Soil micromorphology use for modeling of a non-equilibrium water and solute movement

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ABSTRACT

Soil micromorphology was applied to specify flow domains in different soils and to select a suitable numerical model for simulation of water flow and herbicide transport. Pore structure detected on soil micromorphological images represented in all cases domains of prevailing water flow and solute transport. Depending on pore configuration and boundary conditions either water immobilization or preferential flow was observed and simulated. The benefits and limitations of the soil micromorphology imaging are discussed and compared with the more often used X-ray computer tomography, magnetic resonance imaging and dye tracer imaging.

Keywords: soil pore structure; soil micromorphology; herbicide transport; single-porosity model; dual-porosity model; dual-permeability model

Soil and groundwater contamination by chemicals used in agriculture is a serious environmental problem that is widely studied, both experimentally and theoretically. It was observed that water flow and contaminant transport in structured soils is frequently influenced either by water and solute temporal immobilization or by preferential flow. To describe such non-equilibrium of water flow and solute transport in soils, many numerical models have been recently developed. Overviews of non-equilibrium water flow and solute transport evidence, and various experimental and mathematical approaches to study and describe these phenomena were given by Šimůnek et al. (2003), Gerke (2006), Jarvis (2007), Clothier et al. (2008), Šimůnek et al. (2008a), Šimůnek and van Genuchten (2008), or Köhne et al. (2009a, b). Common physically based models for simulation of water flow and solute transport in structured soils assume (one) continuum and bi- or multi-continuum approaches.

Bi- or multimodal concepts assume that the soil porous system is divided into two (or more) domains, and each domain is characterized by its own set of transport properties and equations describing flow and transport processes. The two-domain models have been mostly tested. The dual-porosity (mobile-immobile) approach defines water flow and solute transport in systems consisting of domains of both mobile and immobile water. The dual-porosity formulation is based on a set of equations describing water flow and solute transport in the mobile domain, and mass balance equations describing soil water and solute content in the immobile domain. The dual-permeability approach assumes that water flow and solute transport occur in both domains. The dual-permeability formulation is based on a set of equations that describe water flow and solute transport separately in each domain (matrix and macropore domains). Various equations may be used to describe water and solute transport in different flow domains. HYDRUS-1D (Šimůnek et al. 2008b) is the software package that includes the single-porosity, dual-porosity and dual-permeability models based on the numerical solution of the Richards equation and advection-dispersion equation in all flow domains.

To apply two (or multi) domain models, the domain fractions and properties characterizing water flow and solute transport within and between domains must be specified. The numerical inversion and parameter estimation from the observed water flow and tracers transport data are usually applied to obtain desired

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information. (See review articles mentioned above.) However, to obtain reliable results many parameters must be independently measured or determined in the literature. The summary of various approaches of independent parameter determination is given by Köhne et al. (2009a).

The X-ray computer tomography (CT), magnetic resonance imaging (MRI), and dye tracer distribution imaging are frequently applied tools to visualize and quantify preferential pathways, and consequently to improve various model parameter estimation. Perret et al. (1999) applied CT for three-dimensional (3D) description of geometry and topology of macropores. Kastell et al. (2000), and Vogel and Roth (2001) used CT to describe regions of different densities. Císlerová and Votrubová (2002) used CT to identify local highly porous zones. Vanderborght et al. (2002) explained two fluorescent dye distributions using the CT imaging. Javaux et al. (2006) presented the CT-derived 3D microscale spatial distribution of hydraulic parameters. Sander et al. (2008) used CT to obtain the 3D distribution of the larger pore systems; the latter were studied before using the dye experiment (Sander and Gerke 2007). Peth et al. (2008) used microtomography to study pores in soil aggregates from different soil management systems. Baumann et al. (2000) applied MRI to asses the 3D pore space arrangement of repacked soil columns with sand and gravel layers. Votrubová et al. (2003) used MRI to study recurrent ponded infiltration into structured soil.

The soil micromorphological images have been recently used for more detail soil pore visualization and detection, flow domains definition, model selection and water flow simulation by Kodešová et al. (2006, 2007). The same procedure was also applied for herbicide transport simulation by Kodešová et al. (2008, 2009). This paper is focused on a review of studies, which used soil micromorphology to improve estimation of parameters characterizing non-equilibrium water flow and solute transport in structured soils.

Soil micromorphology methods for multiple domain parameter estimation

The shapes and sizes of soil pores can be studied by image analysis of thin soil sections at various magnifications. The impacts of pores, which are detectable on micromorphological images, on saturated hydraulic conductivities, K_s, have been mostly investigated. Macropore impact on K_s values was discussed by Bouma et al. (1977, 1979). Differently shaped pores in soils under different management practices and their K_s values were studied by Pagliai et al. (1983, 2003, 2004), and Pagliai and Kutílek (2008) using both micromorphometric and micromorphological investigations.

The effects of macropores (gravitational pores and large capillary pores) detected in micromorphometric images on the shape of soil hydraulics functions was described by Kodešová et al. (2006). The soil pore structure was analyzed in thin section of size 1.5 × 2 cm. Soil hydraulic properties were measured in the laboratory on undisturbed 100 cm^3 soil samples placed in Tempe cells using the multi-step outflow experiment. They showed macropores created by roots and soil microorganisms in the subsurface horizon of Haplic Luvisol and subsequently affected by clay coatings. Their presence was reflected in the soil water retention curve, which displayed multiple S-shaped features as obtained from the water balance carried out for the multi-step outflow experiment. The dual permeability models implemented in HYDRUS-1D were applied to improve the numerical inversion of the multi-step outflow experiment and to obtain van Genuchten (1980) parameters characterizing bimodal soil hydraulic properties. Fraction of the macropore domain was calculated from the porosity detected on the micromorphological images (pores with diameters large than 40 μm) and total porosities evaluated on the 100 cm^3 soil samples.

Kodešová et al. (2007) studied impact of a different vegetation cover on the micromorphology, porous system and hydraulic properties of surface organic matter horizons of forest soils. Micromorphological studies showed that the decomposed organic material in organic matter horizon under the grass vegetation was more compact compared to the decomposed organic material in the organic matter horizon under the spruce forest. The detected soil porous system in the organic matter horizon under the spruce forest consisted of two clusters of pores with different diameters that were highly connected within and between both clusters. The soil porous system in the organic matter horizon under the grass vegetation consisted of one cluster of pores with the larger diameters and isolated pores with the smaller diameter. However, the pore sizes, detected in images of thin soil section made of dry soil samples, did not represented pore sizes under naturally moist conditions due to the large organic matter volume changes of a dry organic matter. Therefore, the two-domain modeling approach was not used in this case. The micromorphological analysis was also used to explain various soil water retention without the extending flow modeling by Constantini et al. (2006), Juhász et al. (2007) and Pires et al. (2008).

Kodešová et al. (2008) investigated the impact of varying soil micromorphology on soil hydraulic properties and consequently on water flow and herbicide (chlorotoluron) transport observed in the field on three soil types (Haplic Luvisol, Greyic Phaeozem, Haplic Cambisol). The field experimental method was described in detail by Kočárek et al. (2005). Similar experimental procedure was also previously used to study chlorotoluron transport in Chernozem (Kodešová et al. 2004, 2005). HYDRUS-1D was applied to simulate water and solute transport in the field assuming the equilibrium herbicide adsorption on soil particles. Before, the same approach as in Kodešová et al. (2006) was used to obtain parameters of single- and two-domains models in HYDRUS-1D. However, depending upon the soil porous structure and the character of observed multi-step outflow, either dual-porosity or dual-permeability models in HYDRUS-1D were applied to obtain soil hydraulic properties from the laboratory data. The micromorphological image of humic horizon of Haplic Luvisol showed higher order aggregates. The majority of detectable capillary pores were highly connected, separating higher order peds with small intra-pores that possibly formed zones with immobile water. Herbicide was regularly distributed close to the soil surface. The single- and dual-porosity models described well the herbicide behavior in this soil. The majority of detectable large capillary pores in a humic horizon of Greyic Phaeozem were separated and affected by clay coatings and fillings. Larger capillary pores formed preferential pathways and sufficient infiltration fluxes, which occasionally filled up these pores, caused the highest mobility of chlorotoluron in this soil. Gravitational pores were detected in a humic horizon of Haplic Cambisol. However, despite the highest infiltration rate, preferential flow only slightly affected the herbicide transport. Large gravitational pores that may dominate water flow and solute transport under saturated conditions were inactive during the monitored period. The dual-permeability model performed better in simulating the herbicide transport in Greyic Phaeozem and Haplic Cambisol.

Finally, Kodešová et al. (2009) studied water flow and chlorotoluron transport in the undisturbed soil samples (taken from the various horizons of the same soils that were explored in previous paper) subjected to ponded infiltrations. Since the preferential flow was observed in all cases, the dual-permeability model in HYDRUS-1D was only applied to improve optimization results compared to the single-porosity model and to obtain bi-modal soil hydraulic properties. Fractions of the macropore domains were calculated from the porosities detected in the larger thin soil sections (7 × 4 cm) and total porosities evaluated on the experimental columns. Both models and numerical inversions were then used to obtain solute transport parameters using the equilibrium and two-site sorption (van Genuchten and Wagenet 1989) models simulating herbicide adsorption in soils. The lowest water flow rates were observed in soils with poorly developed soil structures, a low fraction of large capillary pores, and the absence of gravitational pores. The highest water flow rates were observed in soils with well-developed soil structures, which were affected by clay coatings and high structure stability. However, the prevailing fast chlorotoluron transport through the large capillary pores, and frequently through the gravitational pores, was documented in all cases. Utilization of the dual-permeability model and the concept of a two-site sorption applied to the matrix domain made it possible to fit the measured data more closely than when the single-porosity model with equilibrium adsorption was used.

Benefits and limitations of soil micromorphology approach for multiple domain parameter estimation

The soil porous system analysis, using the soil micromorphology, significantly improved the understanding and description of transport processes in studied soils in all discussed cases. However, Jarvis (2007) and Köhne et al. (2009a) argued that macropores (pores causing the physical non-equilibrium of water flow close to saturation) are pores with an equivalent diameter larger than about 300–500 μm (corresponding to a pressure head of –10 and –6 cm), Kodešová at al. (2006, 2008, 2009) showed that even smaller pores may play a significant role. They defined gravitational pores as pores with an equivalent diameter larger than 1470 μm, corresponding to a pressure head of –2 cm (Watson and Luxmoore 1986), and large capillary pores as pores with a diameter larger than 40 μm (pores detectable on micromorphological images), corresponding to a pressure head of –70 cm, and smaller than 1470 μm. This definition was also based on the bimodal shape of the soil water retention curve (Kodešová at al. 2006) obtained from multiple outflow experiments. In addition, this hypothesis was also supported by the relatively high chlorotoluron mobility, which was observed in the soil samples of a low total permeability and pore diameters detected mainly in the range from 40 to 500 μm.

Three problems arise in this approach. (i) The size of soil thin sections does not allow studying greater system of gravitational pores and fractions as it is possible using the CT, MRI and dye tracer techniques. However, as was shown by Kodešová et al. (2008), the gravitational pores may not have a significant impact on the water flow and solute transport under the natural field conditions. (ii) Scanning of the soil thin sections provides only the two-dimensional (2D) images of the soil porous systems. Analysis of the soil thin section sequence and following reconstruction of the 3D image may partly improve the discussed method. (iii) Soil micromorphological images taken using the optical microscope cannot be used to evaluate pores smaller than 40 μm. The electron microscope scanning and image analyses presented by Rösslerová-Kodešová and Kodeš (1999) may be applied to obtain this information.

In addition to the above mentioned limitations, soil micromorphology imaging does not allow to study actual water flow and solute transport as is possible using the MRI techniques. On the other hand, the standard CT, MRI and dye tracer techniques (except for the microtomography presented by Peth et al. 2008) cannot describe the soil porous system into such details as is allowed using the optical microscope imaging or even the electron microscope scanning. Various combinations of all discussed techniques would be valuable to improve the flow domains detection and parameter estimation. In general, each technique and their combinations are very promising tools for better understanding and conceptual modeling of water and solute movement processes in soils.

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