Water transfer in soil at low water content. Is the local equilibrium assumption still appropriate?

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ABSTRACT

The dynamics of water content in the superficial layers of soils is critical in the modelling of land-surface processes. In arid regions, vapour flux contributes significantly to the global water mass balance. To account for it in theoretical descriptions, most of the models proposed in the literature rely on the local equilibrium assumption that constrains the vapour pressure to remain at its equilibrium value. It implicitly amounts to consider an instantaneous phase change. Recent works underlined a retardation time and a decrease in phase change rate as the water content gets lower. Therefore, the objective is to revisit water transport modelling by rejecting the local equilibrium assumption. This requires developing a non-equilibrium model by taking into account the phase change kinetics. To assess the interest of this approach, a natural soil of Burkina-Faso has been experimentally characterized from independent tests and soil column experiments have been carried out. The comparison of experimental drying kinetics and water content profiles with computational predictions confirms the reliability of this description. Liquid/gas non-equilibrium is significant in a limited subsurface zone which defines explicitly the transition from liquid transport in lower layers to vapour transport in upper layers, i.e., the evaporation front. The overall moisture dynamics is governed by the coupling between water transport mechanisms (liquid filtration, vapour diffusion, phase change) that mainly occurs in this transition zone.

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1. Introduction

Land–atmosphere mass exchanges are concentrated in the superficial layers of soils and control most of biological processes required for plant growth. An accurate description of these layers is of first importance when developing realistic boundary conditions to be implemented in large-scale environmental models. Intensive research has been done to develop efficient numerical models of water transport in the vadose zone. In particular, the quantification of total water evaporation from soil is a crucial issue since it governs the water content dynamics near the surface (Gowing et al., 2006).

Following the pioneered work of Philip and de Vries (1957), most of models have associated the Richard's equation in the liquid phase with a classical diffusive equation in the gas phase while both transport phenomena are coupled through the heat equation (Bittelli et al., 2008; Garcia-Gonzalez et al., 2012; Grifoll et al., 2005; Novak, 2010; Parlange et al., 1998; Saito et al., 2006; Sakai et al., 2009; Thomas and Missoum, 1999; Xiang et al., 2012; Yanful and Mousavi, 2003). Although thermal gradients affect liquid water redistribution in soils, the most important coupling process is the transport of latent heat by vapour flux. These models have

been successfully used to describe the land–atmosphere water and energy balance of various natural field soils over a large period (Bittelli et al., 2008; Garcia-Gonzalez et al., 2012; Grifoll et al., 2005; Novak, 2010; Saito et al., 2006).

Most of these models have been developed for temperate regions where water content evolves in the capillary domain from saturation to the milting point. Since water vapour flow in semi-arid and arid regions can represent a major part of the overall water flow, it is important to take it into account together with liquid water flow when evaluating hydrologic fluxes (Garcia-Gonzalez et al., 2012; Sakai et al., 2009). In this framework, classical models have been extrapolated towards low water contents without carefully checking the validity of such formulations. For instance, usual descriptions of the water retention curve can significantly diverge from experimental points at very low water content (Thakur et al., 2006). Correction functions have been proposed without being fully satisfactory. However, as water content goes to very low values, liquid water takes the form of adsorbed layers onto solid surface and does not behave as "free" water. It has been shown that film flows replace conventional capillary flows at low water content, induces a change in the relative permeability description (Tuller and Or, 2002). It is therefore noteworthy to consider that modelling water transport phenomena at low water content calls for a specific description.

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In particular, the *local equilibrium assumption* is extensively used in most of the theoretical models proposed in the literature (Bittelli et al., 2008; Garcia-Gonzalez et al., 2012; Grifoll et al., 2005; Novak, 2010; Parlange et al., 1998; Saito et al., 2006; Sakai et al., 2009; Thomas and Missoum, 1999; Xiang et al., 2012; Yamanaka and Yonetani, 1999; Yanful and Mousavi, 2003). This hypothesis governs the liquid/gas mass exchange by assuming that the partial pressure of vapour remains equal to its equilibrium value. It is generally written as an explicit relation between the relative humidity and the hydraulic head. It allows combining liquid and vapour mass balance equations in a single one describing the global soil moisture content. Implicitly, it amounts to consider that the evaporation process is instantaneous in comparison with the other transport phenomena. This should be fairly satisfactory when capillary forces are predominant. Nevertheless, under particular conditions, a volatilization retardation time has been observed (Armstrong et al., 1994; Bénet and Jouanna, 1982; Chammari et al., 2008). In the hygroscopic domain where adsorption phenomena predominate, phase change kinetics is strongly influenced by the thermodynamic state of water and evaporation rate is drastically reduced (Bénet et al., 2009; Lozano et al., 2008). These experimental observations conduced us to reconsider the *local equilibrium assumption* in order to assess its reliability.

The aim of this contribution is to revisit water transport modelling in the lower range of water content. The prominence of hygroscopic effects leads us to reject the liquid/gas equilibrium assumption. This requires developing a two-equation model by taking into account the phase change kinetics. It means that, in some specific configurations, the characteristic times of the three transport mechanisms considered (liquid flow, vapour diffusion, liquid–gas phase change) are of the same order of magnitude. To fulfil this objective, a natural soil of Burkina-Faso has been experimentally characterized from independent tests and soil column experiments have been carried out. The comparison of experimental drying kinetics and water content profiles with computational predictions supports the validation of this description. Therefore, the *local equilibrium assumption* can be discussed based on numerical simulations. In particular, the location of the evaporation front is identified as it propagates from the upper surface towards deeper layers.

2. Theoretical and numerical modelling of water transfer

2.1. Liquid and vapour transfer model

A natural soil can be idealized by a triphasic porous medium by considering a solid, a liquid and a gaseous phase, while the gaseous phase consists of two components: dry air and water vapour. Theoretical modelling relies on the following assumptions:

- Temperature is uniform and constant. This hypothesis will be validated *a posteriori* in the last section based on numerical simulations.
- The solid skeleton is undeformable. Assuming a rigid structure is a strong hypothesis since evaporation and dehydration processes in non-consolidated soils generally lead to global shrinkage. However, we focus our attention on the hygroscopic domain where these effects are negligible.
- The total gas pressure is constant and uniform, since the convective transport in the gas phase is negligible. Actually, it means that the gas permeability is large enough to assume that a pressure gradient will be instantaneously equilibrated when compared to the other transport phenomena.

Therefore, three elementary phenomena are considered: liquid filtration governed by capillary and gravity effects, vapour diffusion

in the gas phase and liquid–gas phase change of water. Fundamental mass balance equations of water in liquid and gas phase are written:

$$\frac{\partial \rho_l}{\partial t} + \nabla \cdot (\rho_l \mathbf{v}_l) = -\hat{\rho}_v \tag{1}$$

$$\frac{\partial \rho_v}{\partial t} + \nabla \cdot \mathbf{J_v} = \hat{\rho}_v \tag{2}$$

where ρ_l and ρ_v (kg m^{-3}) are, respectively, the apparent density of liquid water and its vapour, $\mathbf{v}_l$ (m s^{-1}) is the intrinsic velocity of liquid water and $\mathbf{J}_v$ (kg m^{-2} s^{-1}) is the vapour diffusion flux. The phase-change rate $\hat{\rho}_v$ (kg m^{-3} s^{-1}) is thus a volumetric scalar flux, representing the mass of water transforming from a liquid state to a vapour state by unit volume and unit time.

From an experimental point of view, appropriate state variables are the mass water content, w(%), defined as the ratio between the apparent mass densities of liquid and solid:

$$w = \frac{\rho_l}{\rho_s} \tag{3}$$

and the vapour partial pressure in the gas phase, p_v (Pa), linked to the apparent density of vapour, ρ_v, through the ideal gas law:

$$\phi_g p_v = \frac{RT}{M_w} \rho_v \tag{4}$$

where R (J kg^{-1}) is the ideal gas constant and M_w (kg) is the molar mass of water. The volume fraction of the gas phase, ϕ_g, is related to the water content by:

$$\phi_g = \frac{V_g}{V} = 1 - \frac{\rho_s}{\rho_s^*} - w\frac{\rho_s}{\rho_l^*} \tag{5}$$

where ρ_s^* and ρ_l^* (kg m^{-3}) are, respectively, the real density of solid and liquid phase.

2.2. Vapour diffusion

The vapour diffusion flux, $\mathbf{J}_v$, is classically described by a first order Fick's law:

$$\mathbf{J}_v = -D_{vs}\nabla \rho_v^* \tag{6}$$

where D_{vs} is the effective vapour diffusion coefficient in the soil. It generally depends on the tortuosity as presented in next section dealing with experimental characterization.

2.3. Liquid filtration

The liquid filtration flux appearing in Eq. (1) can be expressed by the Darcy's law extended to the non-saturated case. The validity of such description toward very low water content is questionable since the concept of liquid pressure is meaningless (Baker and Frydman, 2009; Low, 1961; Nitao and Bear, 1996). An alternative proposed by Bénet et al. (2012) is to rely on the chemical potential. Therefore, filtration transport is written:

$$\rho_l \mathbf{v}_l = -K(\nabla \mu_l - \mathbf{g}) \tag{7}$$

where μ_l (J kg^{-1}) is the mass chemical potential of liquid water, $\mathbf{g}$ (m s^{-2}) is the gravity acceleration vector. The filtration coefficient, K, refers to the soil effective conductivity by means of:

$$K = K_r K_{sat} \frac{\rho_l^*}{g} \tag{8}$$

where K_r is the relative permeability function and K_{sat} (m s^{-1}) the hydraulic conductivity at saturation.

The chemical potential is a function of the water content described by the soil/water retention curve. It is usually built by merging measurements from classical tensiometry and sorption