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Integrative Environmental Modeling

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Abstract

A fundamental problem that agro-environmental sciences have to face today is the lack of interdisciplinary linkages between the various disciplines dealing with agriculture and environment and the physics of the “soil medium” organization, which is the object of study of the pedology. Currently, the soil medium is far from being considered as the organized physical medium providing the physical conditions for life or development of the numerous biotic and abiotic processes that are taking place in soils. This contribution describes an integrative approach for understanding and modeling the natural environment, in which the soil–plant–atmosphere system is the physical unit of description. We call for distinguishing two kinds of environmental modeling cycles: a local modeling cycle, which is physical and multi-scale according to the soil medium organization, and a global modeling cycle, out of scale of processes, which is necessarily monoscale and statistically based. We propose a way for implementing the physical modeling cycle, inside and at the basis of the global cycle, by using the new concept of Structural Representative Elementary Volume (SREV) for the local-scale description instead of the well-known Representative Elementary Volume (REV) that is valuable only for the global scale. This implementation is possible only with the development of a new discipline in soil science—hydrostructural pedology—that offers a unique theoretical framework for modeling the hydro-functioning of the soil–plant–atmosphere system using physically based equations that take into account the local multi-scale organization of soils and their hydrostructural properties.

INTRODUCTION

High-level meetings between global leaders to develop or outline policies and strategies for global resources security, especially, arable soils and water, are critical for the healthy future of our planet. \[1\] It is clear from these discussions that, to face the climate change challenges, understanding and optimizing of agricultural practices as well as the management of agricultural or ecological systems are key point that require the development of two specific tools: i) a multi-scale model for simulating the functioning and evolution of the agro- or ecosystem being considered; and ii) an associated information system, generally geospatially referenced such as a georeferenced information system (GIS) that stores the characteristics and parameters required by the model. These two tools are used for the modeling of the soil–plant–atmosphere system according to the local conditions of the natural environment (soils, climate) and land use. \[2\] The major problem that these tools have to overcome is the acknowledgment of the hierarchized organization scales and the transfer of information from the local scale of occurrence of processes in the soil medium, where a physical modeling is appropriate, to a global scale of modeling where the effects of these processes are globally and statistically modeled as phenomena appearing at the soil surface. Actually, the questions of interdisciplinary relationships, uncertainties of data, and sustainability of agro/ecosystems, are all arising from the problem of transfer of information across scales. \[3–6\] The two questions that the environmental modeling tools are expected to answer can be formulated as the following:

- How to observe, describe, and model, in a physically based and integrative framework, the water dynamics in the natural environment where soils constitute the natural multiscale infrastructure? The scientific discipline covering the soil and water characterization, mapping, and modeling in the natural environment is the hydropedology. \[7\] It includes numerous specialties of the earth sciences that today are providing more or less empirical responses to that fundamental question. \[8\] The problem lies in the physical characterization and modeling of the hydrofunctioning of the soil–plant–atmosphere system such as that represented in Fig. 1, and is considered as representative of a soil-mapping unit. Its characterization and modeling should be developed considering two fundamental characteristics of the soil medium constituting the infrastructure of this organized system: i) the multiscale organization of soils, both horizontally (the pedological cover) and vertically (the soil profile or pedon), including the internally nested organization of the soil medium, \[9,10\] (horizon, pedostructure, and
primary peds) as schematized in Fig. 2; and ii) the hydrostructural functionality of these internal organizations that determines all the physical properties of the pedon and thus, the corresponding soil-mapping unit of the pedological cover. These two points were specifically treated by Braudeau and Mohtar, leading the authors to propose a new paradigm of characterization and modeling of the hydrostructural functioning of soils represented by the soil–water model Kamel. How do we address the diversity of vision or thinking about soil (typology, criteria of classification, scale of mapping, determinant properties, etc.) and its physical relationship with the object of study of a particular discipline (microbiology, remote sensing, etc.) among the agro-environmental sciences? This question relates to the interdisciplinary coupling between the models elaborated by a particular discipline that studies a specific process in the soil, and the soil medium that actually constitutes the physical environment of this process to be modeled. It becomes obvious that to model and simulate any process in the soil medium, as well as in the air or in a plant, an appropriate description of the thermodynamic environment of the process is needed as shown in Fig. 1. Answering this question means developing a unique theoretical framework of modeling, for generically modeling the hydric dynamics of the soil–plant–atmosphere system, valuable for all the various agro-environmental situations existing in the world. To be generic, the framework must use physically based parametric equations, the parameters of which characterize the multiscaled soil organization locally encountered in each situation. Therefore, to develop this multiscale modeling framework making possible the physical simulation of the hydrodynamics of the complex system described in Fig. 1, an alternative paradigm to the
continuous porous media mechanics, which does not take into account the internal organization of the soil, should be used, as proposed by Braudeau and Mohtar.\cite{9}

We want to show hereafter how the improvement of any agricultural or ecological system can be envisioned based on such a unique framework of modeling, making possible the joint use of physically based simulation models with their associated georeferenced information system, which contains all the needed modeling parameters characterizing the soil medium organization.

CHARACTERIZATION AND MODELING THE NATURAL ENVIRONMENT

Two Cycles of Modeling

A general picture of the activities of characterization and modeling in the agro-environmental sciences is presented in Fig. 3 that represents, in principle, the two environmental modeling cycles, global and local, required to formulate all aspects of the nature–society relationship covered by the agro-environmental sciences. On the right side of these cycles, the assessment (inventory, mapping), hydro-functional characterization, and hydrodynamics modeling (simulation of fluxes, processes, and productions) of the soil–plant–atmosphere system, are necessarily at the core of any problem of optimization and sustainability of the soils and water management in agro- or ecosystems simulated on the left side of the modeling cycles, where all the societal constraints have to be taken into account.

Specific Properties of the Two Cycles

According to Fig. 3, the two modeling cycles already differ from the beginning due to a representation of the internal organization of the physical medium (soil, water, and atmosphere) that is fundamentally different in the two cases: one, represented by the red solid line, recognizes the hierarchical organization of the medium and can be named “local-scale modeling” because it takes a reference to the soil structure; the other, represented by the black line, conceals any internal organization by using the concept of representative elementary volume (REV), and thus cannot be other than a “global-scale modeling” where any reference to the structure of the medium is eliminated.

Therefore, only the gray cycle (gray two-way arrows), where relationships and transfers of scale are based on physical and deterministic laws, allows for a return to the reality of the system.

Fig. 3 The two cycles of the environmental modeling and its applications.
of the natural organization, and thus for a true estimation of the real evolution or changes of this natural organization (e.g., ecosystems).

The current modeling approach of the water cycle in the soil–plant–atmosphere organization (critical zone) is fundamentally based on the REV concept and, because of this, entirely makes it part of the global modeling cycle represented in Fig. 3 (black one-way arrows). In soil–water models based on the REV concept, the internal soil organization is represented as a stack of “black boxes” where the structure of the soil medium is considered as a homogeneous mixture of solids, water, and air. This prevents the modeler to consider the thermodynamic interaction between minerals composing the soil structure and the water at their surface.\[9\] This constitutes the principal reason for the inability of this kind of modeling to physically model and simulate processes in the soil medium that are at the origin of phenomena modeled at the global scale.\[14\]

IMPLEMENTING THE PHYSICAL MODELING CYCLE INSIDE THE GLOBAL CYCLE

The great challenge of the agro-environmental sciences today should be the installation of the physical modeling cycle. According to the questions seen in the introduction and the scheme in Fig. 3, this challenge calls for two new scientific developments: 1) establishing the appropriate methodology for a multi-scale representation of the hierarchized soil organizations, horizontally (pedological cover mapping) as well as vertically (pedon, structural representative elementary volume (SREV) of the soil map unit); and 2) establishing the appropriate system of thermodynamic equations and descriptive variables to physically characterize and model the hydrofunctioning of the soil medium as the conditioning medium controlling the development of all the processes, biotic or abiotic, in soil. These two developments constitute the main objectives of the *hydrostructural pedology* discipline that we present beside the hydropedology in Fig. 4; they consist of the following.

**Mapping the Pedological Cover According to the System Approach**

Soil mapping will be made according to the Kamel paradigm.\[9,11–13\] In principle, primary soil-mapping units are defined by their hydrostructural properties that can be said to be “homogeneous” everywhere in the soil unit. These hydrostructural properties are represented by the shrinkage curve and the water retention curve that can be precisely measured together on the same soil sample (cylinder of 100 cm³) using the Typosoil® apparatus.\[15\] This new methodology for the soil physics characterization matches with the pedogenetic classification of the soil unit and thus, should fully belong to a geomorphological unit of the landscape that is easily defined and delineated by

![Diagram](image_url) **Fig. 4** The hydrostructural pedology, a new discipline in agro-environmental sciences, beside and complementary to the hydropedology, for a physical and multi-scale modeling of the natural environment.
satellite imagery using remote-sensing expertise. Since the pedon is an SREV of the primary soil-mapping units (see Fig. 2), the hydrostructural characterization and modeling of the pedon using Kamel\(^6\) means a quantitative description of the internal organization of the entire soil-mapping units: horizons and pedostructures, along with their hydrostructural behavior at every depth in the soil.

The hydrostructural characterization of the pedostructure in the laboratory is made through the measurement of four hydrostructural characteristics: shrinkage curve, water retention curve, hydraulic conductivity curve, and swelling curve of the primary peds. The two former are simultaneously measured using a new apparatus, Typosoil, allowing for accurately calculating the physical parameters of equations of state of the thermodynamic Gibbs free energy function for the pedostructure.\(^{15}\) The two others are measured using the existing commercialized equipment. This equipment constitutes the chain of measure of all the hydrostructural characteristics of the pedostructure, which is, ultimately, the fundamental structural element constitutive of a soil horizon and, as such, must be archived in pedological data bases for being taken into account through Kamel\(^6\) in every modeling belonging to the local modeling cycle.

Therefore, the pedological map of which the first level of mapping corresponds to soil types units characterized by their pedon provided with its hydrostructural parameters, should henceforth constitute the first layer of any GIS that takes the natural environmental organization as the medium of life and development. We propose to call this particular GIS natural environmental organization georeferenced information system, or “NEO-GIS.”

**Using the Appropriate System of Thermodynamic Equations and Descriptive Variables**

To be part of the local modeling cycle, the modeling approach of the soil–plant–atmosphere organization should be able to describe the true nature of the soil organization as a natural, multiscaled, and structured physical medium, made of mineral particles embedded by water and air according to a specific organization characteristic of the soil medium. It is this specific organization, named pedostructure by Braudeau et al.,\(^{10}\) that offers the hydrothermodynamic conditions (poral space and pedoclimate) to the development and the activity of all biogeochemical processes that take place in the soil medium of the soil–plant–atmosphere system (see Fig. 1). So, these processes must be physically modeled according to the hydrostructural and thermodynamic properties of the pedostructure. Braudeau et al.,\(^{15}\) demonstrated that the adoption and the use of the SREV concept proposed earlier by Braudeau and Mohtar\(^9\) is the necessary condition for researching and finding the correct system of descriptive variables and thermodynamic equations that must be used in the local and physical modeling cycle represented in Fig. 3. This allowed Braudeau and Mohtar\(^{14}\) to present the complete theoretical framework of the hydrostructural characterization and modeling of the soil, as the multi-scale soil component of the soil–plant–atmosphere system considered in agroenvironmental models. The new model represents a pioneer soil–water model that provides the hydrostructural and thermodynamic equilibrium state of the soil medium, at each point of the soil profile and, as such, the changing pedostructural and pedoclimatic conditions for organisms living in the soil depending on the local water content.

**CONCLUSION**

We presented the idea of “local modeling cycle” of the environment, representing the reality on which the global modeling cycle should build. This is made possible through the development of the hydrostructural pedology, a new discipline in soil science based on a new theory of thermodynamics of the soil medium organization, leading to a new methodology of the soil medium characterization, soil mapping, and soil water modeling. One of the important products of the hydrostructural pedology is the NEO-GIS, which is the appropriate system of information containing all georeferenced data needed for the “global modeling cycle” that addresses larger scales of observation (from watershed to regional). Using Kamel associated to the NEO-GIS to cover a zone of study allows us to physically model the natural processes at their local scales of occurrence within the soil medium organization of the soil–plant–atmosphere mapping unit. All characteristic data of these mapping units, including the hydrostructural parameters of pedostructures encountered, must be stored in the NEO-GIS. The physical equations used are the equations of state of the pedostructure locally determining, at each depth of the soil, the hydrostructural and thermodynamic equilibrium of the soil medium, according to the gravimetric water content related to the thermodynamic and gravitational movements of water through the soil–plant–atmosphere system modeled by Kamel. Kamel and the NEO-GIS become the appropriate tools to be used for optimizing the management of soils and water in agro/ecosystems, taking into account the quantity and the quality of water as well as the environmental constraints.

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