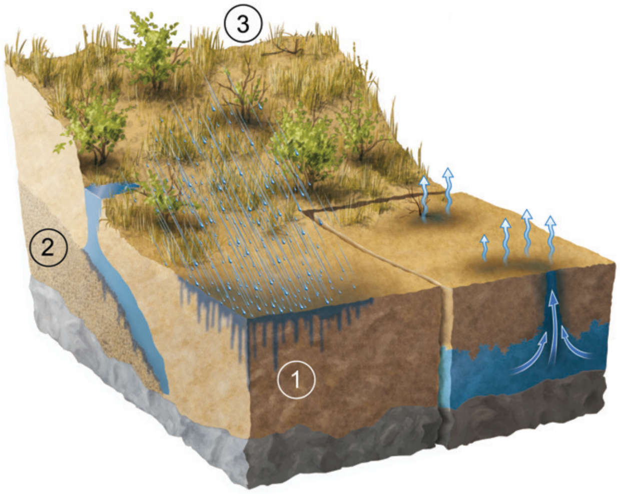

Fig. 1. The role of interfaces on flow and transport in the vadose zone. (1) Fluid displacement is not always a smooth process with constant front velocity but may be controlled by propagation of fingers and other preferential flow paths. Displacements of fluid–fluid interfaces depend on the force balance between capillarity, viscosity, and gravity. (2) The vadose zone is heterogeneous at various scales with sharp contrasts in porosity, texture, hydrophobicity, and reactivity. These material interfaces may result in different time and length scales as manifested in nonequilibrium between water content and pressure in different regions. (3) The interface between soil and atmosphere defines the boundary conditions for soil water flow (evaporating demand, rainfall rate) and the heterogeneity of surface water content distribution.

Fluid–Fluid Interfaces

Water–air interfaces (or interfaces between two fluids in general) are manifested at the pore scale as well as on the Darcy scale, where the pore space is no longer resolved. Their appearance at the pore scale is obvious, with curved interfaces between the air and water phase, defining the capillary forces as main engine of soil water fluxes. At the Darcy scale, the governing flow equation (Buckingham–Darcy law implemented in the mass balance equation or Richards equation) is based on simplifying assumptions such as continuity of air and water phases, uniform distribution of fluids in a control volume, local equilibrium of phase pressures, and slow process velocities with low Reynolds numbers. For fast processes or coarse soils with formation of a sharp displacement front these conditions are not fulfilled. The interplay of driving forces (gravity, capillarity, inertia, and viscous losses) in irregular pore spaces yields complex front patterns (Måløy et al., 1992; Løvoll et al., 2005; Or, 2008) and highly dynamic processes at the pore scale (Moebius and Or, 2012) with fast pressure relaxation and interfacial reconfigurations denoted as Haines jumps (Haines, 1930).

Displacement patterns at the front are often characterized by a front region with fractal properties and burst-like redistribution processes, followed by a compact region with constant fluid contents behind the front, where continuum description at the Darcy scale is valid (Yortsos et al., 1997). At the Darcy scale the variety of these patterns is captured in the one variable, "water content," which determines the hydraulic conductivity and flow velocity. The example of a sharp wetting front above a completely dry soil without liquid phase continuity may reveal the conceptual difficulties of capturing front displacement with standard theory of smoothly varying hydraulic properties. The discrepancy between complexity of front patterns and its simplified representation in one variable is one of the problems of modeling unsaturated flow, which manifests itself in time-dependent and hysteretic hydraulic flow parameters. Possible remedies were discussed in context to gravity fingering and stability (Raats, 1973; Nieber 1996; Cueto-Felgueroso and Juanes, 2008) with special focus on nonequilibrium between water content and capillary pressure (Hassanizadeh et al., 2002; DiCarlo, 2005).

Material Interfaces

Processes in the vadose zone are often controlled by heterogeneity at field scale (Vanderborght and Vereecken, 2006; Vereecken et al., 2007) and the presence of sharp material interfaces, such as layers, aggregates, or wettability contrasts. The hydraulic response of such a heterogeneous system is not the average response of the various materials but depends on the hydraulic coupling between the constituents, leading to preferential flow pathways, trapping or bypassing (Ursino and Gimmi, 2004; Rossi et al., 2008). While aquifers could usually be represented by constant saturated water content, soil processes are dominated by steadily changing water content and its highly nonlinear relation to hydraulic conductivity and water potential. This nonlinear behavior of the water–air system leads to deviations from the classical Richards model (smooth fluid distribution and local equilibrium) already for weakly heterogeneous media (as shown, for example, with stochastic theory by Mantoglou and Gelhar, 1987). For sharp material interfaces, the strong parameter contrasts across material interfaces lead to the generation of different flow domains, where processes happen very fast in one domain and significantly slower in the other one (see reviews of Šimůnek et al., 2003; Gerke, 2006; and Köhne et al., 2009). This nonequilibrium leads to dynamic hydraulic parameters (Hassanizadeh et al., 2002; Barenblatt et al., 2003) and non-Richards types of models taking into account nonequilibrium (Szymkiewicz and Lewandowska, 2006).

An additional difficulty in predicting flow processes in heterogeneous media stems from specific hydraulic properties of the interface itself with fluctuations in porosity across the material interface (Kaestner et al., 2008) that affect the hydraulic properties of a heterogeneous sample and make it impossible to predict hydraulic response without considering interfacial properties (Papafotiou et al., 2008). Similarly to soils with textural contrasts, the response of the soil–plant system also depends strongly on spatial structure and coupling of the components (Kuhlmann et al., 2012). But, neither the properties of the soil–root interface nor the structure of the root system are considered explicitly in soil water flow models (Feddes and Raats, 2004). Therefore, the commonly used simulation tools lack the mechanistic basis that would be required to investigate the interaction between soil and plant interfaces and call for the development of mechanistically integrated soil–root models (Javaux et al., 2008; Draye et al., 2010).

Soil Surface as Interface between Soil and Atmosphere

Practical and theoretical limitations of standard models are accentuated near the soil surface, where fluxes of mass and energy are highly dynamic, with strong alterations in the magnitude of gradient and direction of flow. For modeling fluxes in the vadose zone the soil surface is considered as the upper boundary of the domain with prescribed fluxes. For infiltration into unsaturated soil surface and for evaporation from wet soil, the water flow is often specified as a constant flux over the whole boundary. Such an approach is a simplification of the interaction between the processes above and below the soil surface (Zhang and Foufoula-Georgiou, 1997; Coquet et al., 2005). This is particularly relevant if heterogeneous soil structure is also considered. During infiltration on heterogeneous surfaces, parts of the surface may become saturated, creating conditions favorable for lateral water redistribution on the soil surface, resulting in spatial variations of infiltration rate and reduced lateral variations in water pressure (Foussereau et al., 2000). For evaporation a constant rate is sustained only as long as capillary flow can take place through continuous hydraulic pathways (Lehmann et al., 2008) and when the vapor transport across a thin atmospheric boundary layer is not limited (Suzuki and Maeda, 1968; Schlünder, 1988). In heterogeneous soils, evaporation fluxes at the soil surface can be even more complex due to transversal water fluxes from coarse to fine textured media, increasing evaporation fluxes from the fine region that are not captured in a prescribed constant flux over the whole boundary (Lehmann and Or, 2009). Variations in infiltration and evaporative fluxes are accentuated by heterogeneous surface topography and correlations of hydraulic conductivity with the microtopography (Dunne et al., 1991; Frei et al., 2010). Surface heterogeneities affect the air velocity field (Kondo et al., 2002) controlling the evaporation rate as well as the spatial water distribution during rainfall (Sande and Chu, 2012), leading to scale and rainfall rate dependence of effective hydraulic parameters (Langhans et al., 2011).

Contents of the Special Issue

In the introduction we have shown that the doubts about the predictive power of standard models for flow in the vadose zone stem from the dynamics and complexity of interfacial processes that are not adequately captured in the standard approaches for a variety of conditions (in particular those found close to the soil surface). There is a large research activity to improve descriptions of interfacial phenomena, and this special issue presents 11 contributions on the role of interfaces on flow and hydraulic properties. Below we give a short overview of the studies, covering length scales ranging from microns to several meters. To guide the reader with respect to the addressed scale, we assign each paper to the “pore scale” or “Buckingham–Darcy scale.” In the first case the focus is on the description of processes at the pore scale, while in the second case effective material properties are applied (like the water content dependent hydraulic conductivity used in the Buckingham–Darcy law). In addition, we assign each study to one of the three types of interfaces specified in the discussion above and shown in Fig. 1.

Soil Surface as Interface between Soil and Atmosphere

Buckingham–Darcy Scale

The role of soil surface on water flow was addressed in the paper of Van der Ploeg et al. (2012). For a wetland ecosystem they showed that microtopographic variations create complex patterns of water ponding and redistribution, affecting water flow and solute transport, and creating niches for different plant species. For a raised bog with a shallow groundwater table they quantified surface runoff and groundwater flow, revealing the relevance of characteristic horizontal drainage distances that exist at different scales for the hydraulic response of the system.

Material Interfaces

Buckingham–Darcy Scale

Van der Ploeg et al. (2012) highlighted the role of plants on changing microtopography but also on soil structure and flowpaths in the subsurface. This effect of plant roots was analyzed in detail in the study of Carminati (2012). He showed that the production of root exudates creates a unique type of material interface in the vadose zone with hydraulic properties differing with water content and flow process. Root exudates form a complex porous network that may increase water content and conductivity around roots in drying soils. But, as Carminati (2012) showed in his paper, exudates consist of lipids that make the roots hydrophobic and delay the wetting of a dry root.

Pore Scale

The interface between the soil and rhizosphere is just one of many material interfaces that can be encountered in soils with contrasts in porosity, texture, hydrophobicity, or reactivity. Independent of the nature of the material interface, the characterization and parameterization of the interface is essential to quantify its effect on flow and transport. In his study Gerke (2012) measured the interface between macropores (or interaggregate pores) and fine textured soil matrix based on segmentation of X-ray attenuation images. He is using geometric properties of soils based on surface area/volume ratio, providing more accurate estimates of model parameters that define the mass exchange between the two domains soil matrix and preferential flow paths.

Fluid/Fluid Front Displacements

Buckingham–Darcy Scale

When the structure and material properties of a two-domain system are known, the coupled flow between the domains can be predicted as shown in the article of Neuweiler et al. (2012). They simulated infiltration through a heterogeneous system with gravity driven flow through the “mobile” domain coupled to the embedding fine textured domain with capillary driven flow. To include both domains in an upscaled continuum approach, they used a memory term accounting for equilibration periods of water pressure in the fine textured domain. While in Neuweiler et al. (2012) the "nonequilibrium" between water content and water pressure stems from the heterogeneities with different hydraulic conductivities, Weller and Vogel (2012) quantified the degree of nonequilibrium in homogeneous media. In a series of experiments with stepwise changing infiltration rates, they monitored water content and pressure with high temporal resolution and revealed extreme variations in the relationship between water content and matric potential head. Their data indicate that equilibration between pressure and water content takes place in two steps with fast adaption in response to external forcing, followed by slow equilibration period.

Different origins and manifestation of dynamic nonequilibrium phenomena are reviewed in the study of Diamantopoulos and Durner (2012). They gave a concise overview of physical processes at the pore scale that lead to the ambiguous relationship between soil water content and matric potential head. The paper presents various approaches to model nonequilibrium effects that are not included in the standard form of the Richards equation. An example of such an approach is the concept of dynamic capillary pressure that was used in the model of Kissling et al. (2012) to reconstruct saturation overshoot and wetting front instabilities. They presented a multiscale method to generate and track saturation overshoot waves and applied it for different infiltration studies. Saturation overshoot is a well-known example of nonmonotone fluid saturation profile that cannot be reproduced in standard approaches with monotone constitutive relationship between soil water content and pressure. Another, but rather special, example of nonmonotone saturation profiles is presented in Hilfer et al. (2012). In their numerical study they postulated that due to concurrent drainage and wetting processes within an enclosed system in hydrostatic equilibrium, a non-monotonic distribution of liquid and gaseous phase can be achieved. With a model framework based on the separation between percolating and nonpercolating fluid phases, they reproduced nonmonotonic water content profiles.

Pore Scale

Another limitation of standard theory is the impossibility of describing flow with complex front morphology. Toussaint et al. (2012) discussed the contributions of capillary, viscous, and gravity forces on finger flow and provide estimates of crossover length between capillary and viscous fingering. Based on percolation theory they express the relationship between fluid saturation and capillary pressure as a function of flow velocity (capillary number). They could scale all flow dependent constitutive relationship to a single "master curve" based on the velocity dependent structure of the fingering. Alternatively to the theoretical arguments based on percolation theory, complex interfacial displacements can be simulated with pore network model approaches. Joekar-Niasar and Hassanizadeh (2012) modeled the dynamics of wetting front displacements as a function of initial water saturation. By considering dynamics of pressure relaxation, flow in corners of angular pores, and motion of isolated clusters of liquids, they showed that the front velocity and water content profile were sensitivity to initial water content, trapping of air, and connectivity of corner flow region.

While Joekar-Niasar and Hassanizadeh (2012) highlighted the importance of disconnected water clusters for water flow, Steeb et al. (2012) quantified the effect of water clusters on propagation of seismic waves. By upscaling properties of discontinuous water clusters from the pore scale, they showed that seismic wave velocity and attenuation depends on the number and size of isolated water clusters. They showed that it is possible to deduce the water cluster distribution from wave propagation properties.

The study of Steeb et al. (2012) is representative for this special issue and the research on interfaces in the vadose zone in general:

- Soil hydraulic properties depend on the spatial arrangement and connectivity of the fluid phases and not on the volumetric contents alone.
- A detailed description of physics at the pore scale is required for a more complete understanding of material properties.
- By appropriate upscaling schemes, the main characteristics of complex processes can be captured at the larger scale.

In addition, this study on seismic wave velocity may serve as illustrative example that a better understanding of hydraulic properties and interfacial processes may be achieved by including methods and approaches that are beyond the core disciplines of soil physics (determination of hydraulic conductivity and soil water characteristics, modeling water flow and solute transport). In that sense we hope that this special issue encourages us to pursue collaborations with researchers from other research fields and disciplines.

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