Geoderma 217–218 (2014) 161–172

Contents lists available at ScienceDirect

Geoderma

journal homepage: www.elsevier.com/locate/geoderma

State-space approach to analyze field-scale bromide leaching

Yang Yang *, Ole Wendroth

University of Kentucky, Department of Plant and Soil Sciences, Lexington, KY 40546, USA

ARTICLE INFO

Article history:
Received 12 June 2013
Received in revised form 11 November 2013
Accepted 25 November 2013
Available online 22 December 2013

Keywords:
Bromide leaching
State-space model
Spatial variability
Land use
Soil texture

ABSTRACT

Spatial variability of soil properties complicates the analysis of water and solute transport under field conditions. To meet this challenge, a novel experimental design with a scale-dependent treatment distribution was adopted earlier in a field study to assess the impact of land use and rainfall characteristics on Br^- leaching with the aid of spectral analysis. The objective of the current study was to identify the major underlying processes that controlled Br^- leaching in the previous experiment and to describe the spatial distribution of soil Br^- site-specifically and in different soil layers, using an autoregressive state-space approach. Based on the boundary conditions investigated in this study, the state-space models for Br^- concentration at 40–50 and 60–70 cm exhibited the best prediction quality compared to those at other depths. As indicated by the weight of each variable, land use dominated the spatial pattern of Br^- at shallow depths; whereas, the spatial behavior of Br^- below 40 cm was mainly affected by soil texture and to a smaller extent by rainfall intensity. In addition, the involvement of Br^- concentration and soil texture of the adjacent layer above in the state-space analysis helped to describe the spatial distribution of Br^- typically in the soil layer below 60 cm. These results not only demonstrated the applicability of state-space technique in diagnosing spatial solute transport relationships; but also held important implications for the surface application of chemicals.

1. Introduction

A precise description of water and solute transport in the vadose zone is essential for the management of surface-applied chemicals, which in sustainable agriculture aims to improve crop productivity and food quality while minimizing the groundwater contamination through leaching (Russo, 1991; Corwin et al., 1999; Paramasivam et al., 2002). Many studies have been conducted on soil columns under laboratory conditions and steady-state flow; however, at the field scale, little progress has been made in characterizing the processes of water flow and solute transport, probably owing to the challenge of inherent soil spatial and temporal heterogeneity (Nielsen et al., 1986; Destouni and Graham, 1995; Ashraf et al., 1997). Affected by soil properties such as topography, soil texture, structure and spatial soil water distribution, the spatial transport behavior of water and solute is quite variable (Wendroth et al., 1999; Ersahin et al., 2002; Whetter et al., 2006).

In their field experiments based on classic block design, Kessavalou et al. (1996) and Ottman et al. (2000) used Br^- and ^{15}N as tracers and found the standard deviations were in the same magnitude as the amounts of solutes leached below 1.2 m and 4 m depths, respectively. When such a large inherent variability is present in the set of measurements, it becomes extremely difficult to quantify solute transport and to analyze treatment effects afterwards (Wendroth et al., 2011). In order to yield a representative estimate of solute transport, field experiments aimed at the spatial structures of solute transport variables and their spatial correlations with soil properties have been established since mid-1990s (Ellsworth and Boast, 1996). Nevertheless in many cases, a single spatial range of an individual observation on solute transport could hardly be derived (Netto et al., 1999; Schwen et al., 2012), as it usually varies over different scales (Biggar and Nielsen, 1976; Wendroth et al., 2011). In view of this limitation, a novel experimental design, arranging treatments in cyclic layout at distinct scales has been introduced (Bazza et al., 1988; Shillito et al., 2009). Using frequency-domain analysis, i.e., spectral and cross-spectral analyses, the variances of treatments as well as the related processes can be decomposed among different scales (Kachanoski and De Jong, 1988; Wendroth et al., 2011); thereby allowing identification of the major factors and inherent soil variability-related processes that take effect (Nielsen and Alemi, 1989; Shillito et al., 2009). Thus a field study applying land use and two rainfall characteristics, i.e., rainfall intensity and the time delay between solute application and subsequent rainfall (application time delay), at different scales was conducted earlier (Yang et al., 2013). Including topography complexity and soil texture as boundary conditions, the dominant factors controlling Br^- leaching were found to vary with soil depth.

Spectral analysis and the scale-dependent treatment distribution mentioned above provide an effective way to characterize the spatial associations between boundary conditions and solute transport variables. However, when two boundary conditions, e.g., topography and soil texture, interact, which are typically present between inherent soil processes on which the varying scale-dependent treatments could not

---

* Corresponding author at: Office N-101, Ag. Sci. North Bldg. 1100 Nicholasville Rd., Lexington, KY 40546, USA. Tel.: +1 8592577326; fax: +1 8592573655.
E-mail address: yang.yang@uky.edu (Y. Yang).

0016-7061/$ – see front matter © 2013 Elsevier B.V. All rights reserved.
http://dx.doi.org/10.1016/j.geoderma.2013.11.013

be imposed arbitrarily, the implications of spatial correlations between solute transport and either boundary condition to chemical management are prone to be impaired. Moreover, spectral analysis alone is not able to simulate or forecast the fate of surface-applied chemicals quantitatively, which could be applied in precision agriculture and site-specific solute transport modeling (Loague and Green, 1991; Van Alphen and Stoorvogel, 2000). To further interpret the causes of solute leaching behaviors and to describe their spatial patterns thereafter, the application of state-space technique was suggested (Wendroth et al., 2011; Schwen et al., 2013).

The state-space methodology was introduced by Kalman (1960) and Kalman and Bucy (1961) to filter noisy electrical time series; and then extended to analyze economic series by Shumway and Stoffer (1982) and soil properties by Morkoc et al. (1985). In an autoregressive multivariate state-space model, the variable of interest is related to the same variable and other related variables at the previous location (Shumway and Stoffer, 1982; Nielsen and Wendroth, 2003); and the regression coefficient of each variable reflects the degree of its spatial correlation with the outcome (Morkoc et al., 1985). In the state-space approach, the same variables can be employed as in a classical linear regression analysis. However, the principles behind these two approaches differ conceptually. Assuming that all the observations are independent from each other, the classical statistical method generates an overall response function between two variables. This attempt often fails at the field scale because the observations are commonly spatially correlated (Nielsen and Alemi, 1989) and the underlying processes that are not included in the investigation could modify the response manner across the field. On the contrary, the autoregressive state-space approach takes advantage of the spatial dependence inherent in observations and analyzes the correlations of spatial point-to-point processes between two variables. The change in one variable from one location to the next is related to the change in the other variable. Based on the spatial correlations between point-to-point changes, the state-space model is able to estimate even missing data as well as to forecast the ones outside the domain of observation (Morkoc et al., 1985; Wendroth et al., 2003) while standard error intervals of the estimation increase with increasing distance from a point with an observation. Timm et al. (2004) described the spatial distribution of soil water content in a sugarcane field by clay content, soil organic matter and aggregate stability; and found that compared to multiple regression equations, the estimates based on state-space model by far better agreed with the measured data. Leaving out one third of the measurements along a sorghum transect, Morkoc et al. (1985) successfully estimated the water content by soil surface temperature using state-space model; and for the fifteen omitted locations, the resulting estimates were all within one standard error except for only two locations. Moreover, in contrast to classical statistics, the state-space technique considers the observations as a limited reflection of the real process. With given equipment, sampling volume and analytical device, observations cannot be equivalent to the "true state" but only provide an indirect measure with an unidentified "noise" (Nielsen and Wendroth, 2003). Moreover, inasmuch as the form of a first-order autoregressive model implies limits in the description of the process, the model uncertainty is included in the process description as well. Accordingly, a mathematical algorithm is included in the state-space approach to filter these uncertainties. In view of these merits, this spatial analysis tool has been widely used to quantify the spatial correlations between soil water and temperature (Morkoc et al., 1985; Dourado-Neto et al., 1999), among soil physical and chemical properties (Timm et al., 2004; Wendroth et al., 2006), as well as to predict crop yields based on soil properties (Cassel et al., 2000; Li et al., 2002) or nutrient status (Wendroth et al., 1992) or both (Wendroth et al., 2003). However, few state-space models of solute transport have been developed and presented.

Most researches incorporating the spatial variability of soil properties to analyze water and solute transport only consider the horizontal variation, but ignore the soil heterogeneity in the vertical direction (Russo, 1991; Russo and Bouton, 1992; Vanclooster et al., 1995; Netto et al., 1999). Field soils, however, are often layered and more homogeneous in the horizontal than the vertical direction (Porro et al., 1993). This vertical heterogeneity, typically in soil texture and structure (Butters and Jury, 1989; Heijs et al., 1996; Kulli et al., 2003), exerts an important impact on lateral water flow and solute mixing; thereby affecting solute distribution in both horizontal and vertical directions (Vanclooster et al., 1995; Flühler et al., 1996). Using Brilliant Blue ECF as a dye tracer, Kulli et al. (2003) investigated the stained infiltration patterns at 25 plots over 8 sites; and discovered that besides soil texture and structure, the characteristics of the overlying soil layers could also influence the solute distribution in a given layer and subsequently through the soil profile. With distinct layers above, which control the solute input together with experimental setup (e.g., the amount of solute applied, rainfall intensity) and other boundary conditions (Trojan and Linden, 1992), even similarly textured soil layers are prone to exhibit quite different flow patterns of water and solute (Kulli et al., 2003). Therefore, it would be helpful to involve the solute concentrations and soil properties of the overlying layers into the spatial description of field solute transport.

The hypothesis of the present study is that subsequent to the diagnosis of cyclic variation sources using frequency-domain analysis, the state-space approach more comprehensively characterizes the spatial processes of Br^- leaching in the field experiment conducted earlier by Yang et al. (2013), when natural boundary conditions are taken into account. Adopting autoregressive state-space models, the objective was to: 1) analyze the spatial correlations of soil Br^- among different depths; 2) describe the horizontal distribution of soil Br^- at each depth based on the boundary conditions investigated; and 3) identify the main driving forces, either imposed treatments or natural processes or both, that control Br^- leaching and its spatial distribution at a particular soil depth.

2. Materials and methods

2.1. Experimental design

The field experiment was conducted in late spring of 2012 at the University of Kentucky's Spindletop Research Farm, Lexington, KY. Along a 48-m transect evenly laid out across two land use systems: cropland and grassland, 24 plots each 2 m in length and 3 m in width were established. As a result, half of the plots were located on cropland, which is normally planted with no-till winter wheat, and the other half on grassland, dominated by tall fescue, bluegrass and red clover. In a sampling campaign, undisturbed soil cores of 1 m depth were collected every 1 m along the transect and divided in 10 cm increments for soil texture determination using the pipette method (Gee and Bauder, 1986). The contour maps of sand and clay content along the transect are presented in Fig. 1. Meanwhile, relative elevation at an interval of 25 cm, both along and across, the transect in a 197 × 13 grid was measured and then averaged for every 1 m (Fig. 2c). As an indicator of topographic complexity, the corresponding elevation variance was calculated as the sum of squared differences from the neighboring relative elevations.

One and a half months before the Br^- leaching experiment, Roundup was applied to kill all the plants. KBr solution was applied to the transect at a constant rate of 37.5 g Br m^{-2} with a regular farm sprayer. Using garden sprinklers attached to a metal frame, rainwater collected earlier was applied along the transect at a constant amount of 44 mm, at three levels of intensity, 5, 22 and 44 mm h^{-1}, and with four levels of application time delay, 1, 4, 24 and 96 h, in a repetitive pattern at distinct scales (Fig. 2a, b). As a result of the natural precipitation occurring during rainfall simulation, final amounts and intensities at some plots were slightly different from the ones intended; and the about 10 mm h^{-1} higher intensity at plot 1 and 2 than the one intended was due to an accidental malfunction of the pumping system. After