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► To cite this version:

A. Morvannou, N. Forquet, M. Vanclooster, Pascal Molle. Characterizing hydraulic properties of filter material of a vertical flow constructed wetland. *Ecological Engineering*, 2013, 60, p. 325 - p. 335. 10.1016/j.ecoleng.2013.06.042 . hal-00926091

HAL Id: hal-00926091

<https://hal.science/hal-00926091>

Submitted on 9 Jan 2014

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Characterizing hydraulic properties of filter material of a Vertical Flow

Constructed Wetland

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Abstract

Characterizing the hydraulic properties of filter material used in a vertical flow constructed wetland (VFCW) is a prerequisite to model wastewater treatment using process-based models. The filter material is a matrix of porous mineral material and organic matter that makes hydraulic characterization a difficult task. Here, we present a combined laboratory and in situ approach to assess the hydraulic properties of a VFCW installed at Evieu in Ain, France. The laboratory approach produces prior estimates of the local properties of the different VFCW system layers. These prior estimates are subsequently refined with inversely estimated parameters using the HYDRUS-1D code in combination with in situ hydrodynamic measurements. Laboratory experiments consisted of both direct (sand box, pressure chamber, and permeameter experiments) and inverse estimates (evaporation method) of hydraulic parameters. In situ

Abbreviations

CW, Constructed Wetland; p.e., people-equivalents; RETC, RETention Curve (software); TDR, Time Domain Reflectometry; VFCW, Vertical Flow Constructed Wetland

measurements were based on 5.5-day monitoring of the full-scale filter using 24 time domain reflectometry (TDR) probes installed at different depths. Applying the methodology with successive optimizations led to a reliable assessment of the hydraulic parameters of the VFCW. We conclude that the consistent representation of the hydraulic behavior of the VFCW requires in situ hydrodynamic observations combined with inverse modeling. However, to avoid the ill-posedness of the inverse problem, the number of fitted parameters should be kept to a minimum and parameter initialization need to be based on local-scale laboratory measurements.

Keywords: hydraulic properties; vertical flow constructed wetlands; laboratory measurements; in situ measurements; inverse modeling

1. INTRODUCTION

Constructed wetlands (CWs) are an attractive wastewater treatment technology for small communities (< 2000 people-equivalents; p.e.), as their simplicity of operation, low cost and reliable treatment efficiency often fit with the limited resources small communities can allocate to wastewater treatment (Kadlec, 2000). Irstea (National Research Institute of Science and Technology for Environment and Agriculture) developed an innovative type of first-stage for VFCW, made of gravel instead of sand. This first-stage type directly accepts raw wastewater, without the need for a preliminary settling tank. In a long-term operation, Molle et al. (2005) recorded on this first stage mean removal efficiencies of up to 80% for chemical oxygen demand (COD), 85% for total suspended solids (TSS), and 60% for total Kjeldahl nitrogen (TKN). However,

despite recent optimization trials in terms of media depth and aeration, the first stage of this VFCW still lacks treatment efficiency, making it necessary to upgrade with a second vertical stage that increases the total surface area needed ($1.2 \text{ m}^2 \text{ p.e}^{-1}$ for the first stage and $0.8 \text{ m}^2 \text{ p.e}^{-1}$ for the second stage). Molle et al. (2008) further highlighted that treatment efficiency could be improved if the hydraulic behavior of the VFCW would be better understood.

The hydrodynamic of a VFCW can be analyzed by numerical models such as those included in the HYDRUS software package (Šimůnek et al., 2006). HYDRUS solves the governing flow and transport equations for partially-saturated porous media and contains an extension module called CW2D dedicated specifically to the modeling of bio-geochemical processes in CW for wastewater treatment (Langergraber and Šimůnek, 2005). The bio-geochemical CW2D module incorporates all chemical species and degradation kinetics occurring in the wastewater treatment process. It uses an approach similar to the Activated Sludge Model (ASM) (Henze et al., 2000).

The numerical solution of the flow equation in HYDRUS requires detailed knowledge of the partially-saturated hydraulic properties of the VFCW porous medium. These properties are difficult to estimate because hydraulic functions are both highly non-linear and variable in space. The hydraulic properties of partially-saturated porous media can be assessed by direct and indirect methods applied at laboratory scale, field scale, or both. For example, the constant or falling head method for determining hydraulic conductivity can be applied on soil cores in-lab or in-field using cylinder infiltrometers (Dane and Topp, 2002). However, direct hydraulic characterization

requires restrictive initial and boundary conditions that have limited practicability in the field. Although direct laboratory methods are more accurate, the parameters obtained often fail to reflect real field conditions, and no common procedure exists for transposing laboratory hydraulic properties into field scale hydraulic properties (Russo et al., 1991; Ritter et al., 2003). The differences between laboratory and field assessments are due to several factors, including differences in support volume, measurement scale and structural status (e.g. different macropore compositions), and hysteretic effects (Schuh et al., 1988; Basile et al., 2003). Consequently, in situ measurements are considered more appropriate for assessing the hydraulic properties of partially-saturated porous media (Zou et al., 2001; Ramos et al. 2006), especially in constructed wetlands where the impact of the reeds on the hydraulic characteristics of the filter cannot be easily measured at the laboratory scale.

The indirect methods often rely on inverse modeling and are particularly suited to in situ assessments of hydraulic properties (Beven and Freer 2001; Hopmans et al., 2002; Vrugt et al., 2003; Minasny and Field, 2005; Lambot et al., 2005; Šimůnek et al., 2006; Durner et al., 2008). Inverse methods offer adaptable experimental procedures and impose less restrictive boundary conditions than direct methods. They can therefore be applied on transient flow experiments (e.g. Kool et al., 1987) and include different measurement variables in the objective function. Moreover, with inverse modeling, both hydraulic conductivity and water retention characteristics can be assessed simultaneously from a single flow experiment. In contrast to direct methods, inverse methods can rigorously assess parameter uncertainty (Kool et al., 1987). Furthermore, hydraulic parameters inferred from inverse methods are often more effective at

describing transient flow in real flow systems. The down side is that inverse problems are often ill-posed and can suffer from convergence problems (Russo et al., 1991). Nevertheless, as stated by Durner et al. (2008), inverse-based approaches remain widely recommended, and there are numerous examples of successful estimation of soil hydraulic properties using inverse methods (see Kool et al., 1987; Romano, 1993; Lambot et al., 2002; Hopmans et al., 2002; Ritter et al., 2004; Mertens et al., 2005; Verbist et al., 2009, among many others).

Many studies have addressed the partially saturated hydraulic properties assessment issue in the soil hydrological community, but few studies have attempted to address this issue for particular porous media such as gravels and sands mixed with sludge as retrieved in the VFCW systems. Giraldi and Iannelli (2009) carried out a laboratory-scale experiment to assess the saturated hydraulic conductivity of the material in a VFCW. They combined these measurements with generic estimates of the shape parameters of the hydraulic functions, and subsequently modeled water content distributions measured with capacitance probes in laboratory columns and in a VFCW pilot plant. Using these methods, they were able to simply and rapidly identify the real layout of vertical systems, and consequently highlight operational failures. Moreover, they managed to assess unsaturated hydraulic parameters for the main layers (gravel layers) of a vertical-flow bed using only water content measurements and saturated hydraulic conductivity. Langergraber (2003) carried out an inverse modeling with the HYDRUS-2D software to assess the hydraulic parameters of sand used as filter material. He measured pressure potentials and water contents at different depths (each 10 cm in the main layer) as well as the effluent flow rate. The simulations using the

fitted parameter set showed a good match with the measured data. Toscano et al. (2009) assessed hydraulic parameters using the inverse simulation proposed in HYDRUS-2D software (Šimůnek et al., 1999), with outflow measurements from a pilot-scale VFCW (secondary treatment) used as input data. Although they did not compare their results against laboratory assessments, the flow simulation study resulted in good correlations between measured and simulated effluent flow rates for two successive loadings. Similarly, Maier et al. (2009) used an inverse method considering a global optimization based on a stochastic search strategy for parameters. Hydraulic calibration was also carried out on the outflow rate measurement of two VFCWs filled mainly with a mixture of expanded clay and sand. They maximized the fit between observed and simulated filter discharges and revealed potential parameter correlations between certain hydraulic parameters. Another experiment performed on a laboratory sand column used both water content and suction head measurements to constrain the inversion (Forquet et al., 2009).

Although several studies have reported assessments of the hydraulic properties of VFCWs, none has compared the performance of different hydraulic assessment methods specifically in the VFCW setting. Furthermore, there are no published reports allowing the evaluation of different assessment procedures for the specific case of the French-type VFCW, where a sludge layer develops at the filter surface. In this paper, we compare the hydraulic properties of the first stage of a French-type VFCW estimated by direct and inverse laboratory methods as well as by inverse modeling using water content and outflow data collected on a VFCW. The objective is to determine the most appropriate method to estimate the hydraulic parameters in this type of VFCW.

2. MATERIALS AND METHODS

2.1 The VFCW studied

The Evieu wastewater treatment plant (Ain, France) comprises a sequence of vertical and horizontal sub-surface flow constructed wetlands. The plant has been in operation since 2004. It was originally designed for 200 p.e., but as only 100 p.e. are currently connected, the filter surface has been divided into two stages to work at full capacity. The first stage is made up of three VFCWs receiving raw wastewater. The pump sump at the plant inlet only performs mechanical screening using a 5 cm mesh screen. Each filter is fed according to a feeding/rest regime of 3.5/7 days. Effluent from this first stage is then connected to a second pump sump and separated between the second stage's vertical and horizontal flow constructed wetlands according to the experimental objectives (Molle et al., 2008). All beds are planted with reeds (*Phragmites australis*).

This study focuses on one of the filters of the first stage. The selected vertical filter (28 m², 2.9 m wide x 9.7 m long) is designed according to French recommendations. From the bottom to the top, it contains a 15 cm thick drainage layer (grain size of 30-60 mm), a 10 cm transition layer (grain size 15-25 mm) and a 60 cm gravel layer ($d_{10} = 2.46$ mm; $UC = d_{60}/d_{10} = 1.39$; average porosity of 40.4%). As the filter has been working at nominal load for 7 years, a sludge layer of about 20 cm has developed at the top of the filter. The VFCW is fed by raw wastewater in batches of 5 cm at a rate of 1.23 m h⁻¹ on average. During spells of dry weather, 8 separate batches of 3.4 min on average are

processed per day. Water is drained by a 160 mm diameter drainage pipe (0.42 m of pipe per m²), allowing passive aeration from the bottom as well.

2.2 In situ monitoring of the hydraulic behavior of the VFCW

We monitored the VFCW hydrodynamic behavior to estimate its hydraulic parameters using inverse modeling. To monitor water contents in the VFCW, a set of 24 TDR probes was installed one year before the experiment to minimize measurement disturbances. Six installation pits were dug in the VFCW, 4 probes were installed at different depths in each pit (Fig. 1), and the pits were then refilled. As found in preliminary observations, sludge and gravel proportion varies according to filter depth, with the result that biomass growth and solid entrapment in the porous gravel become increasingly limited with depth. Several layers, each presenting different hydraulic behaviors, can be differentiated. To perform inverse modeling, we hypothesized that the VFCW is composed of 4 horizontal layers (from top to bottom): sludge deposit (Layer 1, $h_1 = 20$ cm thick), biomass-colonized gravel (Layer 2, $h_2 = 20$ cm thick), less biomass-colonized gravel (Layer 3, $h_3 = 20$ cm thick), and almost-clean gravel (Layer 4, $h_4 = 20$ cm thick). Probes were inserted at four different depths corresponding to this layering system, and connected through multiplexers to a signal generator/analyzer (model TDR100, Campbell ScientificTM, Logan, UT). Results were recorded using a datalogger (model CR1000, Campbell ScientificTM Logan, UT). Measurements were made at 1 minute time intervals, end-to-end throughout the monitoring campaign, including the 3.5 batch feeding days and the first two days of the rest period. Three tensiometers were installed at different depths of the VFCW. Unfortunately, pressure

head variations were too small to be recorded by the monitoring device. Therefore, we only used water contents for assessing the hydraulic parameters.

INSERT FIG 1

2.3 Hydraulic parameters of the VFCW materials

In this study, we modeled the hydraulic properties of the VFCW sludge and gravel layers using van Genuchten-Mualem closed-form expressions (van Genuchten, 1980; Mualem, 1976):

$$\theta(h) = \theta_r + \frac{\theta_s - \theta_r}{\left[1 + |\alpha h|^n\right]^m} \quad h < 0 \quad (1)$$

where $h > 0$ and $m = 1 - 1/n$; h (L) is the actual pressure head; $\theta(h)$ ($L^3 L^{-3}$) is the actual water content dependent on h ; θ_r and θ_s ($L^3 L^{-3}$) are the residual and saturated volumetric water contents respectively; α (L^{-1}) and n (-) are shape parameters; and

$$K(\theta) = K_s S_e^\lambda \left[1 - (1 - S_e^{1/m})^m\right]^2 \quad (2)$$

where $S_e = (\theta - \theta_r)/(\theta_s - \theta_r)$ (dimensionless) is the effective fluid saturation; $K(\theta)$ ($L T^{-1}$) is the actual hydraulic conductivity dependent on the actual water content θ ; K_s ($L T^{-1}$) is the saturated hydraulic conductivity; and λ (-) is the Mualem pore connectivity parameter.

Eq. (1) contains four independent parameters (θ_r , θ_s , α , and n), while the hydraulic conductivity equation (Eq. (2)) integrates the saturated hydraulic conductivity (K_s) and the Mualem pore connectivity parameter (λ). This parameter was fixed at 0.5. To limit the total number of parameters to be assessed during the inversion, and following Ramos et al. (2006), we set θ_s for gravel equal to the total porosity. Total porosity is

easy to calculate from the dry bulk and particle densities (Flint and Flint, 2002). Setting θ_s equal to total porosity is challenged by several authors, who suggest that θ_s might be smaller than total porosity due to entrapped air or the presence of flow irregularities (Wessolek et al., 1994; Richard et al., 2001). We hypothesized that this is particularly true for finer-textured porous media or natural soil, but less applicable for gravel. Consequently, we fixed $\theta_{s,gravel}$ to total porosity and only optimized $\theta_{s,sludge}$.

Recalling that (i) in situ measurements provide more representative parameter values than laboratory measurements despite being more difficult to set up, and that (ii) inverse methods take better into account the transient nature of unsaturated flow than the direct methods carried out on permanent flow condition, different parameter assessments were developed using both laboratory and in situ measurements and both direct and inverse methods for the remaining parameters in Eq. (1) and (2).

2.3.1 Laboratory scale experiments

2.3.1.1 Samples

Samples were collected at different depths of the VFCW to assess the local-scale hydraulic properties of the different layers. We used a sampling technique that minimizes sample compaction to keep original sample structure and porosity. A total of six samples were extracted using PVC cylinders (diameter = 15 cm, height = 11 cm): one sample from Layer 1, two samples from Layer 2, three samples from Layer 4. Samples from Layer 3 were not studied because of the damage that occurred during the transport of the sample. The drainage layer was not studied, based on the assumption

that its role in the hydraulic behavior of the filter can be neglected when compared to the hydraulic role of the upper layers.

2.3.1.2 Determination of saturated hydraulic conductivity

The K_s of the VFCW samples was determined directly by applying the constant-head soil core method (Klute and Dirksen; 1986; Reynolds and Elrick, 2002). This technique is suitable for measuring the hydraulic conductivity of highly permeable materials like sand and gravel (10^0 to 10^{-5} cm s⁻¹, Reynolds and Elrick, 2002). The sample cores were first mounted on coarse mesh covered by nylon and then they were saturated by placing them in a tank filled with water for a 24 h period before measuring K_s . Measurements were repeated three times for each sample (except for Layer 1 that was only measured once due to the slow water flow rates). Each sample was then subjected to an evaporation method and subsamples of them were used in a sand box and pressure chamber methods. We also measured the volatile matter content for each sample by loss-on-ignition to compare K_s values with organic matter content: subsamples extracted from the core samples using 100 cm³ stainless steel rings were dried at 105°C and then 550°C to assess the dry matter and the volatile matter contents, respectively.

2.3.1.3 Water retention curves

After determining K_s , one undisturbed subsample of each previous sample was extracted from the core samples using 100 cm³ stainless steel rings. A sand box (Stackman et al., 1969) was used to determine water retention at low suctions up to 10 kPa (0.1, 1, 3.2 and 6 kPa). The samples were subsequently moved to a pressure chamber to determine water retention at high suctions up to 1.5 MPa (0.025, 0.1 and 1 MPa). The van

Genuchten-Mualem model (Eq. (1)) was fitted to the experimental water retention data using the RETC program (van Genuchten et al., 1991). Because θ_s was fixed using the porosity value, only the residual water content θ_r and the shape parameters α and n were fitted for Layers 2 and 4. To make the comparison and interpretation of water retention curves between layers easier, we used a cluster approach. This approach enables to overcome the difficulties related to the number of parameters (3: θ_r , α and n) and the non-linear relationship between them. The aim of this approach is to regroup layers in a limited number of functional layers based on the similarity of the water retention curves, as expressed by the Euclidean distance between them.

2.3.1.4 Evaporation method

The evaporation method is a transient inverse technique for determining unsaturated hydraulic conductivity and water retention curves at the laboratory scale (Wind, 1968; Ciollaro and Romano, 1995; Santini et al., 1995; Hopmans et al., 2002). The method inverts the governing flow equation using measured transient evaporation rates from a saturated soil sample.

The evaporation method was applied on the samples directly after the saturated hydraulic conductivity measurements when samples were still saturated. The samples were sealed at the bottom and placed under a free-evaporation boundary condition at the top (i.e. air humidity and temperature were not controlled). Usually, this method is carried out with some tensiometers to measure matric potentials and TDR probes for monitoring water content evolutions. In this study no tensiometers were used, but only TDR probes. TDR probes were inserted at two different depths (0.03 m from the top,

TDR A, and at 0.03 m from the bottom, TDR B) as illustrated in Fig. 2. Each TDR probe comprises three rods (100 mm length, 3 mm internal diameter, 15 mm spacing between rods). TDR measurements were taken on a Tektronix™ 1503B oscilloscope. The relationship between dielectric constant and water content was obtained by a material-specific calibration (Topp et al., 1980). Samples were weighed two to three times per day at the beginning of the experiment and only once a day after evaporation rate decreased. Once daily losses became negligible (less than 10 mg of water evaporated in 24 h), the experiment was stopped. The weight loss due to the loss of organic carbon during the evaporation experiment was neglected compared to the evaporation process.

INSERT FIG 2

The hydraulic parameters (θ_r , θ_{s_sludge} , α , n and K_s) of the six samples were determined using the inverse modeling tool in HYDRUS 1-D using measured soil water content and evaporation rates. Hydraulic parameter values derived from the earlier constant-head, sand box and pressure chamber experiments were used as starting values for inverse modeling. Samples were considered as initially saturated. Boundary conditions were expressed in terms of water fluxes: no flux at sample bottom and variable flux at top. The measured cumulative evaporation was interpolated, and the instantaneous fluxes were implemented as top boundary conditions. From the water content data we minimized the objective function in HYDRUS-1D model using the Levenberg–Marquardt nonlinear minimization algorithm (Marquardt, 1963). An equal weight was assigned in the model for all water content data during optimization (weight = 1). The mean and the variance of each optimized hydraulic parameter value obtained by this

method are only representative of the quality of the optimization process and are not constrained by physical limits (unphysical values). This may result in parameter intervals which violates the physics of the system. In order to constrain the parameter estimates to physical limits, we updated a-priori physical parameter ranges with information from the evaporation experiment using a Bayesian updating approach. Within the Bayesian framework a prior distribution is specified to reflect an *a priori* knowledge of the physical range of variation (Feyen et al., 2002) of a parameter p : $f(p)$. For example, the prior distribution for the θ_r parameter can range from 0 to the θ_s value. The distribution obtained from the inversion considering the evaporation data set, y , will be called the likelihood function $Ly(p)$, and will be multiplied to the prior distribution to produce a posterior distribution $f(p|y)$ according to Eq. (3).

$$f(p|y) = c \cdot f(p) \cdot Ly(p) \quad (3)$$

where c (-) is a constant adjusted to ensure that the integral of $f(p|y)$ on p is equal to 1.

The choice of the prior distribution is "subjective" but we expect that the likelihood function will "dominate the resulting posterior distribution" (Feyen et al., 2002).

2.3.2 Inverse modeling using in situ measurements

Not all data were used from the in situ monitoring; instead we selected water contents from one particular batch with a long drainage period that was recorded at night (Fig. 5). This reduced the size of the dataset to enable faster optimization, while providing a sufficiently large variation in water content to enable better hydraulic parameter estimates. The mean values of the hydraulic parameters optimized from the evaporation experiment were used as starting values to invert the in situ water content data using HYDRUS-1D. The transition and drainage layers (bottom two layers) were assumed not

to constrain the flow. Furthermore, the design of the drainage system includes a sump that temporarily stocks water between the drainage pipe and the outflow measurement device. Consequently, the measured outflows are not representative of those leaving the drainage pipe and cannot be used for the model inversion. So we restrain the domain to the sludge and filter layers. The one-dimensional mesh used for simulations consisted of 101 nodes. The top boundary condition is a time-dependent atmospheric boundary condition with a threshold value for surface runoff set to 100 cm. Wastewater load duration and flow rate are specified (mean: 1.94 m^3 , 0.05 m s^{-1}), while evaporation is neglected. If the incoming flow rate exceeds infiltration capacity, the ponding of water above the surface is then taken into account until it reaches 100 cm, a value that never observed in our case. The bottom boundary condition is a seepage face. An equal weight was assigned in the model for all water content data during optimization (weight = 1). The setup of initial conditions necessitated a prior initialization step. We could not use observed water contents since they do not provide a continuous pressure head profile at the initial time and cause the model not to converge (Radcliffe and Šimůnek, 2010). The prior initialization step consists in a simulation where loads (1.87 m^3 , 0.04 m s^{-1} , each) are applied at a constant time-lapse until pressure heads reach a pseudo-permanent state starting from hydrostatic distribution. We then selected the time for which water content profile matches the experimentally-observed initial water content. The corresponding water pressure profile was then considered as initial condition. The five van Genuchten-Mualem parameters (θ_r , θ_{s_sludge} , α , n and K_s) were estimated simultaneously, for each vertical profile. However, to avoid ill-posedness problems, the parameters were estimated layer-by-layer, from top to bottom.

Next, parameter distributions obtained from the inverted in situ observations were combined with the same prior distribution (physical limits) as presented in section 2.3.1.4 using the Bayesian data fusion approach. In summary, this procedure yields the hydraulic parameter distribution at the scale of the vertical profile in the filter.

Furthermore, to evaluate the robustness of the inverse approach, we tested different initial parameter values: those obtained from direct laboratory experiments and generic parameter values available in HYDRUS.

2.4 Upscaling hydraulic properties from the vertical profiles to the scale of the filter.

After optimizing hydraulic parameters for each vertical profile, we combined them layer-by-layer to obtain the parameter set probability density distribution (pdf) at the scale of the filter. This final parameter set pdf accounts both for spatial variability of the local properties within the filter and uncertainties associated with the local estimates. However, the pdf of some local scale parameters exhibit large confidence intervals due to a poor optimization or significantly differ from similar parameters obtained for the same layer. These values were considered as outliers and consequently removed before upscaling. In this procedure, we simply considered that the effective filter scale parameter equals the mean of the profile scale parameters. Such upscaling is acceptable if lateral flow between the profiles in the filter can be ignored as compared to the vertical flow. Then, layer-by-layer and parameter-by-parameter, the final value was computed. Since parameter pdfs were not all normally distributed, we used the convolution theory for combining random variables:

$$(f * g)(x) = \int_{-\infty}^{+\infty} f(x-y) \cdot g(y) dy = \int_{-\infty}^{+\infty} f(y) \cdot g(x-y) dy \quad (4)$$

were f and g are the two pdfs for which the convolution product $(f * g)$ is calculated.

We initially combined pdfs of the two first profiles. Then, we successively combined the result with the pdf of the next profile. This is possible because the convolution product is associative.

2.5 Model validation

Following the inverse-modeled parameter identification, hydrodynamic modeling was done using HYDRUS 1D software, including the remaining fraction of the monitoring dataset. Flow domain and boundary conditions were identical to those used for in situ data inversion. The setup of initial conditions was obtained using a prior initialization step as described in section 2.3.2. We calculated the mean square relative error (MSRE, Eq. (5)) to evaluate the agreement between simulation results and measured water contents (precision of the model simulation). The lower value of this MSRE is, the better agreement between observation and simulation is.

$$MSRE = \frac{1}{N} \sum_{i=1}^N \left[\frac{(O_i - P_i)}{O_i} \right]^2 \quad (5)$$

where $i = 1:N$ is the time interval (1 minute) end-to-end throughout the monitoring campaign, with N being the number of data (water contents) collected during the monitoring period (i.e. $N = 7780$); O_i is the water content observed for the time i ; P_i is the water content predicted for the time i .

3. RESULTS AND DISCUSSION

3.1 Parameter optimization

Based on porosity estimates, the θ_s values were fixed to 40.6% for Layers 2 and 3, and 44.0% for Layer 4.

3.1.1 Saturated hydraulic conductivity determination

Table 1 gives the K_s values and the volatile matter contents for all 4 VFCW layers considered.

[INSERT TABLE 1](#)

As expected, K_s values were proportional to pore size. However, for Layer 1, we identified issues over the reliability of the K_s value and the method used. First, the sludge layer is characterized by significant shrinking-swelling behavior. The constant head soil core method is inappropriate for determining the K_s of porous media of variable geometry (Reynolds and Elrick, 2002). Second, the K_s value for Layer 1 is close to the lower boundary of the method's range of validity ($10^{-5} \text{ cm s}^{-1}$). We also noted that the K_s values for Layers 2 and 4 were very close: K_{s-L2} is 1.06 times higher than K_{s-L4} . This is somewhat surprising given that Layer 2 contains more organic matter than Layer 4.

3.1.2 Water retention curves

The water retention curves as determined both on the sand box and in the pressure chamber apparatus are given in Fig. 3. At equal applied pressure, sample water content increases with increasing proportion of organic matter. The shape of the water retention curve is consistent with Aubertin et al. (2003). For all gravel samples, water content

rapidly reaches residual water retention after only few pressure steps. Furthermore, the reliability of measurements close to saturation is debatable, particularly for the coarse gravel material, as there may be significant water loss when handling the samples in the sand box and pressure chamber experiments. For the sludge layer higher residual water content could probably be measured at higher pressure steps.

INSERT FIG 3

Based on these data, and with saturated water content fixed to porosity (except for Layer 1), hydraulic parameters were fitted for every sample. Results are presented in Table 2 and the cluster approach result is presented in Fig. 4. The cluster approach indicates that the curve corresponding to Layer 1 is the most dissimilar from the other curves. The sludge layer has a significantly higher capability to retain water than the other layers. The second node from the top in the tree representation of the cluster approach separates samples from layers 2 and 4 that is consistent with their different organic matter contents. Euclidean distance between samples of Layer 2 is greater than those between samples of Layer 4. Cross-comparison of hydraulic parameters between each sample of Layer 2 revealed significant differences for θ_r and α values ($t-\theta_r = 8.3$, $t-\alpha = -4.3$, $p < 1.10^{-6}$). On the contrary, the Student's t -test applied to parameters of Layer 4 showed that θ_r and α values are close ($t-\theta_r = -0.2$, $t-\alpha = -1.4$, $p > 0.005$), except for the sample 4-3.

INSERT TABLE 2

INSERT FIG 4

Table 2 highlights that the parameter values obtained are consistent with a simple physically-based porous flow modeling concept. Indeed, α will be smaller and θ_r will be higher as organic matter content increases, reflecting the impact of organic matter on the structure of the porous medium. The n parameter values were similar for all gravel-containing samples. Relatively high sludge proportions had no significant impact on this parameter.

3.1.3 Evaporation method

Table 3 presents the hydraulic parameter values obtained from the evaporation experiments. For Layer 2, using the t-test as in section 3.1.2, most of optimized parameter values are dissimilar, except for the θ_r . However, as for the results from the water retention curves, parameters values were similar for two out of three (4-1 and 4-2) of the layer-4 samples. In addition, no clear trend emerged when comparing θ_r , α and n between layers.

The parameter values from the evaporation experiment (Table 3) significantly differed and tended to be lower than those estimated by the direct method (Table 2), with an important exception for the θ_s value of Layer 1 which increased. However, the degree of reliability of parameters assessed by the evaporation method should be considered low, as illustrated by the wide confidence intervals obtained from the inverse optimization method. In addition, the strong correlation between hydraulic parameters (between θ_r and α particularly, the correlation coefficient ranges from 0.53 to 0.99) from inverse optimization (correlation matrix not shown) indicates also that hydraulic parameter values showed a high level of uncertainty (Šimůnek et al., 1998). Indeed, water content

did not decrease very low during evaporation experiments: θ_r and α values are consequently highly uncertain. Several problems may explain this low reliability. First, the evaporation method does not provide reliable estimation of hydraulic properties at near-saturation when sample cores are initially saturated, as was the case in this study. Indeed, for soils with a high structural porosity, Richard et al. (2001) found that the retention properties were overestimated and hydraulic conductivity underestimated when the evaporation experiment started from fully-saturated samples. Stolte et al. (1994) suggested conducting the evaporation method without the preliminary saturation step. Secondly, non-optimal experimental conditions likely biased the evaporation measurements. The contact between TDR probes and porous material may become problematic due to air entry during the measurements. This is particularly problematic for the sludge sample, which strongly shrinks during drying (Vincent et al., 2011). Furthermore, the low frequency of sample weighting leads to poor estimates of the real evaporation rate since we operated in non-controlled climatic conditions. This could had been avoid by continuous monitoring of sample weight.

[INSERT TABLE 3](#)

3.1.4 In situ measurements

Figure 5 presents water content data measured at various depths in the VFCW (13, 31, 47 and 62 cm below the VFCW top surface) for the vertical profile 2 together with the experimental uncertainties estimated by media-specific calibration. The fact that the sludge layer has a high electrical conductivity resulted in fairly significant signal loss in this layer for some water content measurements.

[INSERT FIG 5](#)

Water content variations monitored by TDR probes allow identifying all the batches of water added to the VFCW (Fig. 5). Each batch is easily identifiable by the increase of the water content. In addition, the water retention and hence the water content decreases with depth, as organic matter content is lower deeper in the filter.

INSERT FIG 6

Results from the in situ data inversion are presented in Fig. 6. For Layer 1, parameters are dispersed and the confidence intervals for K_s and n values do not overlap for the different horizontal positions in the VFCW. Mean θ_r values did not significantly differ for Layers 2, 3 and 4 for all vertical profiles ($p > 0.002$). Values for K_s , α and n were also similar between vertical values within a same given layer ($p > 0.0017$), thus demonstrating the reliability of the inversion from field data.

Inverse modeling using in situ data could be even more robust if more information (such as measured VFCW outflow) were included in the objective function. However, this was not possible based on the filter design issue presented in the section 2.3.2. A possible solution could have been to set up a transfer function to account for the buffer effect of the temporary storage between the filter and the outflow measurement device. Because of the issues concerning the tensiometers their values were neither used in the objective function.

3.1.4 Parameter integration

After removing the outliers, the set of parameters validated for each vertical profile was then combined to obtain the overall global VFCW-scale parameter set. Table 4 gives the means and the standard deviations of the global hydraulic parameters. Results mostly differ from values obtained by lab-methods, which is consistent with Mertens et al. (2005). Notice that the residual water content of Layer 1 is very high given that the sludge consists of around 75% water and its desaturation takes a long time. It is a media very difficult to characterize and its physical properties rapidly change (due to swelling/shrinking). While for Layers 2, 3 and 4 the saturated water content was fixed to the porosity, it was optimized for the sludge layer.

INSERT TABLE 4

Comparing laboratory defined (Tables 2 and 3) vs. in situ measured reference parameters (Table 4) showed that laboratory methods gave good estimations of reference K_s value but underestimated the θ_r and α values, and n values were too dispersed to draw any firm conclusions. These patterns contrast with the conclusions of Kumar et al. (2010), who showed that field-scale θ_r , θ_s and n parameters could be estimated from laboratory experiments but that inverse modeling with in situ data was needed for α and K_s . These differences with the conclusions of Kumar et al. (2010) can mainly be explained by the fact that their study was carried out on soil samples and partly explained by the inappropriate operation conditions of the evaporation method in this study.

3.2 Comparison of the different methods

Figs. 7 and 8 present observed and simulated water contents in the VFCW for vertical profile 2. Simulations were performed with parameters obtained from (i) the inversion of in situ water content data (Fig. 7), (ii) the direct laboratory method (Fig. 8, left), and (iii) the inverse laboratory method (Fig. 8, right). Estimated parameters from method (i) were considered as reference parameters. Figure 8 illustrates that parameter sets obtained by the two laboratory methods are unable to properly simulate the water contents observed in the VFCW. We calculated square relative differences (MSRE values) of 11.8% and 5.3% for estimates with direct laboratory parameters and inverse laboratory parameters, respectively.

INSERT FIG 7

INSERT FIG 8

One advantage of the multi-tier approach developed in this article is that we can improve the identifiability of the poorly-posed inversion problem. We experienced convergence difficulties with the inverse modeling of in situ data carried out directly with hydraulic parameter estimates from the direct laboratory experiments. Indeed, when parameter estimates only from direct laboratory experiments for initialization were used, we were able to obtain a parameter set by inverse modeling over one batch, but direct model failed to simulate the entire monitoring campaign. When only using generic parameter databases available in HYDRUS, we failed to obtain a parameter set by inverse modeling. Ritter et al. (2003) showed that laboratory methods are useful to properly initialize inverse methods for estimating hydraulic parameters, and can be used to reduce the number of fitting parameters. Confidence intervals generally decrease over the course of successive hydraulic parameter estimation and optimization processes.

Therefore, a stepwise optimization process maximizes information exploitation from the various experiments while keeping the objective function as close as possible to its global minimum. Furthermore, this method tends to minimize the effect of extreme values stabilizing the solution at the cost of a loss of information.

We found that K_s parameter values were similar for Layer 2 for the different approaches used (Fig. 9). As expected, K_s scales negatively to sludge content and consequently increases with depth as sludge content decreases. This close agreement between the different determination techniques is apparent, given that K_s can normally vary significantly at short distances. These results contrast with many soil science studies showing that K_s at core scale in the laboratory is not effective for modeling in situ transport (e.g. Mallants et al., 1996).

[INSERT FIG 9](#)

Parameter θ_r appeared to be difficult to determine with the inverse method (see max CI, Table 4), particularly when organic matter content was high, as was the case for Layers 1 and 2. For these specific layers, a non-equilibrium flow approach would probably be more appropriate, as not all the porosity would participate in water flow.

The α value was lower for Layer 1 than for Layers 2 and 3, as expected (Table 4). However, the change in values for Layers 2 and 4 when switching from the direct to the inverse laboratory method is not expected. Again, experimental bias in the evaporation method may explain this pattern. For Layers 2 and 4, α was always underestimated by laboratory methods. This could be explained by non-equilibrium flow and hysteresis.

Indeed, non-equilibrium preferential flow may have occurred in the VFCW. In such cases, it is expected that $\alpha_{\text{non-equilibrium flow}} > \alpha_{\text{equilibrium flow}}$ due to a significant effect of macropores on unsaturated flow (Feyen et al., 1998). However, it is still difficult to obtain reliable estimates of non-equilibrium flow parameters using inverse modeling data (Šimůnek et al., 2003; Laloy et al., 2010), and $\alpha_{\text{non-equilibrium flow}}$ is consequently subject to a large degree of uncertainty. Hysteresis may also explain the observed differences, because laboratory methods represent drying processes while field measurements represent drying and wetting processes.

Both the modeling process and the model parameters were validated on the remainder of the monitoring dataset. As shown in Fig. 7, the simulation of water contents was good for most of the layers in the first four batches, where predicted water contents were close to observed water contents (MSRE = 0.6%). For later batches, the MSRE increased, which can be explained by the fact that the applied model does not consider water accumulation due to biomass growth, presence of organic matter, and the build-up of total suspended solids in the filter.

During the rest period, model predictions were unable to accurately reproduce the observed decrease in water content. The lowest absolute difference between observed and simulated water contents was found for Layer 1. Nevertheless, for a mature system like the Evieu VFCW plant, we consider that water content can be adequately simulated over a three-days feeding period. This would probably not be the case for a longer simulation or for a less mature system where biomass growth and suspended solid deposits during a given feeding period is expected to have a greater impact on hydraulic

parameters. Unfortunately, our experimental set-up did not enable us to validate the model in these conditions.

4. CONCLUSION

The calibration of hydraulic properties for a VFCW was carried out using laboratory and field data, and the HYDRUS software. As observed in the VFCW, vertical heterogeneity of hydraulic properties is important. Four layers composing the VFCW (a sludge layer, two layers for the mix between sludge and gravel and a gravel layer) were used in the conceptual and numerical models to describe its hydraulic behavior. However, this number of layer was arbitrary and we did not attempt to optimize it.

We used a multi-tier approach to obtain a hydraulic parameter set for these various layers. Both direct and inverse laboratory experiments and a network of TDR probes inserted within the VFCW were used to obtain specific hydraulic parameters. The applied methodology with successive optimizations as well as a large range of experimental data led to a reliable hydraulic parameter set that is able to predict water contents at different in-VFCW depths. Contrarily, using data sets obtained either from laboratory experiments only or from in situ data inversion using literature values for initialization failed. The fact that the HYDRUS software only features a local search algorithm makes initialization of the hydraulic function a critical issue when inverting HYDRUS on observed VFCW water data. Here, the initialization step can only be done by proceeding step by step with laboratory data. The estimation of hydraulic parameters for the sludge layer was particularly challenging whether it was performed in laboratory or in situ. Further research should be carried out to improve sludge flow modeling by

including the effects of macropore flow and solid deformation. Nevertheless, to improve this methodology, it might be interesting to consider confidence intervals from proposed methods into the inversion algorithm (e.g. using a Bayesian approach). Another way to improve parameter calibration is to account for the correlation among them. A change in one parameter can generate a variation in highly correlated parameters, with the result that none can be accurately determined. Therefore it might be useful to fix one parameter based on prior knowledge and optimize the others. Finally, simulations should be further improved by first considering the inter-dependence between layers and then using non-equilibrium models that are able to reproduce preferential flows. The former could be achieved by performing additional parameter optimizations to test the robustness of the hydraulic parameter optimization and to estimate the influence of layers to each others backward (e.g. by influencing the moisture content at the bottom of the overlying layer).

Acknowledgements

The authors thank Clément Crétollier and Olivier Garcia for their valuable technical assistance in installing the TDR probes in the VFCW. The authors also thank Guido Rentmeesters for his assistance with laboratory experiments (CHSCM, evaporation experiment, sand box and pressure head).

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Figure captions

Fig. 1. Set-up of the in situ experiment: (left) Top view of the VFCW with the six vertical profiles for the time domain reflectometry (TDR) probes. (right) Longitudinal section of the VFCW with the 24 TDR probes inserted within the four layers of the VFCW

Fig. 2. Set-up of the evaporation experiment

Fig. 3. Water retention curves determined during the sand box and pressure chamber experiments

Fig. 4. Cluster analysis of the water retention curves ordered by similarity using the Euclidean distance between them

Fig. 5. Water contents and their uncertainties from time domain reflectometry (TDR) probe calibration at various VFCW depths (vertical profile 2) before and during the monitoring campaign, as well as water contents used for in situ parameter optimization

Fig. 6. Hydraulic parameter estimates and confidence intervals (95%) from the in situ data inversion for the four layers and all vertical profiles (Eq. (1) and (2), HYDRUS software)

Fig. 7. Measured and simulated water content evolution in the VFCW at different depths during the monitoring campaign (Simulation performed with hydraulic parameters from in situ water content data inversion)

Fig. 8. Measured and simulated water contents with hydraulic parameters (left) from direct laboratory methods and (right) from inverse laboratory method

847 Fig. 9. K_s values for the four layers through the various optimizations