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1 **Characterizing hydraulic properties of filter material of a Vertical Flow**

2 **Constructed Wetland**

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9

10 **Abstract**

11 Characterizing the hydraulic properties of filter material used in a vertical flow
12 constructed wetland (VFCW) is a prerequisite to model wastewater treatment using
13 process-based models. The filter material is a matrix of porous mineral material and
14 organic matter that makes hydraulic characterization a difficult task. Here, we present a
15 combined laboratory and in situ approach to assess the hydraulic properties of a VFCW
16 installed at Evieu in Ain, France. The laboratory approach produces prior estimates of
17 the local properties of the different VFCW system layers. These prior estimates are
18 subsequently refined with inversely estimated parameters using the HYDRUS-1D code
19 in combination with in situ hydrodynamic measurements. Laboratory experiments
20 consisted of both direct (sand box, pressure chamber, and permeameter experiments)
21 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

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

30

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

33

34 **1. INTRODUCTION**

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

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

51

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

60

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

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

81

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

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

100

101 Many studies have addressed the partially saturated hydraulic properties assessment
102 issue in the soil hydrological community, but few studies have attempted to address this
103 issue for particular porous media such as gravels and sands mixed with sludge as
104 retrieved in the VFCW systems. Giraldi and Iannelli (2009) carried out a laboratory-
105 scale experiment to assess the saturated hydraulic conductivity of the material in a
106 VFCW. They combined these measurements with generic estimates of the shape
107 parameters of the hydraulic functions, and subsequently modeled water content
108 distributions measured with capacitance probes in laboratory columns and in a VFCW
109 pilot plant. Using these methods, they were able to simply and rapidly identify the real
110 layout of vertical systems, and consequently highlight operational failures. Moreover,
111 they managed to assess unsaturated hydraulic parameters for the main layers (gravel
112 layers) of a vertical-flow bed using only water content measurements and saturated
113 hydraulic conductivity. Langergraber (2003) carried out an inverse modeling with the
114 HYDRUS-2D software to assess the hydraulic parameters of sand used as filter
115 material. He measured pressure potentials and water contents at different depths (each
116 10 cm in the main layer) as well as the effluent flow rate. The simulations using the

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

131

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

141

142 2. MATERIALS AND METHODS

143

144 2.1 The VFCW studied

145 The Evieu wastewater treatment plant (Ain, France) comprises a sequence of vertical
146 and horizontal sub-surface flow constructed wetlands. The plant has been in operation
147 since 2004. It was originally designed for 200 p.e., but as only 100 p.e. are currently
148 connected, the filter surface has been divided into two stages to work at full capacity.

149 The first stage is made up of three VFCWs receiving raw wastewater. The pump sump
150 at the plant inlet only performs mechanical screening using a 5 cm mesh screen. Each
151 filter is fed according to a feeding/rest regime of 3.5/7 days. Effluent from this first
152 stage is then connected to a second pump sump and separated between the second
153 stage's vertical and horizontal flow constructed wetlands according to the experimental
154 objectives (Molle et al., 2008). All beds are planted with reeds (*Phragmites australis*).

155

156 This study focuses on one of the filters of the first stage. The selected vertical filter (28
157 m², 2.9 m wide x 9.7 m long) is designed according to French recommendations. From
158 the bottom to the top, it contains a 15 cm thick drainage layer (grain size of 30-60 mm),
159 a 10 cm transition layer (grain size 15-25 mm) and a 60 cm gravel layer ($d_{10} = 2.46$ mm;
160 $UC = d_{60}/d_{10} = 1.39$; average porosity of 40.4%). As the filter has been working at
161 nominal load for 7 years, a sludge layer of about 20 cm has developed at the top of the
162 filter. The VFCW is fed by raw wastewater in batches of 5 cm at a rate of 1.23 m h⁻¹ on
163 average. During spells of dry weather, 8 separate batches of 3.4 min on average are

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

166

167 2.2 In situ monitoring of the hydraulic behavior of the VFCW

168 We monitored the VFCW hydrodynamic behavior to estimate its hydraulic parameters
169 using inverse modeling. To monitor water contents in the VFCW, a set of 24 TDR
170 probes was installed one year before the experiment to minimize measurement
171 disturbances. Six installation pits were dug in the VFCW, 4 probes were installed at
172 different depths in each pit (Fig. 1), and the pits were then refilled. As found in
173 preliminary observations, sludge and gravel proportion varies according to filter depth,
174 with the result that biomass growth and solid entrapment in the porous gravel become
175 increasingly limited with depth. Several layers, each presenting different hydraulic
176 behaviors, can be differentiated. To perform inverse modeling, we hypothesized that the
177 VFCW is composed of 4 horizontal layers (from top to bottom): sludge deposit (Layer
178 1, $h_1 = 20$ cm thick), biomass-colonized gravel (Layer 2, $h_2 = 20$ cm thick), less
179 biomass-colonized gravel (Layer 3, $h_3 = 20$ cm thick), and almost-clean gravel (Layer 4,
180 $h_4 = 20$ cm thick). Probes were inserted at four different depths corresponding to this
181 layering system, and connected through multiplexers to a signal generator/analyzer
182 (model TDR100, Campbell ScientificTM, Logan, UT). Results were recorded using a
183 datalogger (model CR1000, Campbell ScientificTM Logan, UT). Measurements were
184 made at 1 minute time intervals, end-to-end throughout the monitoring campaign,
185 including the 3.5 batch feeding days and the first two days of the rest period. Three
186 tensiometers were installed at different depths of the VFCW. Unfortunately, pressure

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

189 **INSERT FIG 1**

190

191 2.3 Hydraulic parameters of the VFCW materials

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

$$195 \quad \theta(h) = \theta_r + \frac{\theta_s - \theta_r}{\left[1 + |\alpha h|^n\right]^m} \quad h < 0 \quad (1)$$

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

$$199 \quad K(\theta) = K_s S_e^\lambda \left[1 - (1 - S_e^{1/m})^m\right]^2 \quad (2)$$

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

204

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

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

216

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

223

224 2.3.1 Laboratory scale experiments

225

226 2.3.1.1 Samples

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

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

236

237 2.3.1.2 Determination of saturated hydraulic conductivity

238 The K_s of the VFCW samples was determined directly by applying the constant-head
239 soil core method (Klute and Dirksen; 1986; Reynolds and Elrick, 2002). This technique
240 is suitable for measuring the hydraulic conductivity of highly permeable materials like
241 sand and gravel (10^0 to 10^{-5} cm s⁻¹, Reynolds and Elrick, 2002). The sample cores were
242 first mounted on coarse mesh covered by nylon and then they were saturated by placing
243 them in a tank filled with water for a 24 h period before measuring K_s . Measurements
244 were repeated three times for each sample (except for Layer 1 that was only measured
245 once due to the slow water flow rates). Each sample was then subjected to an
246 evaporation method and subsamples of them were used in a sand box and pressure
247 chamber methods. We also measured the volatile matter content for each sample by
248 loss-on-ignition to compare K_s values with organic matter content: subsamples extracted
249 from the core samples using 100 cm³ stainless steel rings were dried at 105°C and then
250 550°C to assess the dry matter and the volatile matter contents, respectively.

251

252 2.3.1.3 Water retention curves

253 After determining K_s , one undisturbed subsample of each previous sample was extracted
254 from the core samples using 100 cm³ stainless steel rings. A sand box (Stackman et al.,
255 1969) was used to determine water retention at low suctions up to 10 kPa (0.1, 1, 3.2
256 and 6 kPa). The samples were subsequently moved to a pressure chamber to determine
257 water retention at high suctions up to 1.5 MPa (0.025, 0.1 and 1 MPa). The van

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

267

268 2.3.1.4 Evaporation method

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

274

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

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

292 [INSERT FIG 2](#)

293

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

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

$$317 \quad f(p|y) = c \cdot f(p) \cdot L_y(p) \quad (3)$$

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

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

321

322 2.3.2 Inverse modeling using in situ measurements

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

330 to constrain the flow. Furthermore, the design of the drainage system includes a sump
331 that temporarily stocks water between the drainage pipe and the outflow measurement
332 device. Consequently, the measured outflows are not representative of those leaving the
333 drainage pipe and cannot be used for the model inversion. So we restrain the domain to
334 the sludge and filter layers. The one-dimensional mesh used for simulations consisted of
335 101 nodes. The top boundary condition is a time-dependent atmospheric boundary
336 condition with a threshold value for surface runoff set to 100 cm. Wastewater load
337 duration and flow rate are specified (mean: 1.94 m^3 , 0.05 m s^{-1}), while evaporation is
338 neglected. If the incoming flow rate exceeds infiltration capacity, the ponding of water
339 above the surface is then taken into account until it reaches 100 cm, a value that never
340 observed in our case. The bottom boundary condition is a seepage face. An equal weight
341 was assigned in the model for all water content data during optimization (weight = 1).
342 The setup of initial conditions necessitated a prior initialization step. We could not use
343 observed water contents since they do not provide a continuous pressure head profile at
344 the initial time and cause the model not to converge (Radcliffe and Šimůnek, 2010). The
345 prior initialization step consists in a simulation where loads (1.87 m^3 , 0.04 m s^{-1} , each)
346 are applied at a constant time-lapse until pressure heads reach a pseudo-permanent state
347 starting from hydrostatic distribution. We then selected the time for which water content
348 profile matches the experimentally-observed initial water content. The corresponding
349 water pressure profile was then considered as initial condition. The five van Genuchten-
350 Mualem parameters (θ_r , θ_{s_sludge} , α , n and K_s) were estimated simultaneously, for each
351 vertical profile. However, to avoid ill-posedness problems, the parameters were
352 estimated layer-by-layer, from top to bottom.

353

354 Next, parameter distributions obtained from the inverted in situ observations were
355 combined with the same prior distribution (physical limits) as presented in section
356 2.3.1.4 using the Bayesian data fusion approach. In summary, this procedure yields the
357 hydraulic parameter distribution at the scale of the vertical profile in the filter.

358

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

362

363 2.4 Upscaling hydraulic properties from the vertical profiles to the scale of the
364 filter.

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

378 $(f * g)(x) = \int_{-\infty}^{+\infty} f(x-y) \cdot g(y) dy = \int_{-\infty}^{+\infty} f(y) \cdot g(x-y) dy$ (4)

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

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

383

384 2.5 Model validation

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

393 $MSRE = \frac{1}{N} \sum_{i=1}^N \left[\frac{(O_i - P_i)}{O_i} \right]^2$ (5)

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

398

399 3. RESULTS AND DISCUSSION

400

401 3.1 Parameter optimization

402 Based on porosity estimates, the θ_s values were fixed to 40.6% for Layers 2 and 3, and
403 44.0% for Layer 4.

404

405 3.1.1 Saturated hydraulic conductivity determination

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

408 [INSERT TABLE 1](#)

409

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

419

420 3.1.2 Water retention curves

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

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

430 [INSERT FIG 3](#)

431

432 Based on these data, and with saturated water content fixed to porosity (except for
433 Layer 1), hydraulic parameters were fitted for every sample. Results are presented in
434 Table 2 and the cluster approach result is presented in Fig. 4. The cluster approach
435 indicates that the curve corresponding to Layer 1 is the most dissimilar from the other
436 curves. The sludge layer has a significantly higher capability to retain water than the
437 other layers. The second node from the top in the tree representation of the cluster
438 approach separates samples from layers 2 and 4 that is consistent with their different
439 organic matter contents. Euclidean distance between samples of Layer 2 is greater than
440 those between samples of Layer 4. Cross-comparison of hydraulic parameters between
441 each sample of Layer 2 revealed significant differences for θ_r and α values ($t-\theta_r = 8.3$, $t-$
442 $\alpha = -4.3$, $p < 1.10^{-6}$). On the contrary, the Student's t -test applied to parameters of Layer
443 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
444 sample 4-3.

445 [INSERT TABLE 2](#)

446 [INSERT FIG 4](#)

447

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

454

455 3.1.3 Evaporation method

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

462

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

472 did not decrease very low during evaporation experiments: θ_r and α values are
473 consequently highly uncertain. Several problems may explain this low reliability. First,
474 the evaporation method does not provide reliable estimation of hydraulic properties at
475 near-saturation when sample cores are initially saturated, as was the case in this study.
476 Indeed, for soils with a high structural porosity, Richard et al. (2001) found that the
477 retention properties were overestimated and hydraulic conductivity underestimated
478 when the evaporation experiment started from fully-saturated samples. Stolte et al.
479 (1994) suggested conducting the evaporation method without the preliminary saturation
480 step. Secondly, non-optimal experimental conditions likely biased the evaporation
481 measurements. The contact between TDR probes and porous material may become
482 problematic due to air entry during the measurements. This is particularly problematic
483 for the sludge sample, which strongly shrinks during drying (Vincent et al., 2011).
484 Furthermore, the low frequency of sample weighting leads to poor estimates of the real
485 evaporation rate since we operated in non-controlled climatic conditions. This could had
486 been avoid by continuous monitoring of sample weight.

487 [INSERT TABLE 3](#)

488

489 3.1.4 In situ measurements

490 Figure 5 presents water content data measured at various depths in the VFCW (13, 31,
491 47 and 62 cm below the VFCW top surface) for the vertical profile 2 together with the
492 experimental uncertainties estimated by media-specific calibration. The fact that the
493 sludge layer has a high electrical conductivity resulted in fairly significant signal loss in
494 this layer for some water content measurements.

495 [INSERT FIG 5](#)

496

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

501 [INSERT FIG 6](#)

502

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

509

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

517

518 3.1.4 Parameter integration

519 After removing the outliers, the set of parameters validated for each vertical profile was
520 then combined to obtain the overall global VFCW-scale parameter set. Table 4 gives the
521 means and the standard deviations of the global hydraulic parameters. Results mostly
522 differ from values obtained by lab-methods, which is consistent with Mertens et al.
523 (2005). Notice that the residual water content of Layer 1 is very high given that the
524 sludge consists of around 75% water and its desaturation takes a long time. It is a media
525 very difficult to characterize and its physical properties rapidly change (due to
526 swelling/shrinking). While for Layers 2, 3 and 4 the saturated water content was fixed
527 to the porosity, it was optimized for the sludge layer.

528 [INSERT TABLE 4](#)

529

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

540

541 3.2 Comparison of the different methods

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

551 [INSERT FIG 7](#)

552 [INSERT FIG 8](#)

553

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

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

570

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

578 [INSERT FIG 9](#)

579

580 Parameter θ_r appeared to be difficult to determine with the inverse method (see max CI,
581 Table 4), particularly when organic matter content was high, as was the case for Layers
582 1 and 2. For these specific layers, a non-equilibrium flow approach would probably be
583 more appropriate, as not all the porosity would participate in water flow.

584

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

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

598

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

606

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

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

616

617 **4. CONCLUSION**

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

624

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

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

651

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656 experiment, sand box and pressure head).

657

658

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823

824

825 **Figure captions**

826

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

831 Fig. 2. Set-up of the evaporation experiment

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

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

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

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

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

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

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