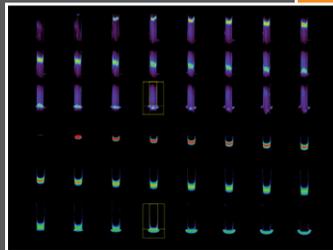


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This paper introduces the special section on Patterns in Soil–Vegetation–Atmosphere Systems: Monitoring, Modeling, and Data Assimilation. It briefly presents three key topics: (i) the development measurement techniques, (ii) the development and improvement of coupled numerical models, and (iii) the long-term monitoring of key state variables and fluxes.

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# Patterns in Soil–Vegetation–Atmosphere Systems: Monitoring, Modeling, and Data Assimilation

In this special issue, we present recent scientific work that analyzes the role of patterns in soil–vegetation–atmosphere (SVA) systems over a wide range of scales ranging from the pore scale up to mesoscale catchments. Specific attention is given to the development of novel data assimilation methods, noninvasive measurement techniques that allow mapping spatial patterns of state variables and fluxes, and two-way coupling of models in a scale-consistent way. “Patterns in Soil–Vegetation–Atmosphere Systems” is also the research topic of a collaborative research center (TR32) between the universities of Aachen, Bonn, and Cologne and the Forschungszentrum Jülich. In this center, which is funded by the Deutsche Forschungsgemeinschaft, on the basis of an international evaluation, scientists covering a broad range of earth science disciplines are working together. During June 11–12, 2010 the center organized its first international workshop in Aachen. The contributions presented in this special issue of *Vadose Zone Journal* include contributions from the collaborative research center and external contributions, both from Germany and worldwide.

Abbreviations: CLR, Community Landsurface Model; CR, capacitive resistivity; DC, direct current resistivity; DTS, distributed temperature sensing; EC, eddy covariance; HHT, Hilbert–Huang transform; MRI, magnetic resonance imaging; NMR, nuclear magnetic resonance; SIP, spectral induced polarization; SVA, soil–vegetation–atmosphere.

**The system of soil, vegetation, and the adjacent atmosphere** is characterized by complex patterns, structures, and processes that act on a wide range of time and space scales. While the exchange of energy, water, and carbon is continuous between compartments, the pertinent fluxes are strongly heterogeneous and variable in space and time. Therefore, quantitatively predicting the systems’ behavior constitutes a major challenge.

Patterns and structures play an important role in controlling and determining the spatial and temporal variability of fluxes of water and carbon dioxide within and between the compartments of the soil–plant–atmosphere system (Flury et al., 1994; Raich and Potter, 1995; Vereecken et al., 2007). They may result from either deterministic processes or from processes causing spatial dependency and autocorrelative behavior or both (Levin, 1992; Borcard and Legendre, 2002). In addition, patterns occur at different hierarchical scales, ranging from the pore scale to the global scale. Patterns and structures in soil–plant–atmosphere systems are intimately linked to the notion of heterogeneity of state variables, parameters, and fluxes. Improving our understanding of soil–plant–atmosphere systems therefore requires (i) the development of measurement techniques that enable us to characterize the spatial structure of key properties across scales, (ii) the development and improvement of coupled numerical models and data assimilation methods, and (iii) the long-term monitoring of key state variables and fluxes for model evaluation.

## ♦ Characterizing Patterns and Structures in Soil–Plant–Atmosphere Systems

Measurement methods mapping state variables and fluxes of key processes are needed to quantify the impact of structures and patterns on these processes. It is well known, for example, that the spatial variability of hydraulic properties determines the fluxes of water and solute transport in soils and aquifers. Stochastic theories have been developed that explicitly require information on the statistics of hydraulic properties in terms of second-order stationary moments. Recent advances have shown, however, that this approach does not capture the impact of connected geological structures over distances larger than the correlation scale (e.g., Zinn and Harvey, 2003). Connectivity in hydraulic properties occurs

on all scales, starting from the pore scale to the regional and catchment scales. At the core-scale level, new noninvasive measurement techniques are being developed that provide the opportunity to identify and characterize these connected structures; examples include magnetic resonance imaging (MRI), spectral induced polarization (SIP), and neutron tomography. At the lysimeter and field scales, hydrogeophysical measurement techniques provide the opportunity to characterize the spatial organization of state variables such as moisture content and bulk electrical conductivity (Vereecken et al., 2004; Robinson et al., 2008). This information can be used in joint inversion approaches by combining forward electromagnetic and hydrological modeling to derive the spatial organization of hydraulic properties.

These new methods also allow characterizing the spatial and temporal dynamics of root systems. Earlier approaches to calculate evapotranspiration at core and field scales used empirical functions, such as those derived by Feddes et al. (1974), which are based on the assumption that water uptake is proportional to root length density. Recent findings have shown that this is not always the case (Draye et al., 2010; Garré et al., 2010). The importance of structural organization of root systems on transpiration fluxes and solute transport at the field scale is not yet fully understood. This is due to the lack of appropriate measurement techniques and numerical models. Recently a combined three-dimensional model for water flow, solute transport, and root water uptake was proposed by Javaux et al. (2008). This model is applicable at the plant level and allows calculating the evapotranspiration fluxes from mechanistic principles.

Remote sensing techniques allow the characterization of spatial structures in terms of vegetation and land use, but also state variables such as temperature and soil moisture. Data assimilation methods can use this information to derive structures of other properties determining fluxes of water and carbon. Recent developments have shown that it is possible to derive parameter estimates in combination with the state update of variables. These methods should be further explored to derive structural information of key parameters.

Wireless sensing networks provide a unique opportunity to characterize, with high spatial and temporal resolution, the dynamics of important state variables such as water content, bulk electrical conductivity, and soil temperature. Bogaen et al. (2010, this issue) developed a wireless sensor network to measure the spatial and temporal dynamics of soil moisture content values at the catchment scale. These networks bridge the measurement gap between local-scale measurements and remotely sensed information (Vereecken et al., 2008). By combining existing and novel satellite platforms, it is now possible to obtain a full spatial coverage of soil moisture patterns across all scales.

Currently, only ground-based and airborne monitoring techniques allow one to monitor the small-scale structures and patterns

induced in the atmosphere by two-way interaction processes with the surface and subsurface. While passive microwave radiometry allows continuous high temporal resolution monitoring of low spatially resolved water vapor and temperature profiles in the planetary boundary layer (e.g., Löhnert et al., 2004; Kneifel et al., 2009), active lidar techniques are able to provide water vapor fields in high spatial resolutions (e.g., Wulfmeyer et al., 2008), although currently at limited temporal resolution. A new generation of Doppler wind lidars is upcoming (e.g., Mann et al., 2009), which will resolve the turbulent structure of the boundary layer wind field in space and time and provide a basis for validating upcoming coupled models with the atmospheric compartment simulated by Large Eddy Simulation models on the meter scale.

## ♦ Coupled Modeling of Soil–Vegetation–Atmosphere Systems

Improving our understanding of SVA systems requires the development of coupled numerical models and data assimilation methods. In recent years, considerable progress has been achieved with a strong focus on a holistic view and theoretical representation of the system under consideration. That is, the interconnection of different compartments has been clearly acknowledged across different scientific disciplines, which resulted in sophisticated coupled modeling approaches from the subsurface into the atmosphere. The goal is to account for various nonlinear fluxes and exchange processes across multiple space and time scales to resolve and explain various structures in the two-way feedback between different compartments.

In the hydrologic sciences, the development has been mainly concerned with relaxing the upper boundary condition at the land surface, which was treated traditionally as simple flux and operational surface water boundary (see review by Ebel et al., 2009). Advancements include fully coupled groundwater–surface water models (VanderKwaak and Loague, 2001; Panday and Huyakorn, 2004; Kollet and Maxwell, 2008; Dawson, 2008; Sulis et al., 2010); incorporation of land surface processes such as evaporation from bare soil and transpiration by plants (Kollet and Maxwell, 2008); and full mass, energy and momentum exchange with the atmosphere via coupled land surface models. On the other hand, in atmospheric sciences, major advancements have focused on improving the lower boundary condition (i.e., the subsurface), which was treated traditionally as simple box or force restore models covering only the top soil layers and ignoring the deeper subsurface and groundwater dynamics. New developments include more sophisticated multi-layer one-dimensional soil columns, parameterized groundwater flow models (Seuffert et al., 2002; Yeh and Eltahir, 2005; Niu et al., 2007) and fully three-dimensional continuum approaches also based on Richards' equation (York et al., 2002; Maxwell et al., 2007).

Application of these coupled models of SVA systems led to considerable insights with regard to patterns and structures observed

in land surface states and fluxes (Kollet and Maxwell, 2008) and in atmospheric processes (Patton et al., 2005). It appears that a general consensus has been established in the hydrologic and atmospheric sciences community that coupled physics-based models of SVA systems are promising tools for understanding patterns and structures due to their better representation of the nonlinear physics and exchange processes across various space and time scales.

Since the aforementioned new research strongly emphasizes physics-based approaches in characterizing SVA systems, state variables and fluxes are included that exhibit a potential predictive capability, lending themselves to data assimilation approaches, that is, the formalized integration of observations and theoretical models. Various data assimilation techniques have been applied in atmospheric sciences in operational forecasting systems for quite some time, including the state of the land surface (e.g., Seuffert et al., 2004; Wilker et al., 2006). Also in hydrologic sciences, data assimilation has been used routinely in flood forecasting for streamflow observations (e.g., Warrach-Sagi and Wulfmeyer, 2010) even in operational environments. Only recently, hydrogeologists have adopted this technique successfully to adjust sequentially parameters and states of groundwater flow models for water management purposes (Hendricks-Franssen and Kinzelbach, 2008). Current scientific and technical challenges deal with efficient assimilation of remotely sensed airborne and satellite information in conjunction with in situ measurements of state variables and fluxes that are available at extremely diverse spatial and temporal scales. More specifically, observation, input parameter, and model structure uncertainty must be honored simultaneously in novel data assimilation approaches to obtain meaningful solutions. Thus, a deep understanding of retrieval algorithms, limitation of model physics, and scaling behavior of coupled, nonlinear processes (among others) is required in a concerted interdisciplinary research effort.

## ◆ Importance of Patterns and Structures for Land Surface–Atmosphere Interactions

Land surface–atmosphere interactions are strongly determined by the spatial and temporal structure and variability in time and space of state variables in SVA systems. These include, for example, soil water content, the leaf area distribution, topographical properties, and meteorological properties. Quantifying the scales of heterogeneity in surface vegetation and soil moisture is essential to understand and model the land–atmosphere interactions (Salmun et al., 2009), but also for correct state parameter retrieval by satellite-borne sensors (e.g., Drusch et al., 1999). Soil moisture fields typically show a clear spatial organization that is closely related to soil properties, vegetation, climate, and topography (Western et al., 1998; Western and Bloeschl, 1999; Hwang et al., 2009). Spatial patterns and temporal dynamics of soil moisture have a major influence on runoff generation, among other watershed

responses (Blume et al., 2009). Western et al. (1998) showed, for example, that connectivity functions and integral connectivity scales provide promising means for characterizing features that exist in observed spatial fields and that have an important influence on hydrologic behavior. Correctly predicting effective fluxes of water (e.g., Schomburg et al., 2010), but also of carbon dioxide, requires a correct parameterization of this spatial organization (e.g., characterization of subgrid variability).

Structures in soil moisture fields not only influence water and energy balances, but also affect the spatial and temporal variability and dynamics of carbon dioxide emissions in SVA systems. The total respiration in many ecosystems is dominated by soil carbon fluxes from heterotrophic and autotrophic respiration (Raich and Potter, 1995; Martin and Bolstad, 2009). Many studies have focused on the analysis of spatial patterns in soil carbon storage (see Bedison and Johnson, 2009, and references cited therein), and the temporal dynamics of CO<sub>2</sub> emissions and its relation to temporal dynamics of temperature and soil moisture (Hanson et al., 1993; Almagro et al., 2009). For example, at the global scale, the rates of soil CO<sub>2</sub> efflux were found to correlate significantly with temperature and precipitation and less with soil carbon pools, soil nitrogen pools, or soil C/N. In addition, soil carbon emissions have a distinct seasonal pattern, with maximum emissions coinciding with periods of active plant growth (Raich and Potter, 1995). Fewer studies have analyzed the joint effect of spatial patterns in soil organic carbon, soil moisture content, and soil temperature on soil CO<sub>2</sub> effluxes in a temporal setting.

## ◆ Content of the Special Section Methods for Characterizing Spatial and Temporal Structures

Characterizing flow processes at the pore to local scale is important for an improved understanding of field-scale processes, such as moisture redistribution and evapotranspiration fluxes. Several contributions have addressed the potential and value of using non-invasive methods to characterize flow and transport processes in soils and subsurface environments. Song (2010) discussed recent progress made in nuclear magnetic resonance (NMR) applications in sandstone and carbonate rocks. Current areas of research include the physics of internal magnetic fields, the use of two-dimensional MRI to characterize pore structures, the decomposition of heterogeneity and the mathematics of Laplace inversion. He also pointed out the potential of these developments, which have been targeted at hard rock environments, for use in partially saturated media such as the vadose zone. Haber-Pohlmeier et al. (2010) used for the first time a Gd-DTPA tracer to monitor the distribution under flow conditions in a packed and undisturbed soil material using MRI. For both soil columns the presence of soil structures on the flow pattern could be identified. Preferential flow paths in the undisturbed soil column were detected and mapped, providing

spatially highly resolved information that can be used to validate mathematical transport models

Mohnke and Klitzsch (2010) present microscale simulations of transverse NMR relaxation in the presence of internal gradients in porous media. They developed a model that simulates transverse NMR relaxation processes in porous media to examine the effect of physical and hydraulic parameters on longitudinal ( $T_1$ ) and transversal ( $T_2$ ) relaxation times. The model explicitly accounts for the presence of coupled pore systems that is typically not considered in conventional models. They found that ratio  $T_2/T_1$  depends on the pore sizes leading to pore size-related effective transverse surface relaxation. This measure can be used to correct estimates of pore-size distributions, and thus permeability values from NMR measurements. In addition to NMR and MRI methods, SIP is increasingly being used to characterize the pore systems of rock and soft sediments, such as soils. Volkmann and Klitzsch (2010) present numerical simulations of frequency dependent complex resistivity of three microscale rock models based on ion transport in the pore fluid and at the fluid-rock interface in an electrical field. With these simulations, they showed the effect of pore length, pore diameter, and fluid conductivity on the polarization signal of porous media. These models will allow better interpretation of SIP signals for estimating hydraulic parameters.

Another widely used method to characterize field scale soil moisture patterns is electromagnetic induction. Martinez et al. (2010) used this method to capture changes in soil conditions and to identify the sources of observed variability in a managed vertisol. Using time lapse measurements they showed the existence of time-stable moisture content patterns that depend on topographical and management characteristics and significant correlations with soil porosity and infiltration properties.

Typically, direct current resistivity (DC) methods used in hydrogeophysics to characterize and image subsurface environments are time consuming leading to a low measurement speed to data density ratio. Neukirch and Klitzsch (2010) show that capacitive resistivity methods (CR) are a time and labor saving alternative to the classical DC methods. They adapted DC inversion programs for CR data to minimize systematic inversion errors and to identify optimal dipole-dipole configurations.

Using NMR relaxometry, Haber et al. (2010) observed water exchange between different pore classes in unconsolidated, saturated soil samples. For the first time, this dynamic behavior is characterized using the two-dimensional NMR  $T_1$ - $T_2$  relaxation exchange that results in distribution functions at constant frequency that can be quantitatively interpreted. Thus, water mobility is distinguishable for heterogeneous soil samples across different pore classes, which is of major importance in soil physics.

Schneider et al. (2010) investigated the influence of the design and internal heterogeneity in waste rock cover systems on the effectiveness prevention of infiltration and enhancement of evapotranspiration in a semiarid, monsoonal climate region. Application of two different cover designs shows the strong impact of internal heterogeneity of the different covers, which results in a strong variability in the drainage rates. This has to be accounted for in the cover design.

## Modeling Coupled Processes in SVA Systems and Data Analysis

Steenpass et al. (2010) explored the potential of using soil surface temperature observations from infrared measurements in the inverse estimation of soil hydraulic properties. Synthetic modeling studies reveal the feasibility of the suggested approach and demonstrate reduction of parameter uncertainty if soil moisture profile measurements are included in the analysis. Application to field data corroborated these findings and showed that the proposed approach is useful in estimating shallow soil properties using areal infrared measurements.

Rudi et al. (2010) applied the Hilbert-Huang transform (HHT) to long-term hydrologic time series of river discharge to extract information on local patterns and structures. The advantage of HHT over commonly applied Fourier and wavelet analyses is its applicability to nonuniform time grids. In addition, the authors showed that the associated Hilbert spectrum offers strongly improved local information, which in the case of the Fourier and wavelet transform may be smeared. With respect to model parameterization, HHT can be used to considerably reduce the time series data and extract only relevant frequencies, arriving at a reasonable approximation containing all important information.

Vanderborght et al. (2010) studied different sources of variability in bare soil evaporation,  $E$ , derived from eddy covariance measurements at the field scale using coupled hydrologic models. The field under consideration is characterized by a distinct topographic gradient and spatial patterns in hydraulic soil properties. While an increased gravel content in the upper part of the field could be linked to decreased  $E$  rates, only the presence of a shallow water table in the applied models fully explained the observed spatial  $E$  patterns. Thus, the unique experimental and theoretical study provides direct evidence of the influence of groundwater dynamics on atmospheric processes via the shallow vadose zone.

Sciuto and Diekkrüger (2010) analyzed the influence of soil heterogeneity and spatial discretization on the water balance modeling in a headwater forest catchment using the coupled subsurface-surface model HydroGeoSphere at 25- and 100-m spatial resolution. The study clearly showed that spatial aggregation of soil moisture more negatively influences the results, because of the nonlinear relationship between soil moisture and soil hydraulic properties, than a simple sampling approach. Thus, preserving the full scale of

nonlinearity in the processes by sampling is the preferred method when modeling with lower resolution compared to state variable aggregation approaches.

Using a fully integrated subsurface–land surface model, Maxwell (2010) studied the impact of subsurface heterogeneity, including fractured bedrock, on infiltration characteristics and the land surface energy balance under varying climatic conditions. He quantified localized and dynamic drainage behavior and structures in different subsurface and land surface state variables and fluxes. The results suggest that land surface observations may be used to inversely gain insight into structural characteristics of subsurface heterogeneity.

Finally, Schwinger et al. (2010) presented for the first time a methodology to use four-dimensional variational data assimilation, a common methodology in weather forecasting, to a land surface model (the Community Landsurface Model, CLM). By developing the tangent linear approximation to the adjoint CLM, they were able to use arbitrarily distributed flux measurements to improve the initial state estimate of the subsurface fields (especially soil moisture). The key innovation of the paper is the implementation of a nonisotropic background covariance matrix, which allows computing analysis increments for regions far from the actual measurements based on modeled covariabilities.

## Monitoring of State Variables and Fluxes

Bogena et al. (2010) presented the potential of wireless soil moisture sensor networks to characterize and capture the spatial variability and dynamics of soil moisture content in a forested catchment. The network consists of 150 nodes and 900 sensors spread across an area of 27 ha. Within a period of 5 mo more than 6 million soil moisture measurements were obtained. This enabled a detailed and profound analysis of soil water content variability as a function of topography, weather conditions, and soil types.

Combining in situ soil moisture measurements with satellite observations, Koyama et al. (2010) demonstrated the usefulness of an empirical retrieval algorithm for soil moisture estimation using a minimum number of fitting parameters. An ensuing analysis of cross-scale variance/mean ratios of the different soil moisture data sets showed a clear linear relationship, with decreasing ratios for decreasing spatial scales. At the catchment scale, this relationship exhibits the largest negative slopes, which is attributed to the different processes and system characteristics acting at the different spatial scales, such as precipitation and variability in soil and vegetation cover.

Wohlfahrt et al. (2010) addressed the measurement quality of turbulent fluxes based on the eddy covariance (EC) techniques. Like many authors, they confirm—especially for a grassland site—the notorious underestimation of EC measurements, by 20 to 30% in comparison with lysimeter measurements and upscaling

techniques. Their analysis of two time periods indicated that the potentially nonresolved larger eddies, which might be the cause for these underestimates, are not generated from sub-field-scale heterogeneity, but must result from larger scale inhomogeneities. Two approaches to correct for these underestimates based on the assumption of a Bowen ratio preserved by the EC methods were proposed and compared.

Rutten et al. (2010) presented a very detailed and thorough evaluation of the distributed temperature sensing (DTS) methodology applied to the near-surface soil layer to observe the spatiotemporal variability of land surface–atmosphere exchange processes of water and energy. Distributed temperature sensing allows monitoring of soil temperature and soil moisture over scales between 1 m and 10 km, with the potential to bridge the gap between point measurements and the scale of a remote sensing pixel or land surface model cell. Four DTS fiber optics were installed in the shallow subsurface and yielded information on both temperature and soil moisture at high spatial and temporal resolution over long distances. The analysis showed, however, that more research is needed to estimate fluxes from DTS, because the role of advection and phase changes within the upper soil is still not known to a sufficient degree. This paper pointed also to the importance of representing these processes correctly in coupled models.

## Outlook

The results obtained within this collaborative research center clearly demonstrated the importance of including patterns in the quantification of exchange processes between the compartments of the subsurface–soil–vegetation–atmosphere systems. In particular, the use of noninvasive methods, such as hydrogeophysical techniques, provides a unique opportunity to further improve the quantification of patterns and structures from the pore to the field scale and even to the catchment scale. At the local scale, combining novel mathematical models with methods such as MRI and SIP has led to improved interpretation of pore-scale processes that should prove valuable when upscaling parameters from the pore to the field scale. Novel measurement techniques, such as soil moisture sensor networks and DTS systems operated at the field- and catchment-scale levels can provide data with high temporal and spatial resolution, which are extremely useful in validating models and in improving model predictions through data assimilation. Combining numerical models that consider the full coupling between different compartments of the terrestrial systems and data assimilation methods is a promising way to improve our understanding and prediction of the dynamics of terrestrial systems.

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