Modeling Soil-Water Dynamics for Diverse Environmental Needs

Pierre Martin[a], **Rabi H. Mohtar**[b*], **Pascal Clouvel**[a], **and Erik Braudeau**[c]

[a] *Centre International de Recherche en Agronomie pour le développement (CIRAD), Montpellier, France*

[b] *Purdue University, Agricultural and Biological Engineering, West Lafayette, Indiana, U.S.A.*

[c] *Institut de Recherche pour le Développement (IRD), UR 179, Pôle de Recherche Agro-environnemental de la Martinique, France.*

[*] *Corresponding author: mohtar@purdue.edu*

Abstract: Accurate representation of the top soil matrix with special attention to the scales present is important to the dynamics of water flow and fate of pollution at field, farm and watershed scales. It is also important from an agronomic stand point since agriculture still constitutes the main source of pollution at a time when many agronomic models still use empirical notions of soil hydraulic properties. The soil dynamics literature describes soil hydraulic properties independently from the soil-water medium hydro-structural dynamics. This leads to an empirical approach to represent and estimate soil hydro-structural properties such as shrinkage, water potential, field capacity, available water, hydraulic conductivity, etc. This study presents a computer model of structured soil-water medium in which the thermodynamic equilibrium is characterized by its internal hydro-structural changes.

Keywords: Soil-water; pedostructure; scale; modelling

1. INTRODUCTION

Soil water models describe soil properties independently from the aggregated organization of soils and their hydro-structural dynamic. This leads to an empirical approach of representing and estimating the physical properties currently used in these models, such as water potential, field capacity, available water, air capacity, and hydraulic conductivity (Braudeau et al. 2005a). Additionally, since the characteristics of the soil organization are not defined, modeling the biophysical and chemical possesses in the soil medium cannot be physically based on a specific soil organization and thus, to a particular type of soil.

Braudeau et al. (2004a) presented a new conceptual and functional model of the soil-water medium organization where the internal structure of the soil horizon is made up of swelling aggregates in a hierarchy of sizes. This representation leads Braudeau and Mohtar (2004a) to define a new paradigm for the soil-water interaction modeling and for the soil hydro-structural properties and parameters characterization. The soil medium organization is represented by two nested Representative Structural Volumes (RSVs), a RSV of the soil horizon and that of the soil fabric, namely the pedostructure, for which the state variables, organisational and functional, are presented in Table 1. Two new functions of the soil fabric are introduced for characterizing these functional RSVs and their dynamic: the shrinkage curve and the swelling curve. The shrinkage curve, S_hC, is defined here as the curve representing the soil fabric specific volume, *V*, in terms of its gravimetric water content, *W*, which results from a standardized experiment where an unconfined and initially water saturated soil core sample is drying at constant temperature. Under these experimental conditions, the S_hC can be assumed to represent the solid-water-air equilibrium configurations (under atmospheric pressure) and thus, define quantitatively the functional organization of the soil fabric. Consequently, the

Table 1. Pedostructure RSV (Representative Structural Volume) characterization inputs including "ideal parameters" issued from lab determination of the shrinkage curve (SC), swelling, potential and conductivity curves and calculations at model initializing.

Symbol	Description	Source	Unit
V_N	Specific volume at point N (dry state)	"	$dm^3 Kg^{-1}$ sol
W_D	Water content at point D	"	Kg soil Kg^{-1} water
W_L	Water content at point L (WC at saturation)	"	Kg soil Kg^{-1} water
W_M	Water content at point M	"	Kg soil Kg^{-1} water
W_N	Water content at point N	"	Kg soil Kg^{-1} water
K_{bs}	Points N and M SC linear phase slope	"	$dm^3 Kg^{-1}$ water
k_N	SC shape parameters at point N	"	Kg soil Kg^{-1} water
k_M	SC shape parameters at point M	"	Kg soil Kg^{-1} water
A	Time coefficient, related to the half time charge	Swelling curve	s^{-1}
E_{ma}	Potential energy of the solid phase resulting from the external surface charge of the primary peds	Potential curve	J Kg^{-1} soil
σ	Micropore water at the surface of the primary peds (empiric determination)	"	Kg water Kg^{-1} soil
K_{sat}	Hydraulic conductivity at saturation	Conductivity curve	dm h^{-1}
kma°	Residual hydraulic conductivity at Wma=0		dm h^{-1}
α	Hydraulic conductivity equation parameter		kg kg^{-1}
Ms	RSV soil mass	Calculated at initialization	Kg sol
V_D	RSV specific volume at point D	"	$dm^3 Kg^{-1}$ sol
V_{REV_D}	RSV volume at point D ($= a^2 \times h_D$)*	"	dm^3
Vs	RSV soil volume	"	$dm^3 Kg^{-1}$ sol

* RSV dimensions as defined according to medium 3D discretization

specific organizational variables, such as specific volumes, pore-volumes, water and air contents, of primary peds and of their assembly the pedostructure, are represented, at equilibrium, by a point (W^{eq},V^{eq}) of the S_hC. These organizational variables at equilibrium are entirely calculated from the S_hC characteristic parameters (Table 2), depending on only one of the two variables V^{eq} or W^{eq} since the parametric equation of the S_hC is known. From the same point of view, the swelling curve, S_wC, is understood as the increase of the specific volume of a soil fabric sample with time, V(t), when the dry aggregated sample is gently immersed in water (Braudeau and Mohtar, 2006). Measurement of the swelling curve provides the unique parameter of the swelling equation (A, Table 1), which is a coefficient of time characteristic of the clay plasma of primary peds. We will use this swelling property of the aggregated soil fabric to represent the dynamics for the soil fabric (or pedostructure) to reach the equilibrium configurations expressed by the S_hC. Thus, the characterization and parameterization of the hydro-structural functions of the pedostructure is defined by the following relations:

1. The shrinkage curve or the specific volume of the pedostructure as a function of its water content $V(W)$;
2. The swelling curve of the pedostructure specific volume as a function of time V(t) during wetting of a dry soil sample put in contact with water;
3. The tensiometric curve or the interped water potential as a function of interped water content $h_{ma}(W_{ma})$;
4. The conductivity curve or the interped conductivity as a function of the interped water content $k_{ma}(W_{ma})$.

The tensiometric and conductivity curves are the parametric variables of Darcy's law extended to the unsaturated soil medium that is described by the pedostructure model. Braudeau and Mohtar (2004b) showed that the tensiometric curve is dependent on the macropore water content and that its equation (Table 1) agrees with the osmotic aspect of the hydration pressure in water layers at the surface of the primary peds. The S_hC allows for distinguishing directly and precisely a macropore space where water flows with no or weak structural volume change from this pore space, and a micropore space (primary peds) where the movement of water is entirely related to the swelling pressure, Ps_{mi}, within the primary peds. Therefore, we will limit the Darcian water flow equation in soil to the macropore space of which the transfer functions, k_{ma} and h_{ma}, are well determined and expressed in terms of the macropore water W_{ma} (Eq. 1). The transfer equation is written such as:

$$\frac{dW_{ma}}{dt} = \rho_w V \frac{\partial}{\partial z}\left(k_{ma}\left(\frac{dh_{ma}}{dz} - 1\right)\right) - \frac{dW_{mi}}{dt} \qquad (1)$$

where the last term dW_{mi}/dt represents the dynamics of the local water exchange between the internal and external porosity of the primary peds. This term is determined by the swelling equation given by Braudeau and Mohtar (2006) and its parameter A (Table 2).

The overall objective of this article is to present a computer model of the soil water medium that can be used in an integrated biophysical or crop system model. This soil module will be able to represent the soil organizational characteristics and variables for each hydro-structural state and to model the water flow in this organization (the vadoze zone) in response to external factors namely; rain and extraction of water by roots.

Table 2. Organizational variables. In the relationships, subscripts mi and ma refer to as micro and macro.

Volume of concern	Specific volume	Specific pore volume	Water content	Non swelling water	Swelling water	Suction pressure
Pedostructure	V		W			h
Interpedal porosity		Vp_{ma}	W_{ma}	w_{st}	w_{ip}	h_{ma}
Primary peds	V_{mi}	Vp_{mi}	W_{mi}	w_{re}	w_{bs}	h_{mi}
Primary soil particles	V_s					

2. MODEL DESCRIPTION

Figure 1 (Martin et al. 2005) shows a schematic representation of the soil horizon showing its four hierarchical structural levels; namely, the horizon, the pedostruture, the primary peds and the primary particles (Braudeau et al. 2004a). In this representation, we define two hierarchical RSVs (Representative Structural Volume, in $dm^3\ kg^{-1}$) which are homogeneous in their specific state variables. The first RSV is that of the soil horizon, V_{hor} which is large enough to include cracks or fissures that open to air when soil dries. It is considered homogenous in the vertical direction with a vertical porosity Vp_{vrt} and density $1/V_{hor}$. This RSV is delimited by the upper and lower limits of the soil horizon. Thus its volume change is limited to the vertical dimension. The second RSV is that of the soil fabric inside the soil horizon RSV that excludes the vertical porosity. This soil fabric RSV corresponds to the pedostructure where the specific volume V and the functional aggregated organization are defined according to Braudeau et al. (2004a,b). The pedostructure is composed of nested functional specific volumes defined based on the shrinkage curve (Table 1). This RSV includes the primary peds (V_{mi}) and the pore space created by their assembly (Vp_{ma}). The primary peds are quantitatively defined by their air entry point which is identified at point B on a continuously measured shrinkage curve.

All the structural specific volumes for all RSVs are summarized in Table 1. All variables of the nested RSVs are in reference to the mass of primary particles. This mass is homogeneously distributed over the horizon RSV. In the absence of vertical porosity, $V_{hor} = V$, which takes place at water contents larger than field capacity. It is important to note that the solid mass is a constant in the two RSVs once they are delimited, and that all their organizational variables are in reference to these fixed masses.

Thus, this representation of the functional soil organisation in two nested RSVs allows us to relate the structural variables between these two RSVs using simplistic geometrical relationships. From this point of view, the in situ shrinkage curve, if measured, represents the equilibrium configurations of the soil water medium for the entire range of water contents. As this in situ shrinkage curve depends on the external pressure on the soil, as well as on the overburden and hydrostatic pressure. The question that arises is how these pressures act on the shrinkage and swelling curves in situ, and if this can be related to the shrinkage and swelling curves measured in the laboratory as characteristic functions of the soil fabric. This problem is being investigated.

A conceptual schematic representation of the soil-water medium dynamics is shown in Figure 2 (Braudeau et al. 2005b). The representation refers to a unit volume of the pedostructure in a hydraulic state between W_C and total saturation W_L. All the variables of this representative volume are "gravimetric" (water contents, specific volumes, and pore volumes) expressed in reference to the mass of the primary particles

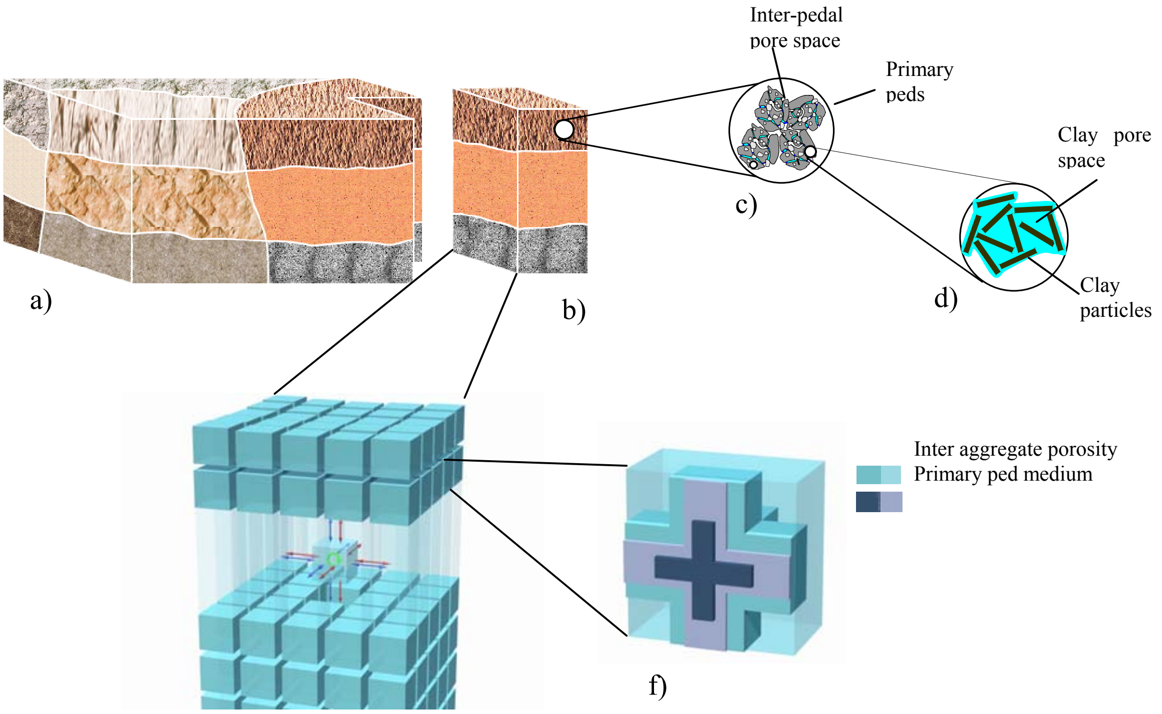

Figure 1. Schematic representation of the soil horizon and its modeling representation: a) Soil horizon, b) Pedon composed of vertical porosity (cracks and fissures) and pedostructures, c) pedostruture description, d) primary ped composed of clay plasma porosity and primary particules, e) conceptual model representation and water flows in the matrix, and f) computational pedostructure unit.

which is considered constant for this unit volume. The clayey plasma of the primary peds (light-gray and gray) defined as micro-porosity (Vp_{mi}) and the inter-ped pore space (dark gray and white) defined as the macro-porosity (Vp_{ma}), are represented by two compartments which are in contact through a transitional zone at the surface of the primary peds (black line). The importance of this transitional zone for the interped water potential determination was outlined by Braudeau and Mohtar (2004b). Micro and macroscopic porosities are considered continuous within and between the representative volumes in all directions. The residual water, w_{re}, which does not contribute to any swelling, shrinkage, nor displacement of water, is represented by the center of the micro-porosity, surrounded by the micro-porosity swelling water, w_{bs}.

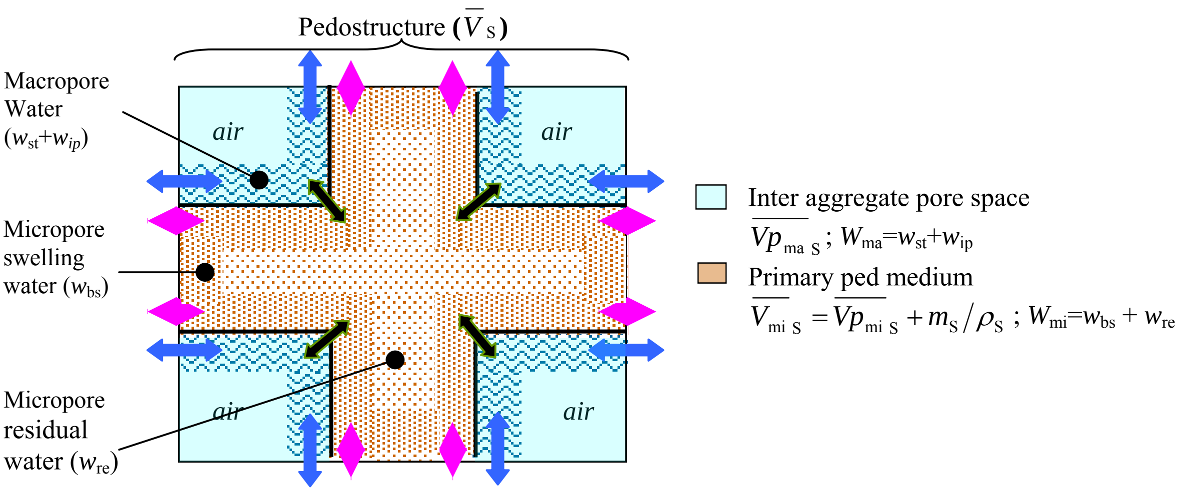

Figure 2. Functional model of the pedostructure, the RSV of the soil fabric. Arrows represent the three types of controlled water flux. In the relationships, subscripts mi and ma refer to as micro and macro, and Vp to as pore volume; and m_S is the mass of the structured solid phase contained in the RSV.

3. MODEL APPLICATION

Sample simulations using the model is shown in Figure 3 (Martin et al. 2005). The figure shows the specific volume as a function of water content during the wetting and swelling cycles. Figure 4 shows a simulation for a constant rain through a soil profile (described in Table 3). The figure shows the steady state equilibrium shrinkage curve (solid line) along with the wetting cycle during irrigation. The soil was initially at wilting point and it follows through a wetting phase (dotted line) until it reaches equilibrium state. The equilibrium state is indicated through the merger of the two lines.

Table 3. Simulation parameters

Description	Values
Percent of sand (%)	19
Percent of clay (%)	21
Bulk density at field capacity ($kg.dm^{-3}$)	1.36
Conductivity at saturation ($dm.h^{-1}$)	0.105
Initial soil status (homogeneous on 2 meters depth) (Kg water.Kg $soil^{-1}$)	0.131
Constant rain input (mm/h)	10

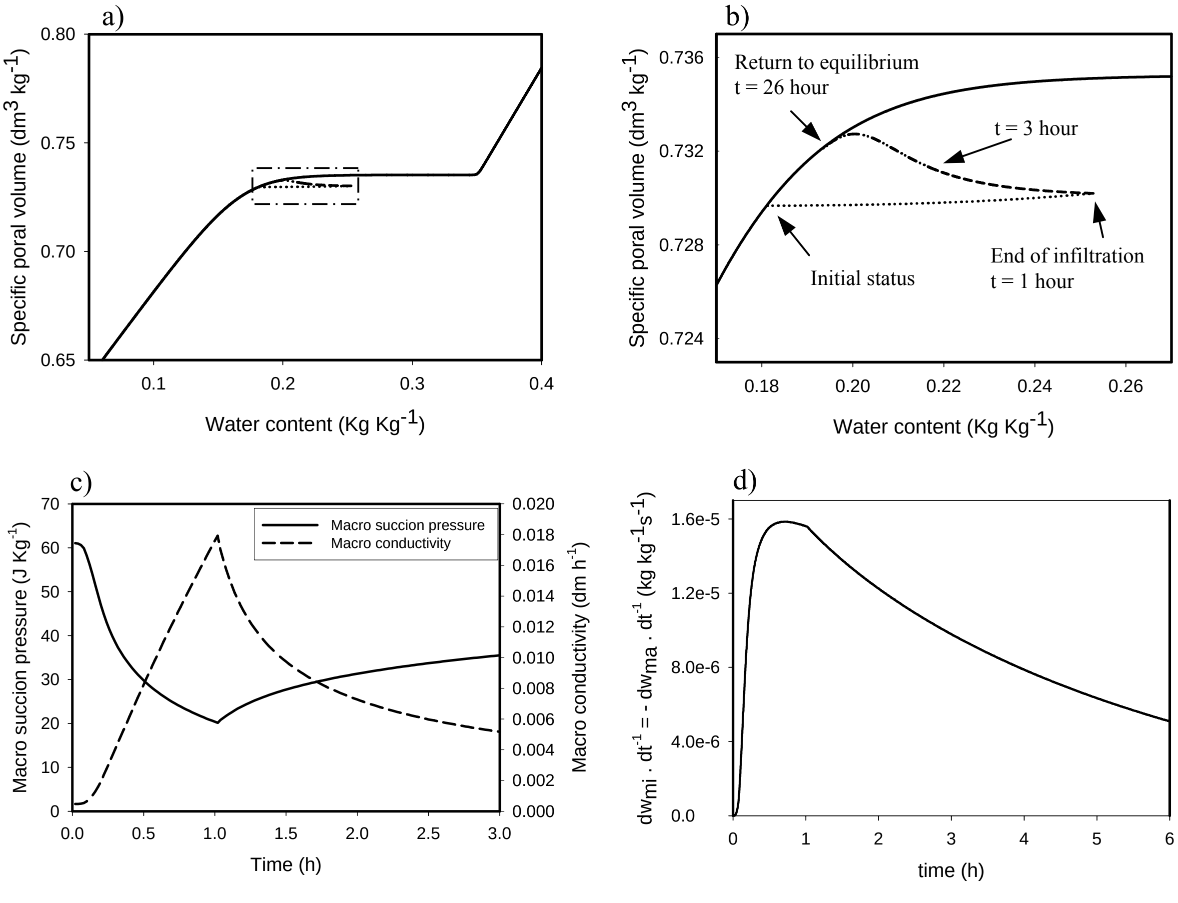

Figure 3. Sample simulation results using the model for a constant rain with a duration of 1 hour. In this situation, the soil requires 26 hours to return to equilibrium. Results are described in the following graphs : a) shrinkage curve for the simulated soil b) a closer look at the shrinkage curve, c) macro pore conductivity (Kma) and macro suction pressure (hma) corresponding to Darcy's law parameters, d) amount of water exchanged between macro porosity and micro porosity per second.

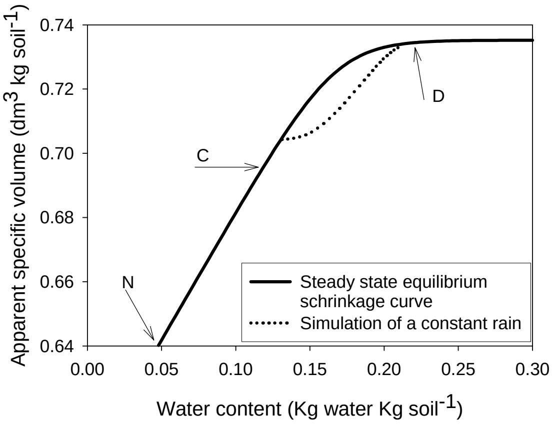

Figure 4. Sample simulation result using the model for a constant rain of 10 mm.h^{-1} .

4. CONCLUSION

A functional model of soil water medium characterization and modelling is presented and demonstrated. The uniqueness of the new model is in its innovative functional characterization of the soil water medium which uses its characteristic properties of shrinkage, swelling, conductivity and water potential. The approach opens the door to further scaling to include field and watershed scales and to more accurately simulate water and solute transfer in pedostructure and field scales.

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