Special Section: Soil Variability and Biogeochemical Fluxes

Core Ideas

- Pattern recognition techniques can help explain biogeochemical flux variability.
- Dynamic factors and their impact on biogeochemical flux variability need better identification.
- Controls on biogeochemical fluxes are time and space scale dependent.

Soil Variability and Biogeochemical Fluxes: Toward a Better Understanding of Soil Processes at the Land Surface

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Soil biogeochemical fluxes in the vadose zone are characterized by a large degree of variability in space and time. This fact leads to the need for the development and application of appropriate methodologies to better understand the high nonlinearity and complex feedback mechanisms responsible for such fluxes. In this sense, there still exists a lack of knowledge in topics such as the scale dependence of the spatial and temporal variability of the controls on soil moisture and biodegradation rates and the dynamic behavior of flow and transport model parameter, and its association with the presence of roots. Knowledge of the variability of biogeochemical fluxes is needed for assorted applications ranging from natural hazards and environmental pollution risk assessment to agricultural production and water resources management. The contributions to this special section epitomize the ongoing effort toward the characterization, quantification, modeling, and understanding of biogeochemical fluxes in the vadose zone at several spatial and temporal scales. The main progress has been the identification of different controls on soil moisture and biodegradation rates depending on the scale of the study as well as the important dependence of the spatial and temporal variability of biogeochemical fluxes on dynamic properties such as vegetation and weather variables.

The vadose zone is a central component of natural systems given its functioning at the boundary between the solid earth and the atmosphere, where most biogeochemical fluxes take place (Seneviratne et al., 2010; Guo and Lin, 2016). The term *biogeochemical fluxes* refers to the dynamics of energy and matter that occur between the terrestrial biosphere and the atmosphere. The quantification of these fluxes is important for natural hazards and environmental pollution risk assessment, climate change adaptation and mitigation, agricultural production, and water resources management, just to mention a few areas.

Soil biogeochemical fluxes are characterized by a large degree of variability in space and time (Baldocchi et al., 2001; Vanderlinden et al., 2012; Vereecken et al., 2008). This fact leads to the need for the development and application of methods to better understand the nonlinearity and feedback mechanisms involved. Among them, variability of the controls on soil moisture and biodegradation rates and the dynamic behavior of water and solute flow parameters and its association with the presence of roots are active areas of research.

Appropriate tools and methods are needed to investigate and to characterize both the temporal and the spatial variability of biogeochemical fluxes in the vadose zone and the system states and soil properties that determine the processes. Spatiotemporal data from vadose zone studies are increasingly available at different spatial and temporal scales and under varying ecohydrological conditions (Vereecken et al., 2014). Such data allow improvements, for example, in modeling across landscapes, satellite- or ground-based sensor data retrieval, and the implementation of experimental designs (Vanderlinden et al., 2012). Moreover, spatiotemporal data can reveal repeatedly appearing features at a range of scales (spatial and/or temporal), as manifested by a pattern, thus contributing to deeper knowledge of the system's functioning (Vereecken et al., 2016).

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Analytical methods, sampling protocols, and the use of covariates and empirical or deterministic environmental models are important in characterizing and quantifying flux variability. Key aspects need to be considered in detail, though, given the important differences that may arise between field and laboratory measurements and depending on different sampling protocols and the particular statistical or mathematical model chosen. Data analysis of biogeochemical fluxes can be conducted in the spatial and temporal domains by means of several methods (Vereecken et al., 2016). Among them, empirical orthogonal functions (Jolliffe, 2002), temporal stability analysis (Vachaud et al., 1985), and geostatistics (Oliver and Webster, 2014) are just a few widely implemented methods. Important outcomes of such methods are their ability to identify the systems' controls and to furnish spatial uncertainty patterns.

Large efforts are being made to deal with the complexity and heterogeneity of biogeochemical fluxes taking place in the vadose zone (Faybishenko et al., 2016). Some examples are the multidisciplinary Unsaturated Zone Interest Group (Nimmo et al., 2009), the Critical Zone Observatories (Guo and Lin, 2016), the International Soil Moisture Network (Dorigo et al., 2011), and the SoilCan lysimeter network (Pütz et al., 2016), as well as the development, improvement, and dissemination of soil models conducted by the International Soil Modeling Consortium (https://soil-modeling.org/). All these efforts strive to improve our understanding of biogeochemical flux controls, interactions, dynamics, and scale dependence as well as to find the most appropriate methods for characterizing and modeling (Brantley et al., 2016; Faybishenko et al., 2016).

This special section arose from a successful session on "Challenges in soil physics" during the 2016 European Geosciences Union meeting held in Vienna, Austria, and it has been complemented with other contributions in response to the call for papers. The first group of works in this section focuses on the temporal variability of soil properties and fluxes, while the second group addresses the variability of biogeochemical fluxes at both spatial and temporal scales.

Temporal Variability of Biogeochemical Fluxes

Water retention dynamics is of paramount relevance to evaluate water flow and solute transport in soils. Temporal variability of water retention has been reported, e.g., Jirků et al. (2013), that limits the use of retention characteristics obtained from small-scale core samples or other widely used methods, e.g., pedotransfer functions or inverse modeling. Herbrich and Gerke (2017) compared water retention data obtained from laboratory soil cores and intact soil monoliths of weighing lysimeters representing field conditions. Their results confirmed, first, that the drying retention characteristic is generally steeper for field than laboratory conditions. Second, the highly resolved soil moisture and matric potential time series indicated complex and dynamic changes in the field water retention occurring at several time scales. Herbrich and Gerke (2017) identified hysteretic, seasonal, and inter-annual behavior in soil water retention dynamics in the lysimeter data by disentangling wet–dry cycles. They associated the short-term dynamics with soil structural and wettability differences in part associated with the presence of vegetation, whereas longer term dynamics reflected soil management and erosion related changes. The soil water retention dynamics revealed the differential role of the factors inducing the intra-seasonal and inter-annual variability and highlighted the need for their consideration in modeling.

Still assuming constant soil hydraulic properties, the modeling framework of Mallmann et al. (2017) served as a tool to evaluate the long-term fate and transport of trace metal contaminants in arable soils due to continuous application of organic fertilizers. Mallmann et al. (2017) described the resident concentrations in the soil profile and the long-term vertical transport of Zn and Cu in a pig-slurry-amended Brazilian Oxisol by means of a mathematical model and tested the impact of considering dynamic root growth and root uptake on the intra-seasonal variability of metal concentrations. They found a better description of Zn concentration profiles when adding a dynamic component of root water uptake and growth to the model. However, this was not the case for Cu, where they suggest considering dissolved organic C facilitated transport to improve predictions.

Spatial and Temporal Variability of Biogeochemical Fluxes

On the one hand, the studies of Martini et al. (2017), Calamita et al. (2017), Schröter et al. (2017), and Wei et al. (2017) tried to identify soil moisture patterns and to characterize the controlling factors at hillslope, field, small catchment, and watershed scales, respectively. On the other hand, Eichert et al. (2017) conducted a multiscale study on evaluating distributed data for analyzing biodegradation patterns of hydrocarbon contamination in the vadose zone.

Martini et al. (2017) explored patterns of soil moisture and apparent electrical conductivity along a hillslope. They found that the dominant pattern within the time-lapse soil moisture and apparent electrical conductivity data set was related to time-invariant properties such as terrain attributes and basic soil properties (i.e., soil texture, bulk density). Also, they observed that the soil moisture condition revealed less dominant patterns than those explained by time-invariant properties. However, observations under dry soil conditions were still important to better characterize the spatial heterogeneity of soil properties. Using principal component analysis, they were able to highlight the potential of pattern recognition techniques to disentangle the complex interactions between different environmental factors (e.g., soil properties, topography) on the spatial and temporal variability of soil moisture and apparent electrical conductivity.

Calamita et al. (2017) characterized spatial patterns of soil moisture at the field scale using soil electrical resistivity measurements within a geostatistical framework. With such an approach, they were able to design an efficient sampling strategy for generating spatial predictions and for evaluating the uncertainty modeling of soil moisture. They also demonstrated that the spatial predictions and uncertainty modeling of soil moisture improved after including electrical resistivity data as a covariate, thus justifying its collection.

Schröter et al. (2017) studied soil moisture patterns at the small catchment scale using multispectral remote sensing (RapidEye) and topographic data. They used a fuzzy *c*-means sampling and estimation approach (FCM SEA) for fusing terrain and vegetation (from RapidEye images) data with the purpose of reconstructing multitemporal soil moisture spatial patterns in the Schäfertal catchment (located in central Germany). Two temporally persistent vegetation patterns were extracted from the RapidEye time series. The persistent vegetation patterns improved the accuracy of the FCM SEA model compared with using only terrain data; however, about half of the variance remained unexplained by the model for most of the dates. They suggest that the addition of soil texture maps and a more precise delineation of soil-landscape units are needed to further improve model accuracy.

Wei et al. (2017) investigated the factors that determine the temporally stable pattern of soil moisture across an 805-km^2, mostly forested watershed in China, using a distributed hydrological model to generate soil moisture data. After collecting the available information on topography, land use, and soil type, they analyzed the temporal stability patterns in the watershed and identified locations that were most representative of the average soil water content of the watershed. They identified vegetation and topographic features as the dominant factors determining the temporally stable soil moisture pattern of this watershed. However, they pointed out that the role of soil properties might have been undervalued due to an insufficient resolution of the soil map. Nevertheless, the available information led to the development of a sampling protocol to monitor the average soil moisture at the watershed scale.

Eichert et al. (2017) conducted a multiscale study focusing on the characterization of the rates of biodegradation of hydrocarbon compounds through natural source zone depletion (NSZD) in the soil of a former oil refinery. They observed a link between the spatial variability in NSZD rates and historical release areas and defined an optimum sampling scheme and method to characterize the spatial variability considering the temporal changes in NSZD rates. Discrepancies between the methods being evaluated to quantify NSZD rates were found and revealed a differential response to the measurement time frame and radiocarbon sampling method. However, they were able to evaluate the temporal variability in NZSD rates that was associated with environmental conditions such as air temperature and precipitation. In addition to improved process understanding, their analysis could also be helpful in setting NSZD expectations at other large sites.

Understanding of the complexity in vadose zone studies is aided by a multidisciplinary approach. This is evident from the diversity of the works presented that focus on exploring how soil variability can control different biogeochemical fluxes, e.g., biodegradation rates of hydrocarbon compounds, soil moisture, water flow, and heavy metal transport. The studies contained in this special section highlight the important role of dynamic factors such as vegetation, temperature, and wetness conditions, especially in the short term, while still showing the need to consider soil properties information to explain the spatial and temporal variability of soil biogeochemical fluxes in the long term.

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