Hydrodynamic characterization of BOF slags through numerical inversion of an evaporation experiment and through water infiltration experiments: a comparison.

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Abstract
Newer urban soils, frequently composed of several types of anthropogenic materials, may contain Basic Oxygen Furnace (BOF) slag, which is a steel industry byproduct. An understanding of the flow and solute transfer processes through urban soils requires a hydraulic characterization of these materials. This article is aimed at characterizing unsaturated hydraulic properties of the BOF slag with the evaporation experiment through parameter estimation method, and comparing the results with the values obtained from the field through water infiltration experiments using the adapted Beerkan Estimation of Soil Transfer Parameters method (Yilmaz *et al*. 2010). The results indicate a creation of a crusted layer at the surface of the column which avoids the characterization, for initial non crusted material. The parameter estimation technique using the experimental data gives acceptable values in agreement with the field data at one year. Such result is discussed in regard to the evolution of the material through carbonatation.

Key words
Soil characterization, unsaturated properties, Evaporation Method, BEST Method.

Introduction
Soils in urban areas are frequently composed of several types of anthropogenic materials whose hydraulic parameters are unknown. For instance, BOF slags that are byproducts of the steel industry are planned to be used as alternative materials in road and civil engineering, despite the fact that little is known in regard to their hydraulic properties. Only a few previous studies have focused on modelling flow through BOF slag (Chaurand *et al.* 2007; Yilmaz *et al.* 2009). Yet, the knowledge of their hydrodynamic properties is required to understand the effect on flows in the works and urban soils where they are found. Moreover, such knowledge is required to understand the pollutant release and transfer processes since flow patterns determine the release and transfer of solutes.

As means of hydraulic characterization, water infiltration experiments are quite common for the hydraulic characterization at the field scale. At the laboratory scale, the use of the evaporation method through analysis of experimental pressure heads at different heights in a vertical column has become widespread in obtaining such properties (Wind 1968; Tamari *et al.* 1993; Simunek *et al.* 1998). Among the various types of analysis of experimental data, the parameter estimation method (Kool *et al.* 1987) involves the coupling of a numerical model for variably saturated water flow with parameter optimization and this can estimate soil properties accurately (Santini *et al.* 1995; Simunek *et al.* 1998).

The present paper is intended (1) to provide a complete characterization of the unsaturated properties of the studied BOF slag using the parameter estimation technique through the Hydrus 1-D software and (2) to compare them with the results from water infiltration experiments performed at a test site and spanned along several dates, and analyzed through an adapted Beerkan Estimation of Soil Transfer Parameters (BEST) method (Yilmaz *et al.* 2010).

Materials and methods
The size fraction of the materials studied was 0 to 6 mm. Chemical properties were characterized by high calcium, iron and silicon contents. The BOF slag targeted in this study was cured for three years in an open area under conditions of atmospheric weathering.

The material was packed into a 17 cm high and a 10 cm in diameter column, placed on a monitored balance. Three tensiometers (T5, Ums Gmbh, Münich, Germany), with cups of 7 cm long and 0.5 cm in diameter were horizontally inserted into drill holes in the material core at 3, 6 and 9 cm from the sample surface.

The specific density ρ_s and the dry bulk density ρ_b of the BOF slag were respectively about 2.97 and 1.84 g/cm^3, leading to a porosity of 38 %. The volumetric saturated water content θ_s was equalized to the porosity. The system was saturated with water during a sufficient time to reach hydraulic equilibrium. A fan was used to ensure a potential evaporation rate of 0.8 cm/d. The measurement of the mass was performed by weighing with mass balance every hour and the measurements of pressure heads each five minutes. Initial pressure heads of -14 cm for the tensiometer at 3 cm was measured. The experiment was performed till the water pressure heads reach the limiting value of -750 cm. The experiment lasted eight days. At the end, the material was extracted from the columns and dried for the determination of the water content profile with 6 points.

Modelling was performed using HYDRUS 1D code that resolves the Richards' equation. The unsaturated soil hydraulic properties are described by the following expression (Van Genuchten 1980), in junction with Mualem capillary model (Mualem 1976):

$$\frac{\theta-\theta_r}{\theta_s-\theta_r}=\left(1+\left|\frac{h}{h_g}\right|^n\right)^{-m} \qquad (1)$$

$$K(\theta)=K_S\left(\frac{\theta-\theta_r}{\theta_s-\theta_r}\right)^{0.5}\left[1-\left(1-\left(\frac{\theta-\theta_r}{\theta_s-\theta_r}\right)^{1/m}\right)^m\right]^2 \qquad (2)$$

where n, $m(=1-1/n)$ are the hydraulic shape parameters, and h_g, θ_s, θ_r and K_s the hydraulic scale parameters. h_g is the scale parameter for water pressure head, and K_s is the saturated hydraulic conductivity. The value of θ_r was assumed to be close to zero, as is typically considered for coarse materials (Haverkamp *et al.* 2006).

The evaporation setup was simulated through a 17 cm length mesh with 0.1 cm length elements. Observation points were introduced at the tensiometer depths. The initial conditions corresponded to pressure equilibrium with -17 cm at the surface and 0 cm water pressure head at the bottom. The boundary conditions correspond to no flux at the bottom and a potential evaporation rate of 0.03 cm/h at the surface. The hydrodynamic parameters were estimated through the HYDRUS 1D inverse procedure. The data to be fitted correspond to the evolution of the pressure heads at the observation points and the total water loss at the end of the experiment. The additional hydraulic parameters to be fitted were the parameter n, the scale parameter for water pressure (h_g) and the saturated hydraulic conductivity (K_s).

Results and discussion

The soil hydraulic parameters were estimated from the evaporation experiment using a parameter inversion technique. For this purpose, we used the tensiometer readings as a function of time and the final water contents. As described before, mass measurements were used to calculate the evaporation rate at the top of the column for upper boundary condition. All data were introduced in Hydrus 1D. The tensiometers response and the numerically fitted *h(t)* function are shown in Figure 1.

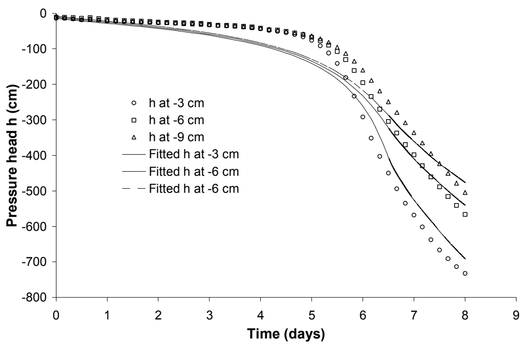

Figure 1. Experimental and numerical pressure head h (cm) in function of time (days).

The experiment was stopped after 8 days after the first tensiometer reached a value of -750 cm. The fitting of numerical data with experimental points can be considered correct. Moreover, the inverse procedure provided accurate values with the following values: estimated value for the scale parameter h_g of -33 cm with a confidence interval width of 6%, an estimated value for the saturated hydraulic conductivity *Ks* of 547 cm/d with a confidence interval width 50%, and an estimated value for *n* of 1.64 with a confidence interval width of 6%.

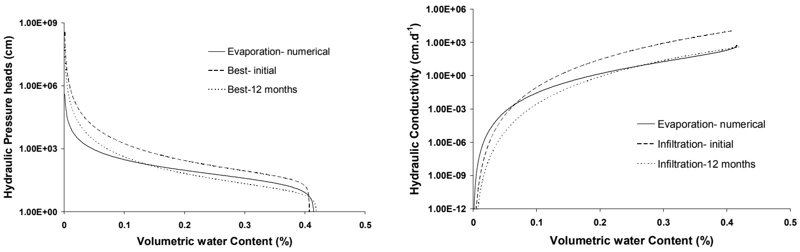

Figure 2. Water retention and hydraulic conductivity curves compared with curves from inverse analysis of infiltration experiments in the coarse zone of the experimental site

The field experiments were performed on an experimental embankment, built with the studied BOF slag. During the setup of the site, two zones appeared, a zone with fine materials (bulk density: 1.95 g/cm^3) and another zone with coarse materials (bulk density: 1.72 g/cm^3). Infiltration experiments were done immediately after the construction of the embankment was completed and then one year after. During this experiment, we found that the hydraulic properties of the BOF slag changed after 12 months due to the atmospheric events causing a carbonatation reaction at the surface of the slag material. These changes are assumed to be due to the clogging of pores through the formation of a coating of carbonates around the grains (Yilmaz *et al.* 2010). The water retention curves $h(\theta)$ and hydraulic conductivity curves $K(\theta)$ are illustrated in (Figure 2) in comparison with the hydraulic properties from the water infiltration experiments related to the coarse zone (Yilmaz *et al*. 2010).

As regards the Figure 2, the water retention curves from field experiments after 12 months and from evaporation experiments resemble. The hydraulic conductivity curve of the evaporation experiment is characterized by a similar tendency with the infiltration inversion of 12 months. During the evaporation experiments, it was noticed that a crusted zone formed at surface after a few days (coating of grains by carbonates). This may explain such agreement. In fact, the time required for the evaporation experiment is sufficient to crust the material by carbonatation. The evaporation experiment seems to be inappropriate to characterize a non crusted BOF slag.

However, as the crust occurred on the top of the column, in order to characterize the non crusted material below; the inverse modelling approach should be integrated with a double layer material. If the implementation of the two materials for the inversion of evaporation based experiment data could have been performed, this could have resulted in the following problems: (1) the increase in the number of parameters to be estimated and (2) the unknown variables such as the thickness of the crust versus time. These results point to the need for methods that may implement the evolution of the material with time and the need to adapt the base evaporation method to such material.

Conclusions

We characterized the hydrodynamic properties of the BOF slag using the parameter estimation technique through an evaporation experiment. During the evaporation experiment and due to a formation of a layer of crusted material, the inversion of the evaporation data by the parameter estimation technique gives similar results to the field infiltrations experiments after one year. In order to characterize the non crusted zone, a double layer material approach should be used; however, this would result in the need to estimate more parameters and difficulties to provide accurate values. The evaporation method for the material as BOF slag needs to be adapted, the evolution in time of the initial material has to be implemented in the parameter estimation technique. These aspects will be the subject of further research.

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