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TECHNICAL ARTICLE

Modeling of Water Flow in Reclaimed Mine Spoil with Embedded Lignitic Fragments Using Hydrus-1D

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Abstract Lignitic mine soils represent a dual-porosity medium consisting of a technogenic mixture of overburden sediments that include porous fragments embedded within a mostly coarse-textured matrix. Flow and transport process in such soils are not sufficiently understood. The objective of this study was to identify the most appropriate conceptual model for describing small-scale heterogeneity effects on flow based on the physical structure of the system. HYDRUS-1D was used to simulate water flow under field conditions. We compared a dual-porosity (mobile–immobile) model simulation of the field soil water with field monitoring results. The predicted and observed water content were in good agreement. Since the heterogeneity of the lignitic mine soil may lead to preferential flow, Coomassie brilliant blue dyes were applied to the reclaimed surface, revealing preferred flow paths through macropores surrounding the numerous, large rock fragments.

Keywords Dual-porosity · Mobile–immobile · Spatial heterogeneity · Hydrus-1D · Preferential flow · Coal mine waste · Vadose zone

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Introduction

In opencast mining, overburden sediments are first removed from the coal seams using, for instance, dragline excavators. This destroys the original sediment layers; the sediments are then transported to a site where they are dumped, thereby creating large initially unsaturated spoil heaps. At our study sites, the resultant mine soil is a mixture of predominately sandy, overburden sediment with lignitic fragments of various geometries and sizes. The fragments are highly porous, so the mine soil represents a dual-porosity sandy soil system.

Despite a number of experimental (Gerke et al. 2001b; Hangen et al. 2004, 2005) and modeling attempts (Buczko and Gerke 2005, 2006; Buczko et al. 2001; Gerke et al. 1998, 2001a), flow and transport in heterogeneous mine soils is not well understood. In contrast to naturally developed soils, a finger-type preferential flow process (Hangen et al. 2004) seems to result from several interacting and temporally varying causes. Among these are the effects of the lignitic fragments, funneling along inclined structures, and finger-type flow regions influenced by spatially and temporally changing water repellence (Gerke 2006a, b; Gerke et al. 2001b).

Classically, water flow through variably-saturated soils is described by Richards' equation with a uniform flow domain (Simunek and van Genuchten 2008). Recently, efforts have been made at simulating contaminant transport under the influence of preferential flow using dual-porosity models (Gerke and van Genuchten 1993, 1996; Jarvis 2007; Simunek and van Genuchten 2008; Simunek et al. 2001, 2003). These dual-porosity models assume the coexistence of two separate pore domains: fractures (or inter-aggregate pores, cracks, and macro-pores); and matrix pores, with water exchange between the two domains. The two-domain concept, assuming either mobile–mobile or dual-porosity model flow domains, i.e. a mobile–immobile model (MIM), has mostly been used to describe flow and solute transport in aggregated or otherwise structured soils under variably saturated conditions. Our objective in this paper was to use HYDRUS-1D as a tool to understand the effect of preferential flow on water flow in mine soil containing porous, lignitic components. For the analysis of water movement, we compared 1D dual-domain (i.e. MIM) approaches with field monitoring data. We focused on conceptually understanding and describing the flow processes rather than on parameter optimization or stochastic model analysis.

Materials and Methods

Soil Site Description and Experimental Data

The mine soil samples were from the reclaimed Shenshan mine soil heap (39°45′N, 110°11′E; 1,476 m above sea level), which is located approximately 23 km west of the city of Ordos (Inner Mongolia, China). The soil heap was created in 2009 by removing quaternary overburden sediments from nearby opencast lignite mines. The annual mean temperature is 8.7 °C and average annual precipitation rate is 357 mm.A 1 m deep and 2 m long trench was excavated for experiments and soil sampling at a location where quaternary sediments dominate. The soil profile had a clearly separate top soil and subsoil. The sandy tertiary sediments contained differing amounts of lignitic fragments. Large fragments can be identified as dark spots in Fig. 1. Volumetric water content was measured with time domain reflectometry (TDR). Fourteen TDR probes were installed along the trench at four locations spaced 50 cm apart laterally, at seven depths of 5, 15, 25, 40, 50, and 60 cm.

Fig. 1 Photographs of the 0.55 m vertical lignitic mine soil profile, about 0.9 m in width

Rainfall was measured and recorded continuously near the trench across a catchment area of 200 cm^2. The trench was filled after all devices were installed. Field measurements started on 3 Aug 2012. We used 48 days of data.

Flow Modeling

To consider the significant effect of preferential flow on the mine soil with embedded lignitic components, a dual-porosity flow model (based on mass transfer driven by differences in soil water pressure head) was selected from HYDRUS-1D. The dual-porosity formulation for water flow is based on a mixed formulation of the Richards equation to describe water flow in the macropores (mobile water region) and a mass balance equation to describe moisture dynamics in the matrix (immobile water region), as follows (Simunek et al. 2003):

$$\frac{\partial \theta_m}{\partial t} = \frac{\partial}{\partial z}\left[K(h)\left(\frac{\partial h}{\partial z} + 1\right)\right] - S_m - \Gamma_w \quad (1)$$

$$\frac{\partial \theta_{im}}{\partial t} = -S_{im} + \Gamma_w \quad (2)$$

The subscripts m and im refer to the mobile and immobile water regions, respectively; $\theta = \theta_m + \theta_{im}$ and is the volumetric moisture content, S_{im} and S_m are sink terms (root water uptake) for both regions [T^{-1}], and Γ_w is the transfer rate for water exchange between macro-pores and matrix [T^{-1}]. We assumed that root water uptake was preferentially from macro-pores, so that $S_{im} = 0$.

In the dual porosity flow model based on mass transfer driven by differences in soil water pressure head, the exchange rate of water between the macro-pores and matrix regions, Γ_w, was assumed to be proportional to the difference in pressure heads between the two pore regions (Gerke and van Genuchten 1993; Simunek et al. 2003):

$$\Gamma_w = \omega(h_m - h_{im}) \quad (3)$$

Here, ω is a first-order mass transfer coefficient (L^{-1} T^{-1}). Since pressure heads are now needed for both regions, this approach requires estimating retention curves for both pore regions. That means each region has its own values of: θ_r, θ_s, α, and n. As a result, soil hydraulic properties are now described by six parameters for macropores (θ_r, θ_s, α, n, K_s, l), four parameters for the matrix (θ_{r-im}, θ_{s-im}, α_{im}, n_{im}), and a parameter (ω) for mass transfer between the two zones (Simunek et al. 2003).

Soil Hydraulic Properties

Soil hydraulic parameters of both domains are described (van Genuchten 1980) using

$$\theta = \theta_r + (\theta_s - \theta_r)(1 + |\alpha h|^n)^{-m} \quad (4)$$

$$K(S_e) = K_S S_e^{0.5}\left(1 - \left(1 - S_e^{1/m}\right)^m\right)^2; \quad m = 1 - 1/n \qquad (5)$$

where: $\theta_s(-)$ is saturated and $\theta_r(-)$ residual water content parameter, $\alpha(L^{-1})$, $n(-)$, and $m(-)$ are empirical coefficients, K_s is the value of K at water saturation, and $S_e = (\theta - \theta_r)/(\theta_s - \theta_r)$ is the reduced water content.

Measured Hydraulic Parameters

Because of the destructive method of soil block excavation, hydraulic parameters could not be determined directly for the analyzed 2D cross-section. Instead, mine soil water retention characteristics were measured using samples from a profile a few meters from the study site. In May 2012, 35 undisturbed soil cores (100 cm^3) were sampled from depths of 5, 15, 25, 40, and 50 cm. Water retention characteristics (Fig. 2) were determined using ceramic suction plates (Romano et al. 2002) in the suction range of 0–745 cm at 20 different pressure steps.

Estimation of Hydraulic Parameters

Hydraulic conductivity and the mine soil matrix water retention function were estimated using pedotransfer functions in which the parameters were calibrated for mine soil properties (Buczko et al. 2001). Here, available data from the Shenshan study site were utilized and the effect of lignitic fragments and particles on the hydraulic functions was considered. The pedotransfer function approach for the lignitic mine soil is based on the Arya–Paris-model (Arya and Paris 1981) for the water retention [$\psi(\theta)$] function. For estimating $\psi(\theta)$, the Arya and Paris (1981) model was applied in a first step to the mineral fraction, V_s (<2 mm) (i.e. the 'fine' soil excluding V_s (>2 mm) of lignitic fragments and gravel) of the spoil heap. The pore radius, $r_i[L]$, corresponding to the particle size class, i, is calculated as:

$$r_i = R_i\left[\frac{2\varepsilon}{3(1-\varepsilon)}\left(\frac{3M_i}{4\pi R_i^3 \rho_s}\right)^{1-\alpha_{AP}}\right]^{1/2} \qquad (6)$$

with R_i, the mean radius of particles of particle size class $i[L]$, $M_i$is the mass fraction of particle size class i, ρ_s is the density of particles [ML^{-3}], and α_{AP} is a scaling parameter (the subscript AP denotes Arya and Paris). The matrix potential, $\psi_i[L]$, is calculated from the pore radii using the capillary rise equation:

$$\psi_i = -\left(\frac{2\sigma\cos\beta}{\rho_w g r_i}\right) \qquad (7)$$

Here, σ denotes surface tension of pore water [MT^{-2}], β is the wetting angle of the water menisci on the pore walls, and ρ_w the density of water [ML^{-3}]. The volumetric water contents, θ_i for the matrix potentials, ψ_i, and the drained pore sizes corresponding to the ith particle size class are obtained by summing up the volumes of all pores, $V_{P,i}$, of the size class, i, as:

$$\theta_i = \sum_i V_{P,i}\rho_b \qquad (8)$$

In a second step, the water retention curve for the lignitic particle (Fig. 3) was derived from the volumetrically-weighted difference between the mean measured water retention curve in Fig. 2 (i.e. 100 % soil volume comprising both mineral particles and lignitic fragments) and the mean curve of the mineral soil matrix obtained with the Arya–Paris approach. It reflects the distinctly different pore size distribution and the much higher water retention

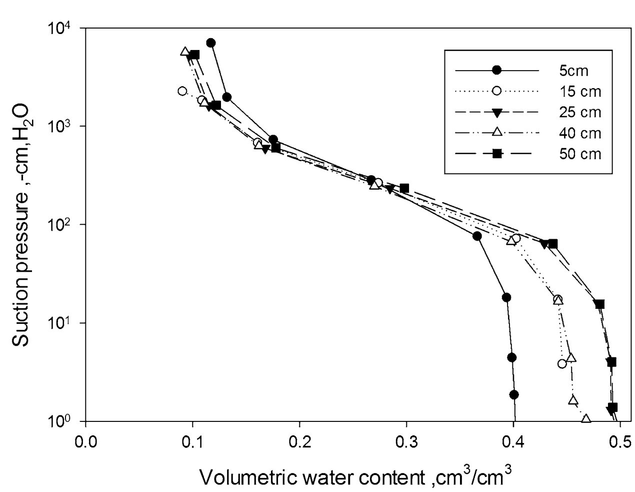

Fig. 2 Measured water retention characteristics at different soil depths

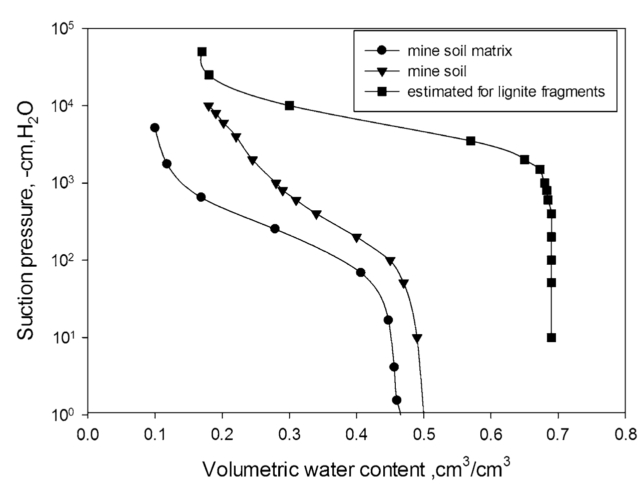

Fig. 3 Estimated water retention curve for lignitic fragments, mean measured data for the total soil, and Arya–Paris retention data predicted for the mineral soil matrix

Table 1 Average values of soil properties at the monitoring depths

Depth (cm)	No. of samples	Soil		Textural %(w/w)	Fraction		Bulk density (g cm^{-3})	Organic C %(w/w)
		>50 μm	50–20 μm	20–10 μm	10–2 μm	<2 μm		
5	7	31.02	23.09	18.49	12.63	14.76	1.58	2.73
15	8	24.8	24.57	20.36	13.49	16.79	1.57	3.84
25	7	29.06	23.3	18.45	12.32	16.86	1.47	4.08
40	8	25.09	26.35	19.51	12.34	16.72	1.53	7.48
50	5	24.73	24.89	20.06	12.89	17.44	1.36	3.01
60	3	29.88	23.21	17.95	12.06	16.9	1.74	3.21

capacity of the lignite fragments as compared to the mineral soil matrix.

In this paper, the saturated hydraulic conductivity, K_s was estimated from a pedotransfer functions (PTFs) (Wosten 1997). Wosten (1997) presented a function for determining K_s, as follows:

$$K_s = 1.15741 \cdot 10^{-7} \exp(x) \quad (9)$$

where x for sandy soil is:

$$x = 9.5 - 1.471(BD^2) - 0.688(Om) + 0.0369(Om^2) - 0.332 \ln(CS) \quad (10)$$

and where BD is bulk density in g cm^{-3}, CS is the sum percentage of clay and silt, and O_m is the percentage of organic matter.

The HYDRUS-1D model (Simunek et al. 2008) was used to simulate flow at the field site using hydraulic parameters obtained with PTFs. The HYDRUS-1D software (Simunek et al. 2008) was used to run the simulation. This software gives options to run simulation with the van Genuchten Eq. (4). The unsaturated hydraulic conductivity (K) function was calculated using Eq. (5) for the van Genuchten–Mualem model.

A separate simulation run was performed with HYDRUS-1D for each PTF. Water retention was estimated by applying the PTFs to the soil properties for each individual layer at the Shenshan field site (0–10, 10–20, 20–30, 30–50, and 50–70 cm; see Table 1).

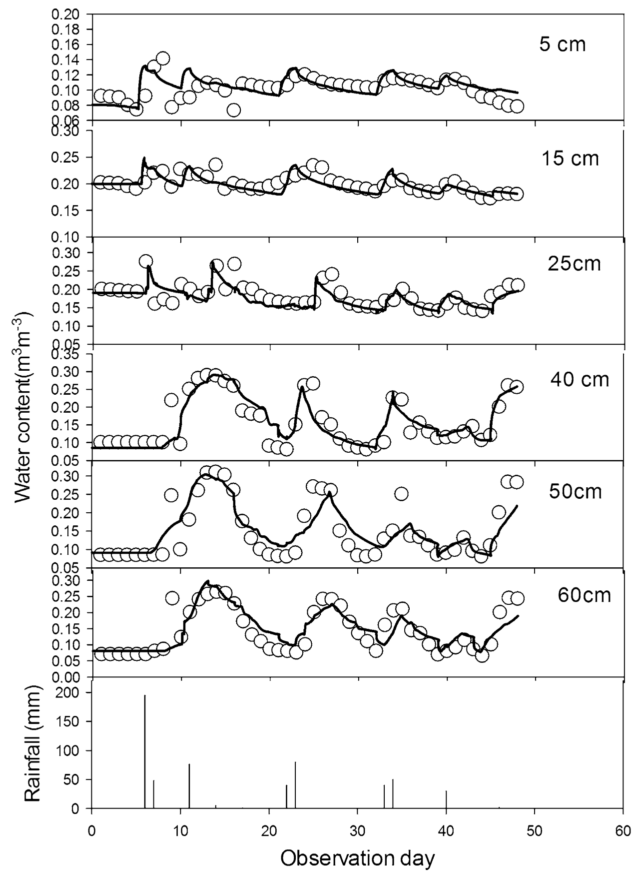

Fig. 4 Observed (*symbols*) and simulated (using the HYDRUS-1D model, lines) daily average water content; Observed values are averages across a transect for each depth and each day

Results and Discussion

Observed and simulated soil water contents are shown in Fig. 4. The topsoil (5, 15, and 25 cm) exhibited more weather-related variation in water content than the subsoil or mine soil (40, 50, and 60 cm), and the water content in the subsoil or mine soil (40, 50, and 60 cm) was greater than that of the topsoil. Figure 4 also shows that the mine soil water flow lagged behind initiation of rainfall. Yet in the second event, water flow responded very quickly to rainfall, which indicates that the mechanism of mine water flow must be dominated by rapid preferential flow through macro-pores in the mine soil rather than saturated flow through the mine soil matrix.

Discussion of Flow Paths

Still, it remains unclear how to explain how water in the lignitic fragments can be more mobile than in the matrix domain. The assumption that the lignitic fragments as a whole form a continuous pore domain would be difficult to verify. Nevertheless, the model analyses suggest the existence of non-equilibrium conditions and of a continuous pore system in which rapid water movement may take place. Observations show that the fragments itself can be heterogeneous and may not be homogeneously distributed; other observations indicate that a more continuous pore domain may be formed by lignitic components along surfaces of the fragments and smaller structures formed by lignitic in the mine soil matrix (Fig. 5). The integration of macro-pores in the mine soil horizon provides a mechanism for rapid downward movement of water through the unsaturated mine soil matrix.

In an attempt to verify the above formulated hypotheses on local flow paths in an unsaturated mine, we applied brilliant blue dye tracer in the waste dump of the Hei Dai Gou opencast coal mine, Ordos (Inner Mongolia, China). The Hei Dai Gou opencast coal mine is not at the same location as the Shenshan spoil heap, but they are only about 60 km apart. One liter of water containing Coomassie Brilliant Blue dye was slowly poured directly onto the surface of the mine soil. The dye readily penetrated into cracks surrounding surface fragments and into cracks beneath the fragments to an additional depth of 10 cm. Where cracks were absent, the dyed water penetrated <1 mm into the mine soil. The general vertical depth of penetration was 10–12 cm. In general, dyed water tended to flow along narrow, discrete paths, the length of which depended on the abundance and proximity of coarse fragments.

Infiltration of dyed water into the macro-pores and subsequent excavation revealed preferential flow paths along macro-pores developed around and connecting coarse fragments within the mine soil matrix (see Fig. 5). The integration of surface and subsurface cracks into a mine soil macro-pore network provides an important pathway for water flow to occur.

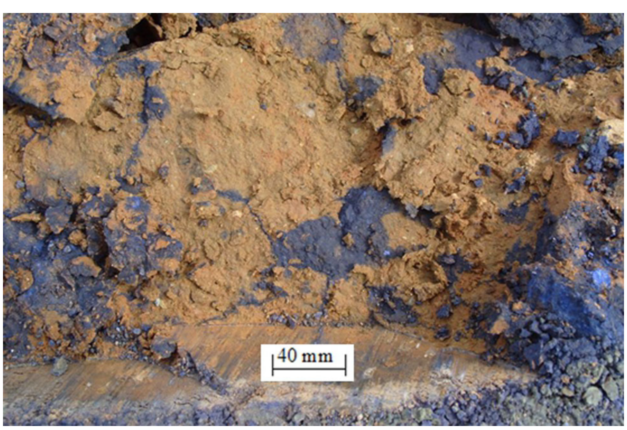

Fig. 5 Macropores in the mine soil of the Hei Dai Gou opencast coal mine dump site beneath coarse fragments that are embedded within a sandy mine soil matrix

Most dyes consist of relatively large organic molecules and, as such, interact to some degree with the solid matrix in soils and aquifers. Dyes have the ability to stain the travel paths of water and solutes in soils and are thus useful for visualizing water flow patterns. In general, organic dyes have amphiphilic characteristics, i.e. the molecule has both hydrophobic and hydrophilic properties. In addition, the functional groups of organic dyes can protonate and deprotonate depending on pH, thereby changing the net charge of the molecule. Because of these characteristics, interaction of the dye molecule with soil surfaces is rather complex. Sorption of dyes to solid surfaces involves one or a combination of the following interactions: hydrophobic, van der Waals, ion exchange, covalent bonding, and hydrogen bonding. The Coomassie Brilliant Blue dye is zwitterionic (amine and sulfonic acid groups) and has a solubility of 200 kg m^{-3}. It is nontoxic and, depending on pH, the dye is either neutral or dissociates to a mono- or bivalent anion (Flury and Flühler 1995). The Coomassie Brilliant Blue dye is a charged organic molecule that consists of polar and non-polar portions; sorption studies indicate that hydrophobic interactions are much less important than electrostatic or sorbate-mineral surface interactions (Flury and Flühler 1995; Ketelsen and Meyer-Windel 1999). The non-conservative nature of the Coomassie Brilliant Blue tracer is probably enhanced by relative slow volumetric flow through the highly absorbent materials in the mine soil.

The pH of the solution determines the degree of dissociation of the sulfonic acid groups and directly influences the net charge of the dye molecule. At the low pH of the soil, the molecule is predominantly in its neutral form, and may be more prone to adsorption in soils than anionic species. Qualitatively, the data are consistent with the presumption of increased sorption at low pH, although pH and soil texture can often interfere with sorption (Judit and Markus 2000). For tracing in field soils, a dye should preferably be mobile, distinctly visible, and nontoxic. The two criteria of visibility and mobility are to a certain degree mutually exclusive, because to stain the flow paths of water or solutes, the compound has to be retained. The advantages of Coomassie Brilliant Blue, especially for mine soil use, are its visibility against the color of the soil and its low toxicity. From the point of view of mobility, however, Coomassie Brilliant Blue is not ideal for tracing the travel times of water, but used in combination with conservative tracers, such as Cl^{-} or Br^{-}, Coomassie Brilliant Blue is useful for detecting flow patterns. We believe that, in terms of toxicity, visibility, and mobility, Brilliant Blue may be one of the best compromises available as a dye tracer in vadose zone hydrological studies.

Discussion of Model Concepts

Figure 5 indicates that the network of flow paths within the mine soil follows a small-scale structure, especially connecting the interface regions surrounding lignitic fragments. A network of flow paths may develop where the fragments are close together and where, with the sandy matrix, large pores are bridged by lignitic particles or by slightly more compacted regions formed locally during the sedimentation process. Further assessment of flow in small-scale heterogeneous media was beyond the scope of this study.

Summary and Conclusions

We studied the effects of local heterogeneity (here in the form of embedded porous lignitic fragments) on observed preferential flow. Such lignitic mine soils represent a typical two-scale dual-porosity medium. The results were used to assess the most appropriate conceptual model for describing small-scale heterogeneity effects on flow. One hypothesis is that at the interface between the sandy matrix and the inner parts of lignitic fragments, a more conductive porous network exists. This 'interface' flow domain probably consists of the outer, more weathered and cracked regions of fragments and those sandy regions that have a higher lignitic content. The latter could be due to particle segregation and compaction within the spoil piles during sedimentation, which is one major difference between mine soils and naturally developed and aggregated soils.

This flow model fit reasonably well to the monitoring data (Fig. 4). Our attempts to use HYDRUS-1D (MIM) model simulations based on the Richards' equations were hence warranted.

Development of macro-pores, predominantly in the mine soil horizon, is the fundamental control on increases in infiltration rates following reclamation of surface-mined land. Macro-pores in the mine soil horizon provide a mechanism for rapid downward movement of water through the unsaturated mine soil matrix.

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