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1 **Determining the effective properties of a highly heterogeneous horizon: Estimations by**
2 **numerical simulations and calculations by analytical equations**

3

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17 Abstract

18 In this study, we have attempted to determine the effective hydraulic properties of a highly
19 heterogeneous soil horizon composed of two elementary pedological volumes (EPVs). Our
20 upscaling approach was guided by the scaleway approach introduced by Vogel and Roth
21 (2003), in which the properties of a complex system can be estimated by multiple discrete
22 upscaling steps. This approach was tested on a dataset from laboratory measurements of
23 hydraulic conductivity at EPV scale, while explicit 3D soil structure was considered at
24 horizon scale. We then formulated a decision tree to guide the user to choose the appropriate
25 upscaling method to determine effective hydraulic conductivity at horizon scale. In the case of
26 low contrast between hydraulic conductivities at EPV scale, the effective hydraulic
27 conductivity at horizon scale can be achieved by calculating the Wiener bounds, which
28 requires only the proportion of the different EPVs. In the case of high contrast between
29 hydraulic conductivities at EPVs scale, we recommend either calculating the Cardwell and
30 Parson bounds, or performing a direct 3D numerical simulation to solve Richard's equation,
31 which requires an explicit representation of the 3D structure of the soil horizon. The Cardwell
32 and Parsons bounds remain a good and easily available approximation. Otherwise, more
33 accurate estimation can be obtained by numerical simulation though this is time-consuming.
34 A decision map is proposed to help choosing the best method for estimating effective
35 hydraulic conductivity.

36

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37 1. Introduction

38 Hydraulic properties are often key parameters in environmental simulations and it is usually
39 necessary to obtain them at horizon scale. In this context, soil horizons represent the reference
40 soil volume in terms of soil functioning. Nevertheless, in many cases soil horizons are
41 heterogeneous, for example, in stony horizons (Cousin et al., 2003), cultivated horizons
42 (Richard et al., 2001), and also specific weathering horizons like those in Albeluvisols (Diab
43 et al., 1988; Frison et al., 2009). In these cases, the determination of hydraulic properties
44 remains difficult. Consequently, two possibilities are offered. The soil horizon can be
45 described either by an explicit structure with distinctive hydraulic properties, or by effective
46 soil hydraulic parameters. The first possibility requires 2D or, even better, 3D modeling,
47 though the latter is not always practical to carry out. The second possibility is based on the
48 assumption that the soil horizon can be represented by a homogeneous structure if it is
49 possible to take into account the hydraulic properties at a lower scale. Nevertheless, the
50 determination of effective hydraulic properties in heterogeneous horizons cannot be done by
51 classical laboratory experiments on decimetric samples, such as the Multi-Step-Outflow (van
52 Dam et al., 1994) or the Wind evaporation experiment (Wind, 1968). According to the WRB
53 (1998), these heterogeneous horizons can be described as a combination of different
54 elementary soil pedological volumes that have different chemical and mineralogical
55 compositions and physical properties. For example, in the case of an Albeluvisol we can
56 distinguish ochre and pale volumes resulting from soil evolution; in the case of a cultivated
57 horizon, compacted and uncompact soil clods result from mechanical stress. Here, we
58 propose to determine the effective properties at the horizon scale based on the scaleway
59 upscaling approach introduced by Vogel and Roth (2003). In this upscaling approach, spatial
60 variability is considered to exist at multiple scales, and the system can be divided into
61 multiple discrete upscaling steps. Indeed, this approach permits dealing with multiscale

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62 heterogeneities without making assumptions about the heterogeneities of the underlying
63 structure, because the latter is taken into account explicitly.

64 The aim of this paper is threefold: i) to determine the hydraulic properties at the scale of the
65 soil's elementary volume, ii) to discuss benefits and disadvantages of the different analytical
66 methods for upscaling, and iii) to compare these methods with the estimation of the effective
67 hydraulic conductivity by using a direct 3D numerical simulation.

68 First, the determination of the hydraulic properties at the elementary scale of soil pedological
69 volumes is done by adapting the method proposed by Meadows et al. (2005). The second step
70 consists in developing different strategies to determine the effective hydraulic properties at
71 horizon scale. Renard and de Marsily (1997) discussed of different analytical methods based
72 on the simple calculation of bounds to estimate the effective hydraulic conductivity in
73 heterogeneous porous media. Until now, these methods have mostly been used in petroleum
74 engineering and in hydrogeology. Moreover, recent research to determine the effective
75 hydraulic properties of soil has often neglected natural soils and opted for simulated structures
76 (Knudby et al., 2006; Samouëlian et al., 2007; Durner et al., 2008). Here, we propose to apply
77 the analytical methods put forward by Renard and de Marsily (1997) in the context of Soil
78 Science, to natural soil heterogeneities and real data measurements of hydraulic properties at
79 local scale. To achieve this, we use an explicit representation of 3D soil structure measured by
80 electrical resistivity tomography (Frison 2008). We also test the accuracy of analytical
81 characteristics which can be easily computed once the structure of hydraulic properties is
82 known.

83 2. Material and Methods

84 2.1 Soil characteristics and structure

85 The soil studied was an Albeluvisol that exhibited several horizons composed by the
86 juxtaposition of two Elementary Pedological Volumes (EPVs). Here, we have focused on the
87 E&BT horizon, from 30 to 55 cm depth. The EPVs in this horizon can be visually
88 distinguished by their colours (ochre and pale). Their chemical and mineralogical
89 compositions (Montagne et al., 2008) and their different modes of hydraulic functioning
90 (Frison et al., 2009) were analysed on clods of the two types of EPVs, each clod being large
91 enough to be a Representative Elementary Volume of the EPV. This is consistent with
92 previous studies on E&Bt horizons (Diab et al., 1988; Wopereis et al., 1993). The pale EPVs
93 contained more silt whereas the ochre EPVs contained more clay (Table 1), but the proportion
94 of clay increased with depth inside the whole sample volume whatever the EPV. The bulk
95 density of the EPVs was around 1.5 g.cm^{-3} and was not significantly different between the
96 two types of EPV (Table 2). Further works conducted by Frison (2008) provided the 3D
97 structure of the soil horizon, and the proportion of each EPV. The characterisation of this
98 E&Bt horizon was done during autumn 2006, when no macropore was observed in the field.
99 As a consequence, only two types of EPVs, ochre EPV and pale EPV, represent the structure
100 of the horizon. The 3D structure of this heterogeneous horizon was obtained by electrical
101 resistivity measurements (fig. 1). A 3D soil block (90 cm x 52 cm x 30 cm) with the explicit
102 localisation of the ochre and pale EPVs was obtained after a simple binary threshold of the
103 electrical resistivity data. The threshold was chosen by comparison between the binary
104 resistivity image of the top of the horizon and its picture from photography (Frison, 2008).
105 Moreover, the proportion of each EPV type was calculated on this soil block: 57% for the
106 ochre EPVs and 43 % for the pale EPVs respectively.

107

2.2. Determining hydraulic properties at EPV scale

To calculate the effective hydraulic properties at horizon scale, experiments were first conducted at EPV scale. Large undisturbed blocks of the E&BT horizon – about 10,000 cm³ – were sampled when the soil was near field capacity during the autumn season. They were carefully stored at 4°C to avoid both structural disturbance by biological activity and loss of water. Before the experiments, each soil block was gently cut by hand, to separate the ochre EPVs and the pale EPVs, without destroying their structure. Each EPV was roughly cylindrical, with a diameter of at least 2 cm and a height of about 4 cm.

To keep the soil sample intact and avoid destruction during the experiments, the EPVs were embedded in paraffin wax and then placed in small plastic cylinders (6 cm in diameter, 6 cm in height).

Saturated hydraulic conductivity was determined with the constant-head method (Stolte, 1992) by using a mini-permeameter whose diameter was equal to the diameter of the plastic cylinder. After this experiment, the method proposed by Meadows et al. (2005) was adapted. The cylinder was placed on a mass balance and a mini tensiometer was inserted horizontally at the centre of the saturated EPV and equipped with a pressure transducer to continuously measure soil water potential. From these experimental data, the water retention curve and the unsaturated hydraulic conductivity were estimated by inverse modelling using HYDRUS-1D (Simunek et al., 2005). The water retention curve was parameterized by the modified van Genuchten equation with an air-entry value equal to -2 cm, and the unsaturated hydraulic conductivity was parameterized by the Mualem-van Genuchten equation (Mualem, 1976; van Genuchten, 1980):

$$\begin{cases} \theta = \theta_{sat} & \text{if } h \geq -2 \text{ cm} \\ \frac{\theta - \theta_r}{\theta_s - \theta_r} = [1 + (\alpha|h|)^n]^{-(1-1/n)} & \text{if } h < -2 \text{ cm} \end{cases} \quad [1]$$

$$\begin{cases} K(Se) = K_0 & \text{if } h \geq -2 \text{ cm} \\ K(Se) = K_0 Se^l \left[1 - (1 - Se^{1/m})^m \right]^2 & \text{if } h < -2 \text{ cm} \end{cases} \quad [2]$$

$$\text{with } Se = \frac{\theta - \theta_r}{\theta_s - \theta_r} \quad [3]$$

135 where h is the water potential (m), θ the volumetric water content (m^3m^{-3}), θ_s the saturated
136 water content (m^3m^{-3}), θ_r the residual water content (m^3m^{-3}), l the tortuosity factor, here taken
137 as equal to 0.5, K_0 ($\text{m}\cdot\text{s}^{-1}$) the hydraulic conductivity at $h = 0$, m , and n and α (m^{-1}) are fitting
138 parameters.

139 We chose the following conditions for the inversion:

140 Boundary conditions: no flux occurred at the lower EPV boundary while the flux at the
141 surface of the EPV was recorded during the experiment and corresponded to the loss of mass
142 of the whole sample, i.e. the loss of water through evaporation.

143 Initial condition: a linear distribution of water potential with depth was used.

144 The objective function of the inverse problem was defined with both the values of the water
145 potential recorded in the middle of the sample by the microtensiometer, and the values of the
146 water content calculated from the loss of mass recorded by the mass balance. Among the
147 parameters to be determined, two of them were fixed before the inversion: parameter K_0 was
148 taken as equal to the measured value ($K_0 = K_{sat}$) with K_{sat} being the saturated hydraulic
149 conductivity; parameter θ_s was taken as being equal to the porosity and estimated with the
150 EPV mass and the EPV volume, assuming a particle density equal to 2.65 g cm^{-3} . Quality of
151 the fit was checked through the mass balance error.

153 2.3. Determination of effective hydraulic properties

155 2.3.1 Case studies

156 Three case studies were analysed from the results at EPV scale: case 1: the highest contrast
157 between the hydraulic properties of the ochre and pale EPVs was taken into account; case 2:
158 the mean value of the hydraulic properties calculated for each type of EPV was taken into
159 account; and case 3: the lowest contrast of hydraulic properties between the ochre and the pale
160 EPVs was taken into account.

162 2.3.2 Effective water retention curve

163 The effective water retention curve was obtained from the additive properties of the water
164 retention curves at local scale, introduced by Durner (1994). This was achieved by an
165 expansion of the modified van Genuchten parametrization to a k-modal form (Vogel et al.,
166 2008):

$$167 \quad S_e(h) = \sum_{i=1}^k \omega_i \left[(1 + \alpha_i h)^{n_i} \right]^{-1+1/n_i} \quad [4]$$

168 where $S_e(h)$ is the effective water saturation. The relative weight of the different modes ω_i
169 fulfilled the condition $\sum_i \omega_i = 1$ while n_i and α_i are the related van Genuchten parameters (van
170 Genuchten, 1980). In our study, ω , the volume proportion of the different EPVs was equal to
171 0.43 for the pale EPVs and to 0.57 for the ochre EPVs.

173 2.3.3 Effective hydraulic conductivity

174 The effective hydraulic conductivity was determined with two different methods: numerical
175 3D variably saturated flow modeling, and an analytical method with the calculation of
176 mathematical bounds. It should be noted that the analytical method consisted in fast and easy
177 calculation, compared to the numerical one that requires a numerical 3D code to solve
178 Richards equation.

179

2.3.3.1 Numerical simulation of the effective hydraulic conductivity calculation

The effective hydraulic conductivity $K_{eff}(h)$ of the E&Bt horizon was obtained by solving Richards equation using Hydrus 3D (Simunek et al., 07). The 3D soil structure at horizon scale (fig. 1) was used to allocate each node (15 600 in total) of the finite element mesh to ochre or pale soil hydraulic properties. We used a modified hexahedral mesh with 80 850 elements to spatially describe the soil horizon. The average size of each element was about 2 cm³, whereas the sizes of the pale and ochre EPVs ranged from some centimeters to decimeters.

Numerical simulations were the same as described by Samouëlian et al. (2007). A steady-state flow regime was simulated by applying a constant water potential h at the upper and the lower boundary, so that gravity was the only driving force and the soil potential was approximately constant throughout the domain. The initial condition was a constant pressure head, whereas the vertical boundaries were considered as no-flux boundaries since the flow was assumed to be mainly vertical. This calculation was done for 102 pressures starting from saturated ($h = 0$ hPa) to unsaturated conditions ($h = -10000$ hPa). For each water potential value, the simulation time was chosen so that the steady-state flow condition was reached. The highest mass balance error that was accepted was 0.003%. Finally, we obtained $K_{eff}(h)$ which is equal to the simulated flux.

2.3.3.2 Calculation of the analytical bounds

Three types of analytical bounds, namely those of Wiener (1912), Matheron (1967), Cardwell and Parsons (1945), were calculated to estimate the hydraulic conductivity of the heterogeneous E&Bt soil horizon.

The calculation of the Wiener and Matheron bounds is based on an assumption of the spatial arrangement of the different EPVs constituting the soil horizon and takes into account their

205 proportion. The Wiener bounds assumed a layered model structure. When the flux is parallel
206 to the main direction of organization of the two types of EPVs, the effective conductivity at
207 each water potential, $m_a(h)$, is given by the arithmetic mean of the hydraulic conductivity of
208 each EPV:

$$209 \quad m_a(h) = \sum_{i=1}^2 \omega_i K_i(h) \quad [5]$$

210 where ω_i represents the volume proportion of each EPV and $K_i(h)$ represents the hydraulic
211 conductivity of EPV i at water potential h .

212 When the flux is perpendicular to the main direction of organization of the two types of
213 EPVs, the effective conductivity at each water potential, $m_h(h)$, is given by the harmonic
214 mean of the hydraulic conductivity of each EPV:

$$215 \quad 1/m_h(h) = \sum_{i=1}^2 \omega_i / K_i(h) \quad [6]$$

216 In a more complex arrangement of the different types of EPV, the effective hydraulic
217 conductivity of the E&BT horizon $K_{eff}(h)$ is comprised between these two theoretical bounds:

$$218 \quad m_h(h) \leq K_{eff}(h) \leq m_a(h) \quad [7]$$

219 In the calculation of the Matheron bound, we consider that the geometry of the porous
220 medium is isotropic. In this case the effective hydraulic conductivity $K_{eff}(h)$ is equal to:

$$221 \quad K_{eff}(h) = m_a(h)^\alpha m_h(h)^{1-\alpha} \quad \text{with } \alpha = (D-1)/D \quad [8]$$

222 where D is the spatial dimension.

223 Cardwell and Parsons (1945) proposed to take account of the spatial 3D arrangement of the
224 soil horizon to define the upper and lower bounds. The effective conductivity in a given
225 direction is bounded by: 1) the arithmetic mean of the harmonic means calculated on each cell
226 line parallel to the main flow direction (lower bound); 2) the harmonic mean of the arithmetic
227 means on each slice of a cell perpendicular to the main flow direction (upper bound). If the

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228 main flow is orientated along the vertical z axis, the effective conductivity $K_{eff}(h)$ is then

229 bounded by:

230
$$m_a^x(h)[m_a^y(h)(m_h^z(h))] \leq K_{eff}(h) \leq m_h^z(h)[m_a^y(h)(m_a^x(h))] \quad [9]$$

3. Results

3.1. Water retention curves of each pair of EPVs and the effective water retention curve at horizon scale

3.1.1 Comparison of the water retention curve for the pale and ochre EPVs

Figure 2a presents the water retention curve estimated from evaporation experiments for 17 pale and ochre EPVs. For potentials higher than about -1000 hPa, the volumetric water content was generally higher in the pale EPVs than in the ochre ones, which was in agreement with higher porosity due to biological structures (earthworm and plant roots) observed in the field in the pale EPVs. On the contrary, for water potentials lower than -1000 hPa, the water content was higher in the ochre EPVs, due to their higher clay content (Table 1) (Montagne et al., 2008; Frison et al., 2009). Nevertheless, the variability in the water retention curve within the different EPVs was high. Statistical tests on water content for water potentials equal to -10 hPa, -33 hPa, -100 hPa, -330 hPa, -500 hPa and -1000 hPa showed that the difference in water content between the two types of EPV was significant for water potentials equal to or higher than -100 hPa and non significant for water potentials equal to or lower than -330 hPa. The hydraulic parameters of the three cases are summarized in Table 3.

3.1.2 Calculation of the effective water retention curve at horizon scale

According to equation [4], the effective water retention curve at the horizon scale must be localized inside the domain defined by the water retention curves of the pale and ochre EPVs. Because the proportion of ochre EPVs was slightly higher (57%) compared to the pale EPVs (43%), the resulting effective water retention curve was closer to the ochre EPV water retention curve. Figure 2b presents the results for case 1; nevertheless the tendency was the same for the other cases 1 and 2, but the amplitude of the contrast between the water retention curves at EPV scale became decreasingly significant (results not shown here).

3.2. Hydraulic conductivity of each pair of EPVs and determination of effective hydraulic conductivity

3.2.1 Comparison of the hydraulic conductivity curve for the pale and ochre EPVs

Figure 3a presents the hydraulic conductivity curve for 8 pale and 9 ochre EPVs. Statistical tests performed on the logarithmic value of hydraulic conductivity for water potentials equal to those already studied for the water retention curve, i.e. -10 hPa, -33 hPa, -100 hPa, -330 hPa, -500 hPa and -1000 hPa, showed that hydraulic conductivity was always significantly different for the pale EPVs and for the ochre EPVs: hydraulic conductivity was higher in the pale EPVs whatever the water potential.

As shown in figure 3b, the contrast in hydraulic conductivity between ochre and pale EPVs was different for the three cases. The difference in hydraulic conductivity between pale and ochre EPVs was maximal for a water potential around -1000 hPa for case 1, and around -400 hPa for case 2. For more negative water potentials, the difference decreased slightly. Concerning case 3, the difference in hydraulic conductivity between the ochre and pale EPVs was negligible. To check this difference, we also calculated the surface area, defined by integral differences, between the two hydraulic conductivity curves for each case (fig. 4). As seen in Table 4, this surface area varied by one order of magnitude between case 1 and case 3.

3.2.2 Calculation of the effective hydraulic conductivity curve at horizon scale

The estimation of the effective hydraulic conductivity curve by the numerical simulation was assumed to be the closest to the real hydraulic conductivity and was thus considered as the reference hydraulic conductivity curve. As expected, whatever the case, it was between the hydraulic conductivity curves of each EPV, and was closer to the hydraulic conductivity of the pale EPVs (fig. 4), although the proportion of ochre EPVs was higher. This example backs up the argument that hydraulic conductivity is above all correlated to the soil structure.

281 For case 3 (fig. 4c), the effective hydraulic conductivity curves estimated by the numerical
282 simulation and calculated by the analytical bounds merged as the contrast in hydraulic
283 conductivity was low. Contrary to case 3, cases 1 and 2 presented distinct effective hydraulic
284 conductivity curves. As seen in figure 4a and 4b, the Wiener bounds and the Cardwell &
285 Parsons bounds delineated a surface area inside the domain of the hydraulic conductivity
286 curves of the ochre and pale EPVs. These domains included the effective hydraulic
287 conductivity curve estimated by the numerical simulation. By definition the Cardwell &
288 Parsons domain is included inside the Wiener domain. Indeed the heterogeneous structure is
289 taken into account by the Cardwell & Parsons bounds. The Wiener bounds assume an extreme
290 geometric structure of soil with a layered structure. This is in agreement with calculation of
291 the surface areas of the two domains: $S_{\text{Wiener}} \geq S_{\text{Cardwell-Parsons}}$, whatever the case (Table 4).

292 The results of our study showed that the high Wiener bound (calculation of the arithmetic
293 mean) was closer to the numerical simulation than the low Wiener bound (calculation of the
294 harmonic mean). This means that the general structure of the E&BT horizon was more or less
295 parallel to the water flow. This was consistent with field observations of vertical tongues of
296 pale EPVs and image analysis observations (Cornu et al., 2007).

298 4. Discussion

299 As shown previously, for the estimation of the effective hydraulic conductivity at horizon
300 scale, different situations could occur, depending on the contrast of the hydraulic conductivity
301 of each elementary EPV. Here, we propose a decision tree to guide the user in choosing the
302 method best-adapted for estimating the effective hydraulic conductivity of a heterogeneous
303 soil horizon (fig. 5). First of all, for any anisotropic medium like soil, the structure must be
304 studied roughly, for example, by qualitative soil profile observation. The two extreme cases
305 consist in a layered porous medium, where the elementary pedological volumes would be

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306 either parallel or perpendicular to the water flow. Between these two extreme structures,
307 various possibilities of structure topology and connectivity can be considered, as is often the
308 case for the natural soil horizon. Indeed, recent research has pointed out that the topology of
309 the sub-scale structure may be of crucial importance for upscaling hydraulic conductivity
310 (Western et al., 2001; Zinn and Harvey, 2003; Knudby et al., 2006; Samouëlian et al., 2007).
311 Here, we propose to take into account not only the topology but also the contrast between the
312 hydraulic conductivity curves at EPV scale to choose the appropriate upscaling method: either
313 estimation by numerical simulation or calculation using the analytical bounds.

- 314 i) When the contrast between the hydraulic conductivity curves of the two types of
315 EPV is low, the effective hydraulic conductivity can be rapidly and easily
316 estimated by the calculation of the domain defined by the Wiener bounds. This
317 method requires only the volume proportion of the different EPVs.
- 318 ii) When the contrast between the hydraulic conductivity curves of the two types of
319 EPV is high, we recommend either estimating the effective hydraulic conductivity
320 by numerical simulation, or calculating it with Cardwell-Parsons bounds. Both
321 methods require the 3D structure of the soil horizon. An initial estimation could be
322 given quickly by the calculation of the Cardwell and Parsons bounds. Depending
323 on the required accuracy, this first estimation can be sufficient. Otherwise, a more
324 accurate estimation can be provided by numerical simulation. Nevertheless, it
325 should be noted that this numerical simulation is much more time consuming than
326 the calculation of analytical bounds.

327 Nevertheless, determining an absolute value for a “high” or a “low” contrast of hydraulic
328 conductivity at EPV scale remains difficult. One way of deciding whether Wiener bounds can
329 be used consists in calculating their ratio, which itself depends on the ratio between the

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330 hydraulic conductivity curves of the two types of EPV and the volume percentage of each
331 EPV. This ratio R_w is equal to:

$$R_w = \frac{\left[\omega_p \frac{K_p(h)}{K_o(h)} + (1 - \omega_p) \right] \left[\omega_p + (1 - \omega_p) \frac{K_p(h)}{K_o(h)} \right]}{\frac{K_p(h)}{K_o(h)}} \quad [10]$$

333 where $K_p(h)$ and $(K_o(h))$ represents the hydraulic conductivity of the pale EPVs the ochre
334 EPVs respectively, while ω_p is the volume fraction of the pale EPV. When the contrast
335 between the hydraulic conductivity curves is low, the R_w ratio between the two Wiener
336 bounds is close to one. This means that the Wiener bounds enclose a rather narrow region in
337 which the actual effective hydraulic conductivity is located. For more complex cases, we
338 propose a decision map based on the R_w ratio, in order to simultaneously track the effect due
339 to the contrast between hydraulic conductivity at EPV scale, and that for each possible
340 proportion between the two EPVs. The hydraulic conductivity contrast was extended up to 4.5
341 in log scale, covering by this way the range of hydraulic properties proposed by Vogel et al.,
342 (2006) between macropores and a soil horizon. In our study, we consider that the Wiener
343 bounds could be correctly applied when the R_w value is lower than 3 (fig. 6). Nevertheless the
344 R_w threshold value has to be considered case to case by the user, depending i) on the accuracy
345 of the measurements themselves at the lower scale, and ii) on the expected accuracy required
346 for the simulation. In our survey, the cases 1 and 2 have R_w ratios lower than 3 and the use of
347 Wiener bounds remained then acceptable. Consequently, by calculating effective hydraulic
348 conductivity it is possible to avoid the difficulties related to numerical simulation. For case 3,
349 the R_w ratios were from around 3 to 100; the contrast between the hydraulic conductivity
350 curves of the pale and ochre EPVs therefore remained too high (around 2.5 in log scale) to
351 estimate the effective hydraulic conductivity by using the Wiener domain. In this case, the

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352 calculation of the effective hydraulic conductivity curve by the Cardwell and Parsons bounds
353 remained the best and most easily available approximation.

354
355 This decision tree was built with the assumption that the structure was bimodal at horizon
356 scale. Nevertheless, according to the scaleway upscaling approach introduced by Vogel and
357 Roth (2003), the applied concept could be generalized to estimate effective hydraulic
358 conductivity at scale n from knowledge of scale $n-1$. With respect to Wiener bounds assuming
359 a layered structure this suggest a simple way for upscaling to the scale of soil profiles or even
360 watershed. Nevertheless, this approach only allows the calculation of the vertical flux
361 component, so that this concept would be valid only when lateral flows are negligible or else
362 can be neglected.

363 At profile scale, the general structure of the soil is layered, with horizons sub-parallel to the
364 soil surface and generally perpendicular to the main water flow. Consequently, an easy way to
365 estimate the effective hydraulic properties at profile scale would be to calculate the low
366 Wiener bound, that is to say the harmonic mean of the hydraulic conductivity of the different
367 superimposed soil horizons weighted by their thickness (fig. 5).

368 At small watershed scale, it can be assumed that the general organization of the pedological
369 mantel consists of a juxtaposition of soil units. If we hypothesize that the general
370 hydrodynamic functioning of this watershed is vertical, and that the hydraulic conductivity
371 curve of each soil unit is known, we can calculate the effective hydraulic conductivity curve
372 of the watershed from the high Wiener bound, that is to say the arithmetic mean weighted by
373 the surface area of each soil unit.

5. Conclusion

In this study we investigated the impact of using different analytical bounds to upscale the effective hydraulic properties of a complex horizon, and especially hydraulic conductivity. The calculations of the analytical bounds were either based on the volume proportion of the different EPVs (Wiener and Matheron), or on the 3D structure (Cardwell and Parson), which included additional topological and connectivity information about soil structure. As already acknowledged in the literature, prior knowledge of topology and connectivity leads to more precise determination of effective hydraulic conductivity. However, because calculating analytical bounds is much easier than performing a numerical simulation based on a 3D structure, we defined the case in which the first method would lead to satisfactory results. We demonstrated that the contrast of hydraulic conductivity between the two EPVs was crucially important for choosing the most appropriate method to estimate effective hydraulic conductivity. Indeed, for a low contrast between these two EPVs, it was shown that the Wiener method, which requires only the volume proportions of each EPV, provided satisfactory results. For high contrast between the two EPVs, an adequate upscaling method required the 3D soil structure, i.e. topology and connectivity. For a hydraulic contrast equal or higher than the case 3, the use of Wiener bounds is then inadvisable. The calculation using Cardwell and Parson bounds is recommended at first because it is simpler to compute. If the accuracy of the calculated effective hydraulic conductivity is not sufficient, the numerical simulation is then the most relevant method.

We then used our results to propose a decision map that can be used for other studies to help choosing the appropriate analytical bounds as a function of the accuracy expected up to a conductivity contrast of 4.5 in log scale.

Our results are based on a natural soil horizon defined by only two EPVs, but extrapolation to more than two EPVs is easy. The sole restriction is the need to define the hydraulic properties

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399 at EPV scale. Moreover this approach was tested on real measurements at EPVs scale
400 combined with an explicit 3D structure at horizon scale, but it can be generalized for
401 estimating effective hydraulic conductivity at other scales. For example, this approach could
402 be applied to define effective soil hydraulic properties for each soil unit at watershed scale,
403 leading to better account being taken of heterogeneous soil horizons in simulations of
404 environmental functioning.

405
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5. References

- 409
410 Cardwell, W.T. and Parsons, R.L. 1945. Average permeabilities of heterogeneous oil sands. Trans.
411 Am. Inst. Mining. Met. Pet. Eng: 34-43.
- 412 Cornu, S. Montagne, D., Maguin, F., Le lay, C., Chevallier, P. and Cousin, I. 2007. Influence of
413 human impacts on Albeluvisol analysed by X-ray microfluorescence: Relative evolution of the
414 transforming front at the tongue scale. Science of the Total Environment, 377(2-3): 244-254.
- 415 Cousin, I., Nicoullaud, B. and Coutadeur, C. 2003. Influence of rock fragments on the water retention
416 and water percolation in a calcareous soil. Catena, 53(2): 97-114.
- 417 Diab, M., Merot, P. and Curmi, P. 1988. Water-Movement in a Glossaqualf as measured by two
418 tracers. Geoderma, 43(2-3): 143-161.
- 419 Durner, W. 1994. Hydraulic conductivity estimation for soils with heterogeneous pore structure. Water
420 Resources Research, 30(2): 211-223.
- 421 Durner, W., Jansen, U. and Iden, C. 2008. Effective hydraulic properties of layered soils at the
422 lysimeter scale determined by inverse modeling. European Journal of Soil Science, 59, 114-124.
- 423 Frison, A., Cousin, I., Montagne, D. and Cornu, S. 2009. Soil hydraulic properties in relation to local
424 rapid soil changes induced by field drainage: a case study. European Journal of Soil Science,
425 60(4): 662-670.
- 426 Frison, A. 2008 Analyse et modélisation des propriétés hydriques d'un horizon hétérogène de sol.
427 Thèse de l'Université d'Orléans, 228 p.
- 428 Knudby, C., Carrera, J., Bumgardner, J.D. and Fogg, G.E. 2006. Binary upscaling - the role of
429 connectivity and a new formula. Advances in Water Resources, 29: 590-604.
- 430 Matheron, G., 1967. Eléments pour une théorie des milieux poreux, Paris.
- 431 Meadows, D., Young, M.H. and McDonnald, E. 2005. A laboratory method for determining the
432 unsaturated hydraulic properties of soil peds. Soil Science Society of America Journal, 69: 807-
433 815.
- 434 Montagne, D. Cornu, S., Josière, O., Le Forestier, L., Daroussin, J. and Cousin, I. 2008. Soil drainage
435 as a factor of human-induced soil evolution: quantification of such an evolution in an
436 Albeluvisol. Geoderma, 145(3-4): 426-438.

Postprint

Version définitive du manuscrit publié dans / Final version of the manuscript published in :
Vadose Zone Journal, 2011, 10(1), 450-458, <http://dx.doi.org/10.2136/vzj2010.0008>

- 437 Mualem, Y. 1976. A new model for predicting the hydraulic conductivity of unsaturated porous
438 media. *Water Resources Research*, 12: 513-519
- 439 Renard, Ph. and de Marsily, G. 1997. Calculating equivalent permeability: A review. *Advances in*
440 *Water Resources*, 20(5-6): 253-278.
- 441 Richard, G., Cousin, I., Sillon, J.F., Bruand, A. and Guerif, J. 2001. Effect of compaction on the
442 porosity of a silty soil: influence on unsaturated hydraulic properties. *European Journal of Soil*
443 *Science*, 52(1): 49-58.
- 444 Samouëlian, A., Vogel, H.J. and Ippisch O. 2007. Upscaling hydraulic conductivity on the topology of
445 the sub-scale structure. *Advances in Water Resources*, 30, 1179-1189.
- 446 Šimůnek J., Sejna M. and van Genuchten M.Th., 2007. Software package for simulating the two and
447 three dimensional movement of water, heat and multiple solutes in variably saturated media,
448 user manual, version 1.07 203 p.
- 449 Šimůnek, J., van Genuchten, M. Th. and Šejna, M. 2005. The HYDRUS-1D Software Package for
450 Simulating the Movement of Water, Heat, and Multiple Solutes in Variably Saturated Media,
451 Version 3.0, HYDRUS Software Series 1, Department of Environmental Sciences, University of
452 California Riverside, Riverside, California, USA, 270 pp.
- 453 Stolte, J. 1992. Determination of the saturated hydraulic conductivity using the constant head method.
454 *Manual soil physical measurements*, version 2.0. Technical Document sc-dlo, Wageningen, 4p.
- 455 van Genuchten, M.T. 1980. A Closed-Form Equation For Predicting The Hydraulic Conductivity of
456 Unsaturated Soils. *Soil Science Society of America Journal*, 44(5): 892-898.
- 457 Vogel, H.J., Samouëlian, A. and Ippisch, O. 2008. Multi-step and two-step experiments in
458 heterogeneous porous media to evaluate the relevance of dynamic effects. *Advances in Water*
459 *Resources*, 31:181-188.
- 460 Vogel H.J., Cousin I., Ippisch O., Bastian P., 2006. The dominant role of structure for solute transport
461 in soil: experimental evidence and modelling of structure and transport in a field experiment.
462 *Hydrology and Earth System Sciences*, 10, 495-506.
- 463 Vogel, H.J. and Roth, K. 2003. Moving through scales of flow and transport in soil. *Journal of*
464 *Hydrology*, 272(1-4): 95-106.

Postprint

Version définitive du manuscrit publié dans / Final version of the manuscript published in :
Vadose Zone Journal, 2011, 10(1), 450-458, <http://dx.doi.org/10.2136/vzj2010.0008>

- 465 Western, A.W., Blöschl, G. and Grayson, R.B. 2001. Toward capturing hydrologically significant
466 connectivity in spatial patterns. *Water Resources Research*, 37(1): 83-97.
- 467 Wiener, O. 1912. *Abhandlungen der Mathematisch. Physischen Klasse der königlichen sächsischen*
468 *Gesellschaft*(32): 309.
- 469 Wind, G.P. 1968. Capillary conductivity data estimated by a simple method. In: E. P.E. Rijtema and
470 H. Wassink (Editor), *Water in the Unsaturated Zone*, Gentbrugge, Belgium, pp. 181–191.
- 471 Wopereis, M.C.S., Kropff, M.J., Wösten, J.H.M. and Bouma, J. 1993. Sampling strategies for
472 measurement of soil hydraulic properties to predict rice yield using simulation models.
473 *Geoderma*, 59: 1-20.
- 474 WRB, 1998. A world reference base for soil resources. In: O.C.S. J.A. Deckers, F.O. Nactergaele,
475 L.R. Oldeman, R. Brinkman (Editor), *World Soil Resources*, Report n°84. FAO-ISRIC-AISS,
476 Rome, Italia.
- 477 Zinn, B. and Harvey, C.F. 2003. When good statistical models of aquifer heterogeneity go bad: A
478 comparaison of flow, dispersion, and mass transfer in connected and multivariate hydraulic
479 conductivity fields. *Water Resources Research*, 39(3): 1-18.

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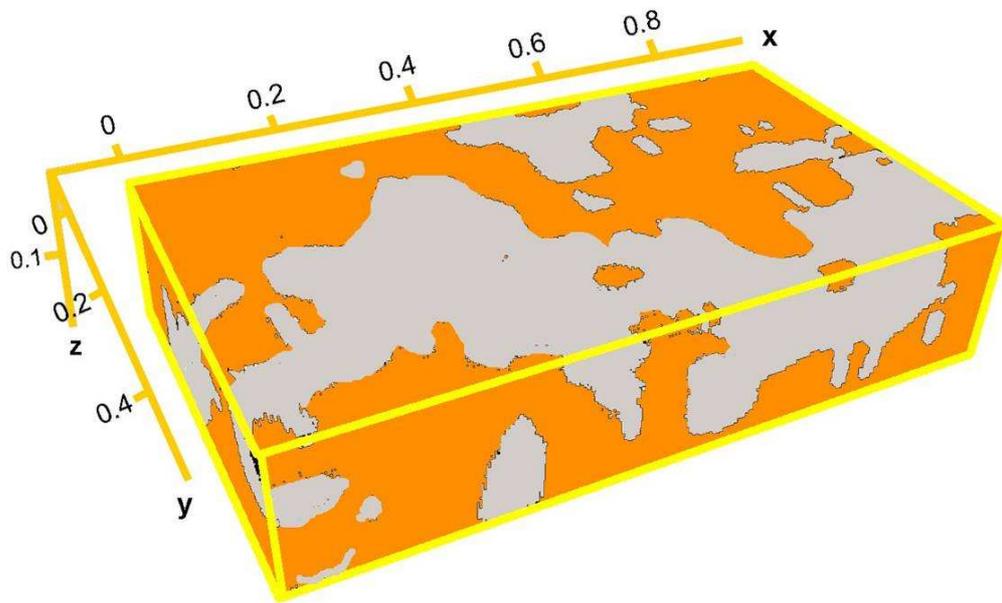
526

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Figure 1

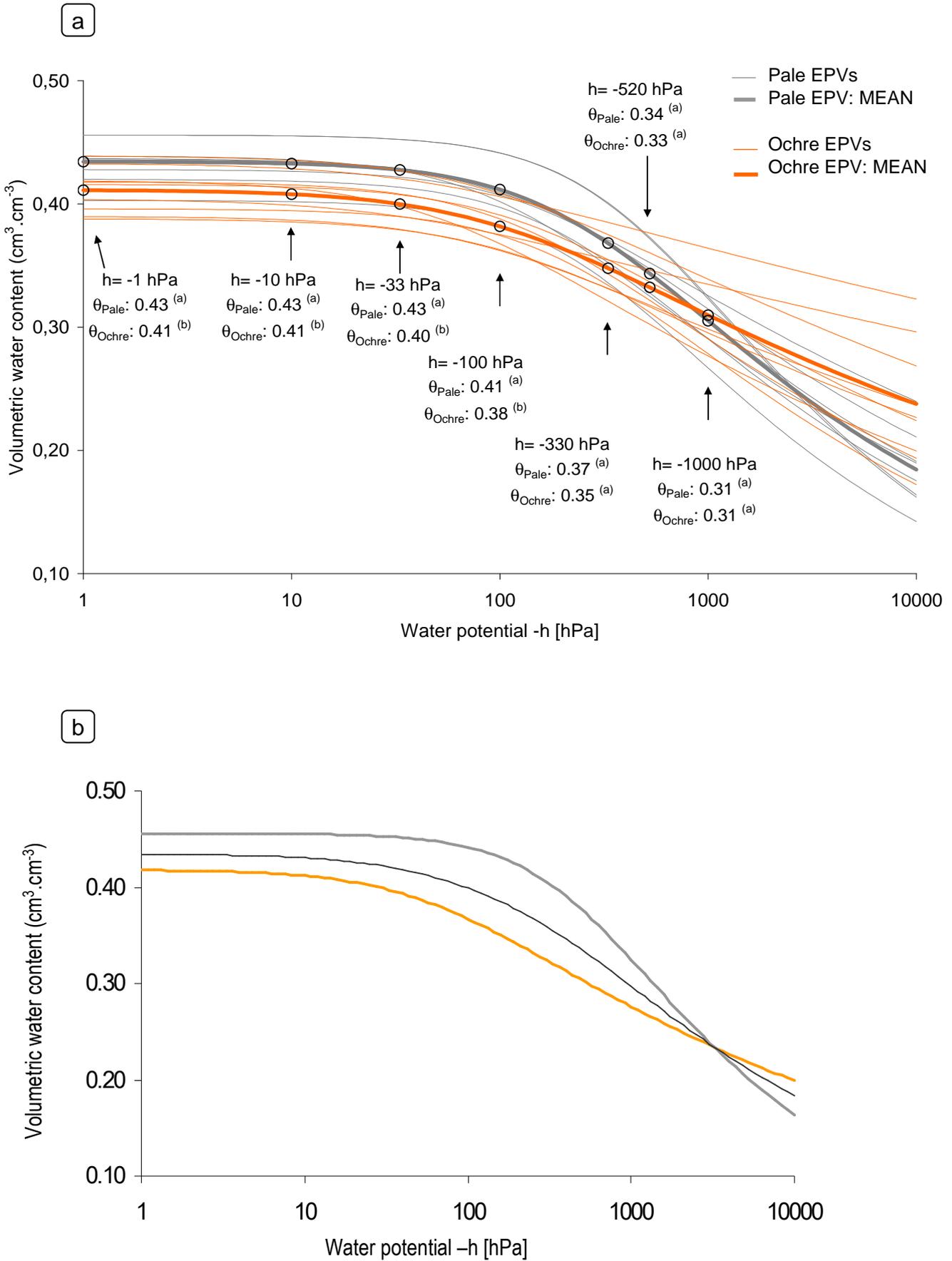


Figure 2

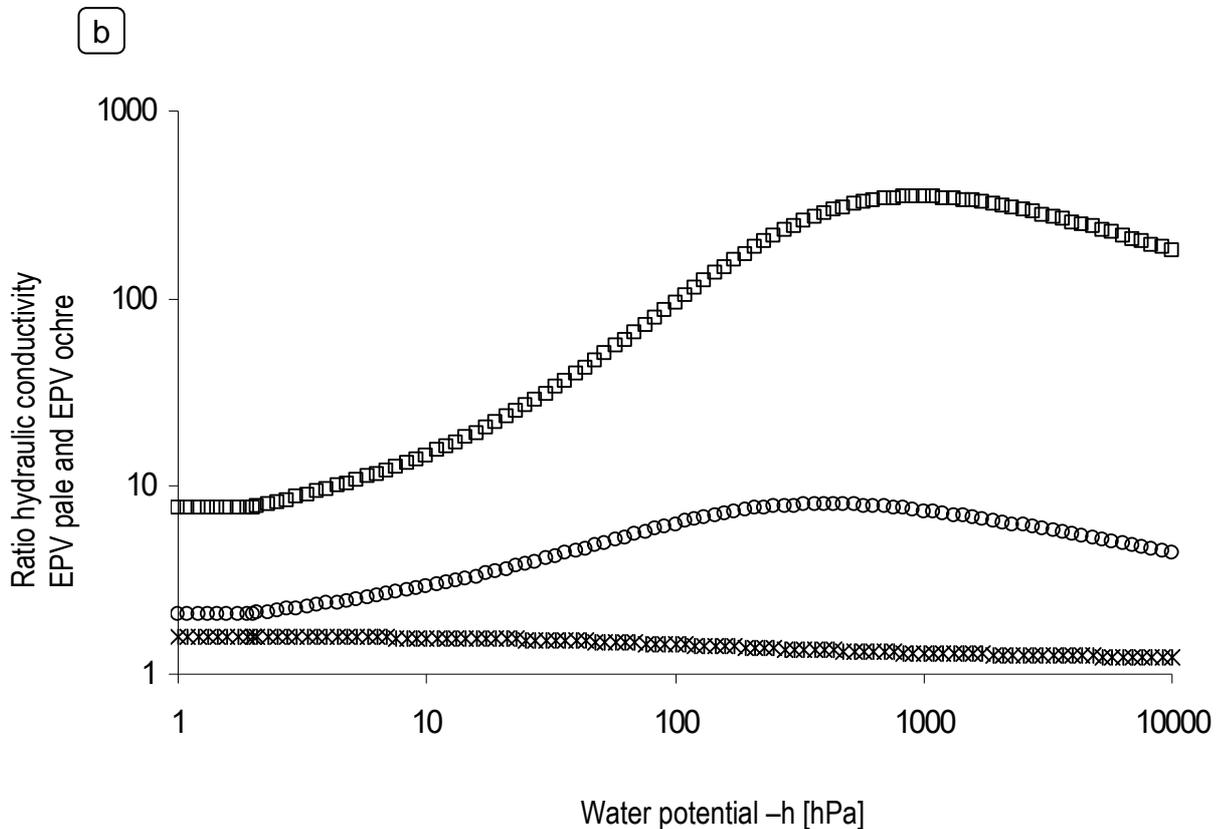
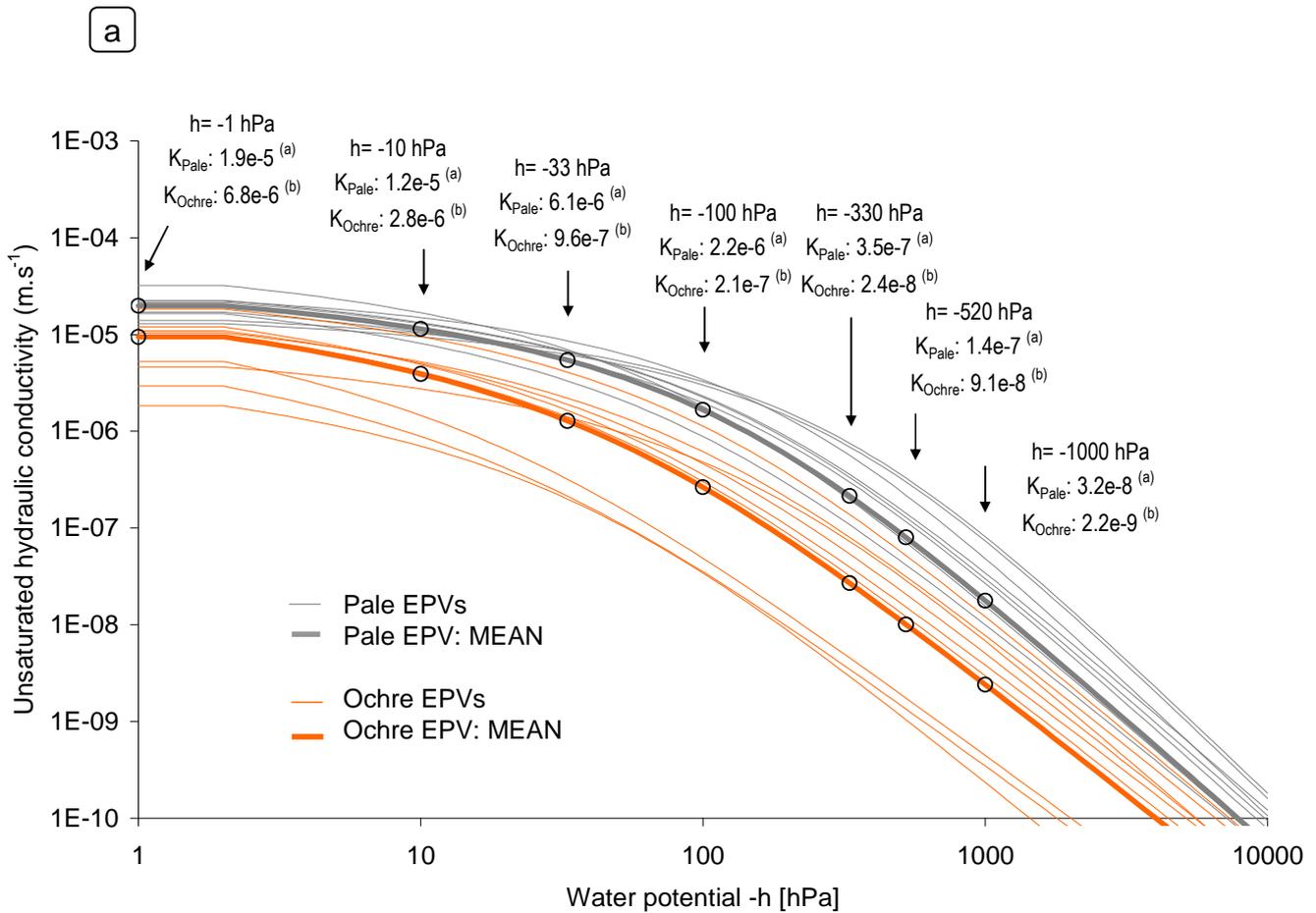


Figure 3

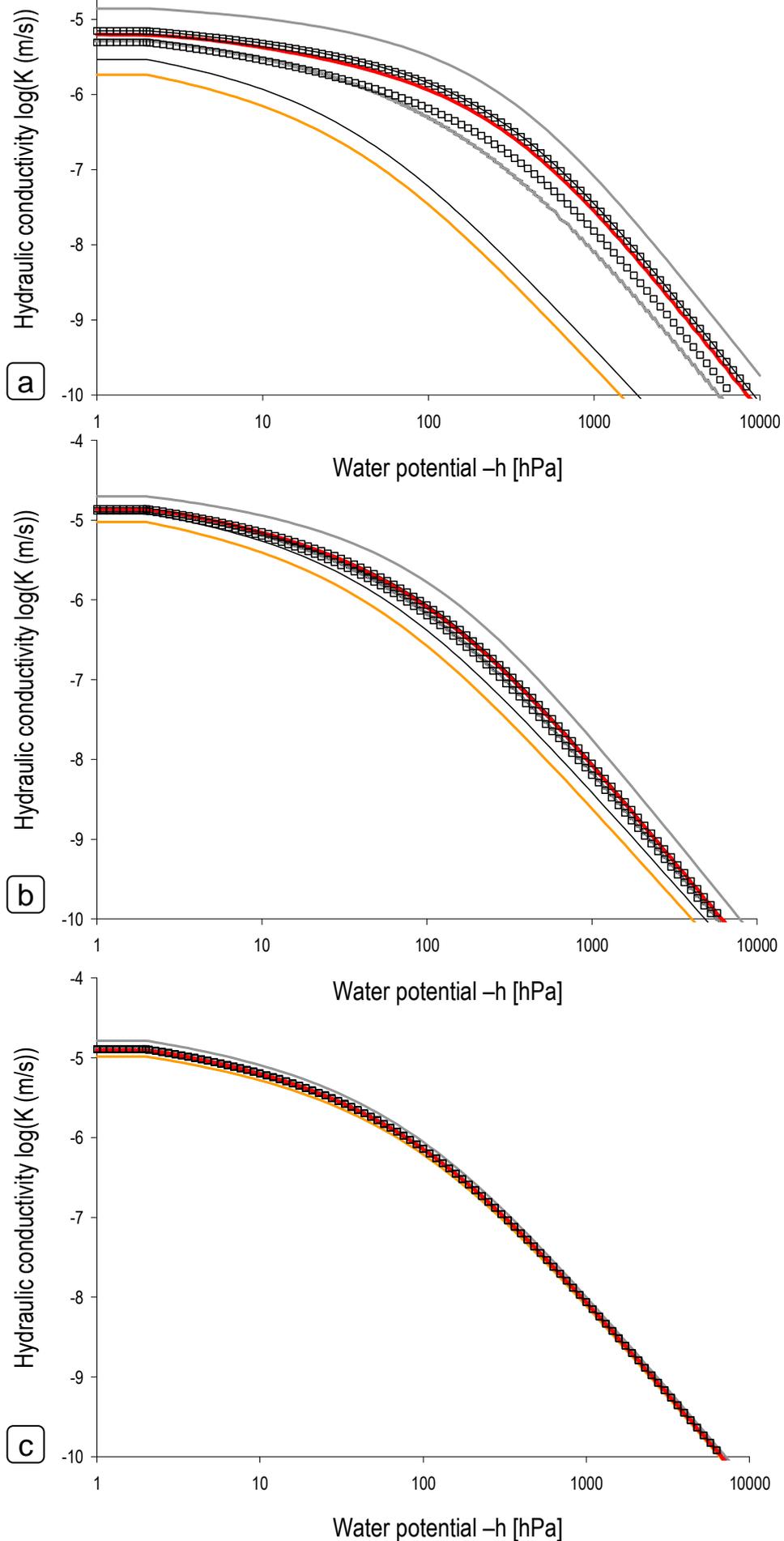


Figure 4

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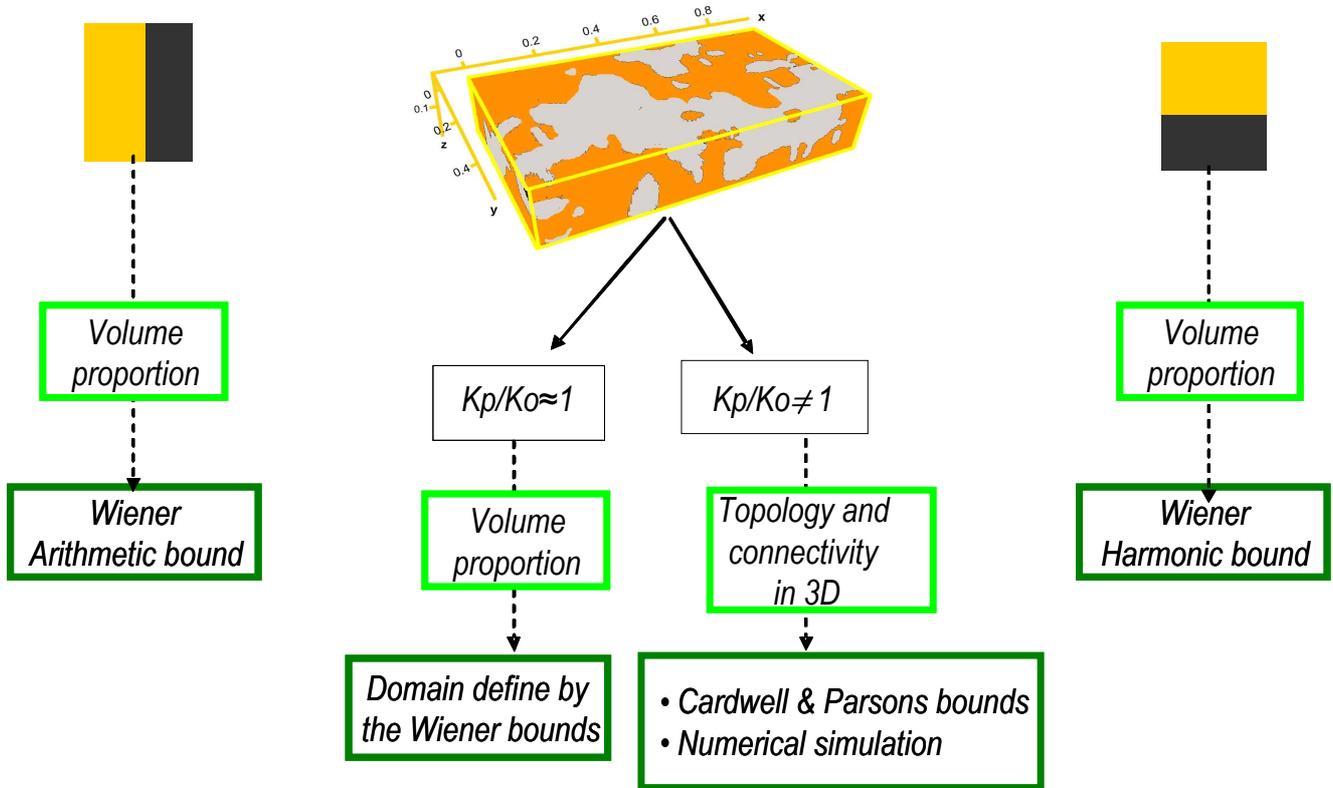


Figure 5

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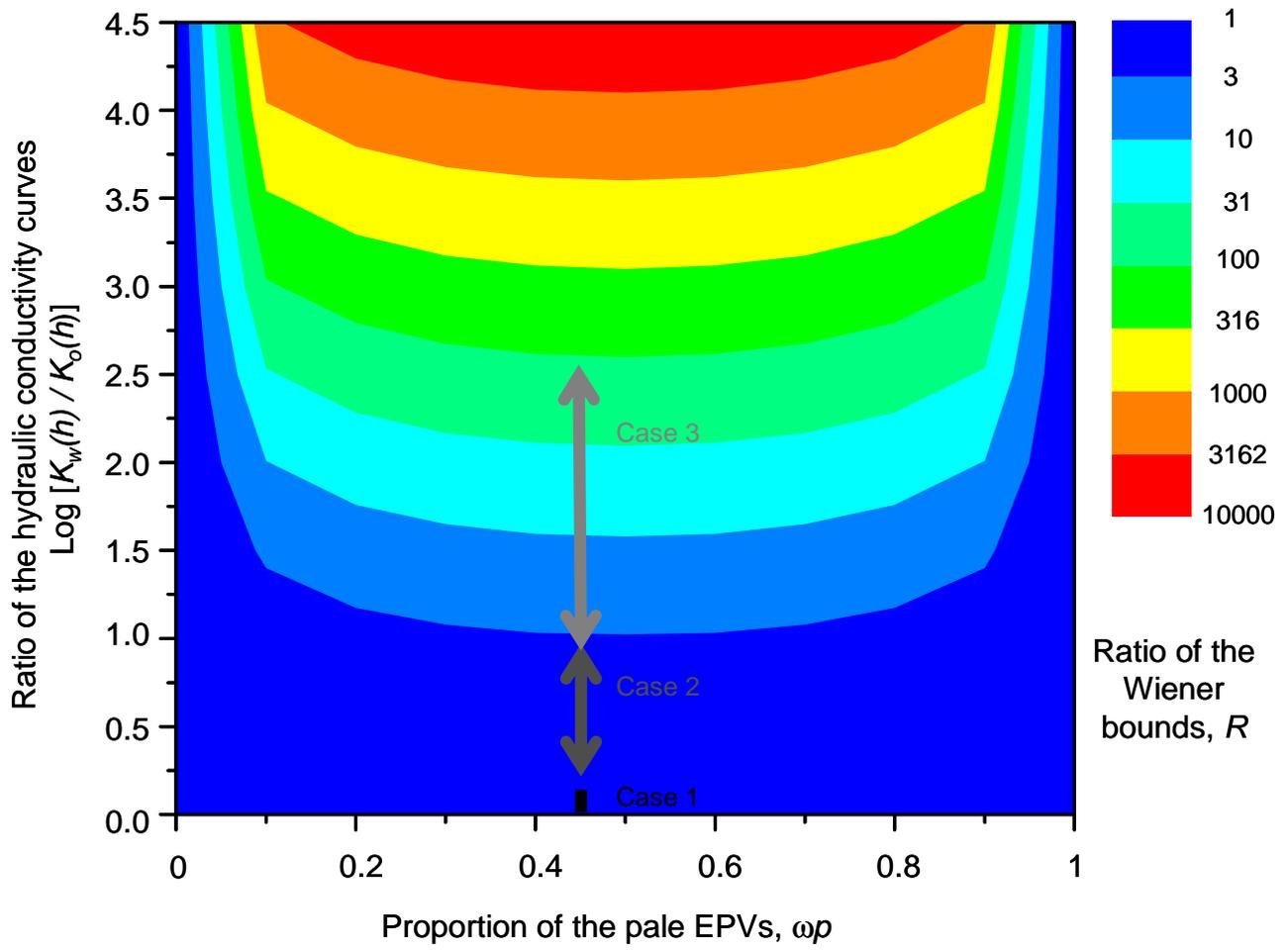


Figure 6

Depth (m)	Particle-size distribution (g kg ⁻¹)		
	< 2 μm	2 – 50 μm	50 – 2000 μm
0.35 – 0.45	182 ^p / 248 ^o	714 ^p / 659 ^o	104 ^p / 93 ^o
0.45 – 0.55	213 ^p / 322 ^o	706 ^p / 620 ^o	81 ^p / 58 ^o

.p: pale EPV
 .o: ochre EPV

Table 1

	Nb (-)	Mean bulk density (g cm ³)	Mean saturated water content (cm ³ cm ⁻³)	Coefficient of variation (%)
Pale EPV	15	1.53	0.423	2.76
Ochre EPV	18	1.57	0.408	3.75

Table 2

	case 1		case 2		case 3	
	pale	ochre	pale	ochre	pale	ochre
$\theta_s / \text{cm}^3 \text{cm}^{-3}$	0,46	0,42	0,43	0,41	0,44	0,42
$\theta_r / \text{cm}^3 \text{cm}^{-3}$	0,001	0,016	0,033	0,021	0,034	0,005
α / m^{-1}	0,23	1,64	0,55	1,21	0,72	0,66
n	1,33	1,15	1,23	1,13	1,16	1,15
$K_s (m s^{-1})$	1,40E-05	1,83E-06	1,98E-05	9,46E-06	1,64E-05	1,04E-05

Table 3

	SEPV	SWiener	SCardwell-Pearson	SCardwell-Pearson _ Numerical simulation		SWiener _ Numerical simulation	
				Upper Bound	Lower Bound	Upper Bound	Lower Bound
case 1	184,54	125,67	29,40	7,58	21,82	8,29	117,38
case 2	66,63	24,15	9,86	1,59	8,27	1,98	22,17
case 3	15,47	1,40	0,61	1,02	0,42	1,09	0,58

Table 4

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