

## Determining the effective hydraulic properties of a highly heterogeneous soil horizon

Anatja Samouëlian, Isabelle Cousin, Cécile Dagès, Anthony Frison, Guy Richard

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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

4 Samouëlian A.<sup>1,\*</sup>, Cousin I.<sup>1</sup>, Dagès C.<sup>2</sup>, Frison A.<sup>1</sup>, Richard G.<sup>1</sup>

5

6 <sup>1</sup>INRA, UR 0272 - Unité de Science du Sol, Centre de recherche d'Orléans, 2163 Avenue de  
7 la Pomme de Pin, CS 40001 Ardon, 45075 Orléans Cedex 2, France

8 <sup>2</sup>INRA, UMR LISAH - Bat 24, 2 place Viala, 34060 Montpellier Cedex, France

9

10 \*Corresponding author:

11 Phone: + 33 2 38 41 78 49

12 Fax: + 33 2 38 41 78 69

13 E-mail: [Anatja.Samouelian@orleans.inra.fr](mailto:Anatja.Samouelian@orleans.inra.fr)

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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.

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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  $1.5 \text{ g.cm}^{-3}$  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 cm<sup>3</sup> – 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),  $\theta$  the volumetric water content ( $\text{m}^3\text{m}^{-3}$ ),  $\theta_s$  the saturated  
136 water content ( $\text{m}^3\text{m}^{-3}$ ),  $\theta_r$  the residual water content ( $\text{m}^3\text{m}^{-3}$ ),  $l$  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  $\alpha$  ( $\text{m}^{-1}$ ) 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  $\theta_s$  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  $2.65 \text{ g cm}^{-3}$ . 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  $\omega_i$   
169 fulfilled the condition  $\sum_i \omega_i = 1$  while  $n_i$  and  $\alpha_i$  are the related van Genuchten parameters (van  
170 Genuchten, 1980). In our study,  $\omega$ , 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 cm<sup>3</sup>, 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  $\omega_i$  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



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:

$$332 \quad R_w = \frac{\left[ \omega_p \frac{K_p(h)}{K_o(h)} + (1 - \omega_p) \right] \left[ \omega_p + (1 - \omega_p) \frac{K_p(h)}{K_o(h)} \right]}{\frac{K_p(h)}{K_o(h)}} \quad [10]$$

333 where  $K_p(h)$  and  $(K_o(h))$  represents the hydraulic conductivity of the pale EPVs the ochre  
334 EPVs respectively, while  $\omega_p$  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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408

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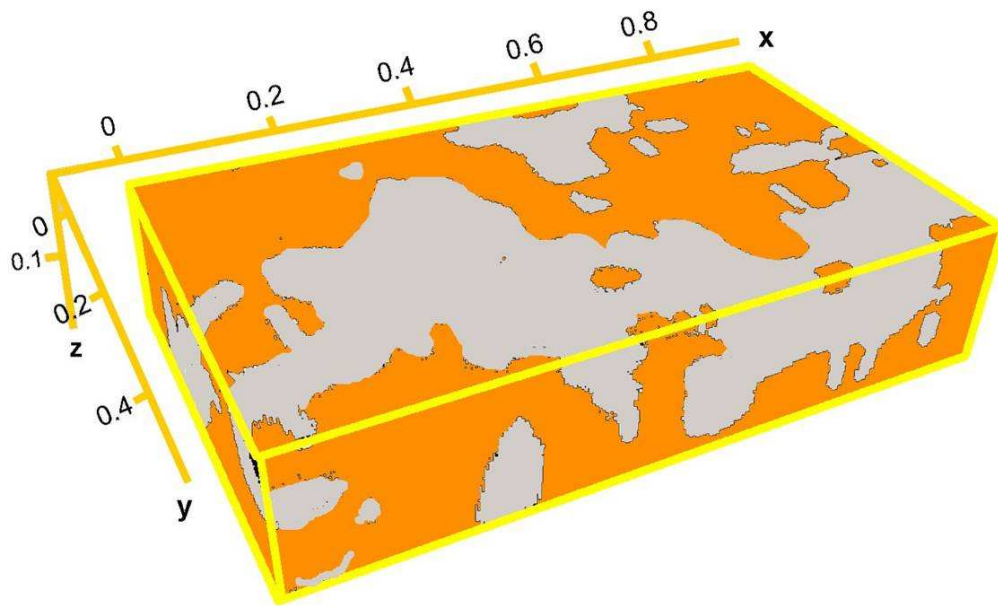
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Figure 1

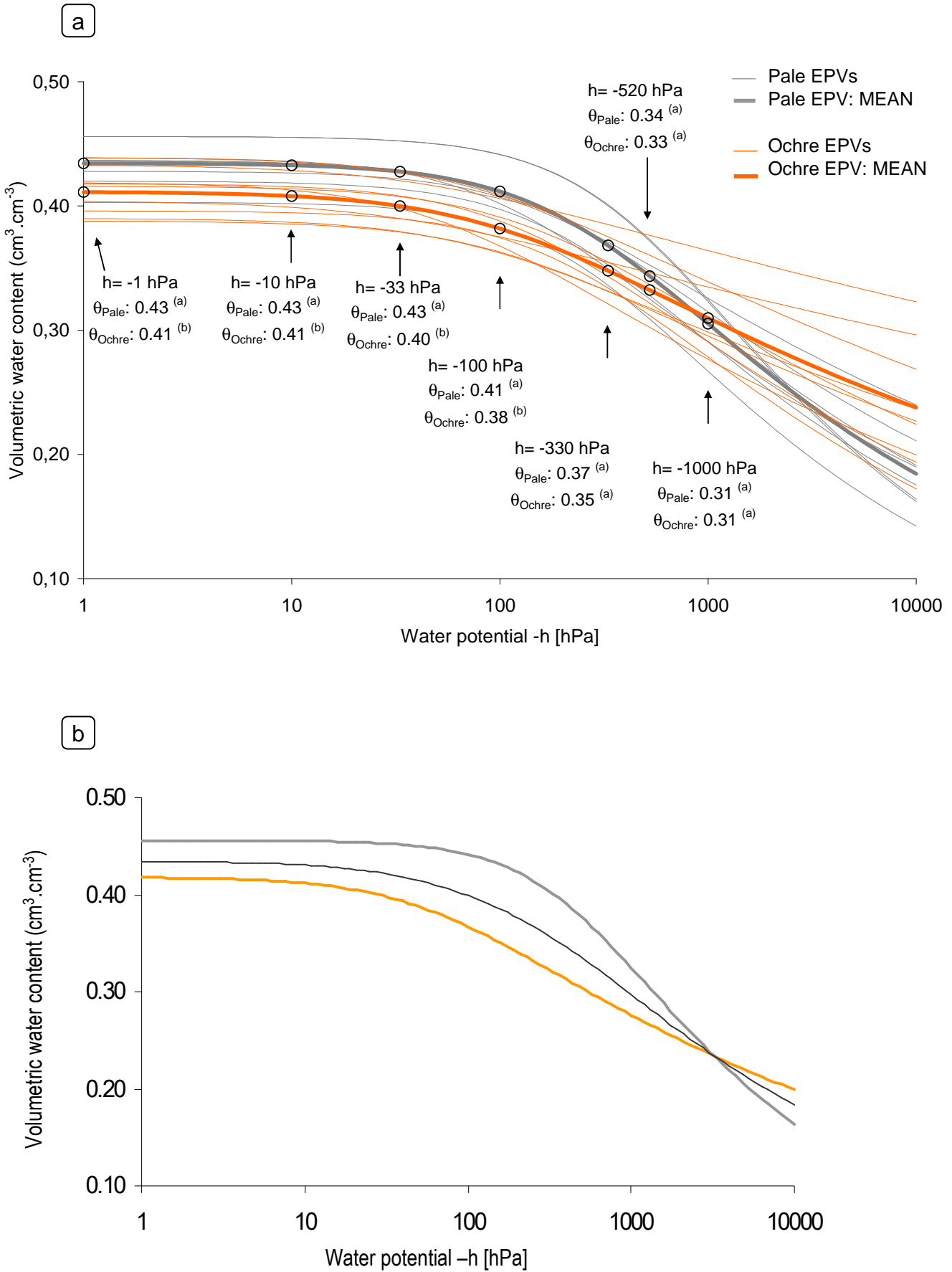


Figure 2

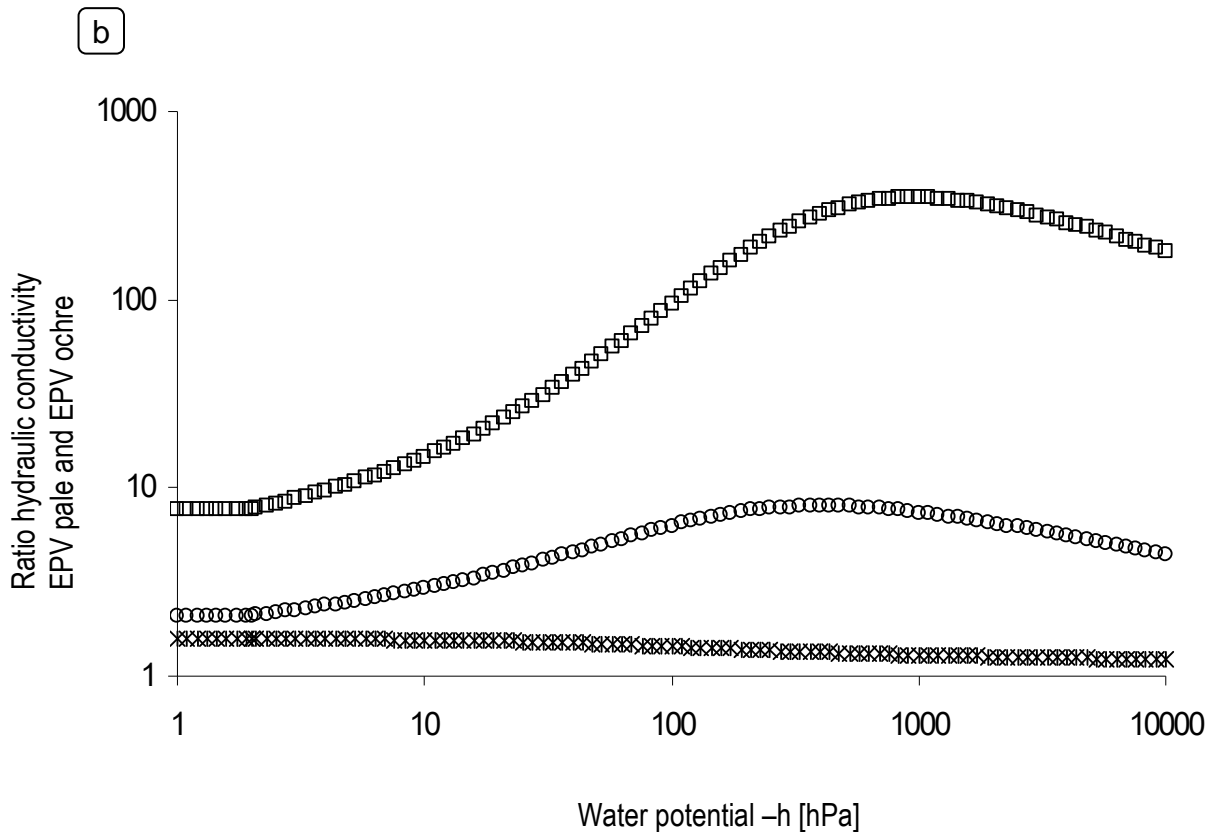
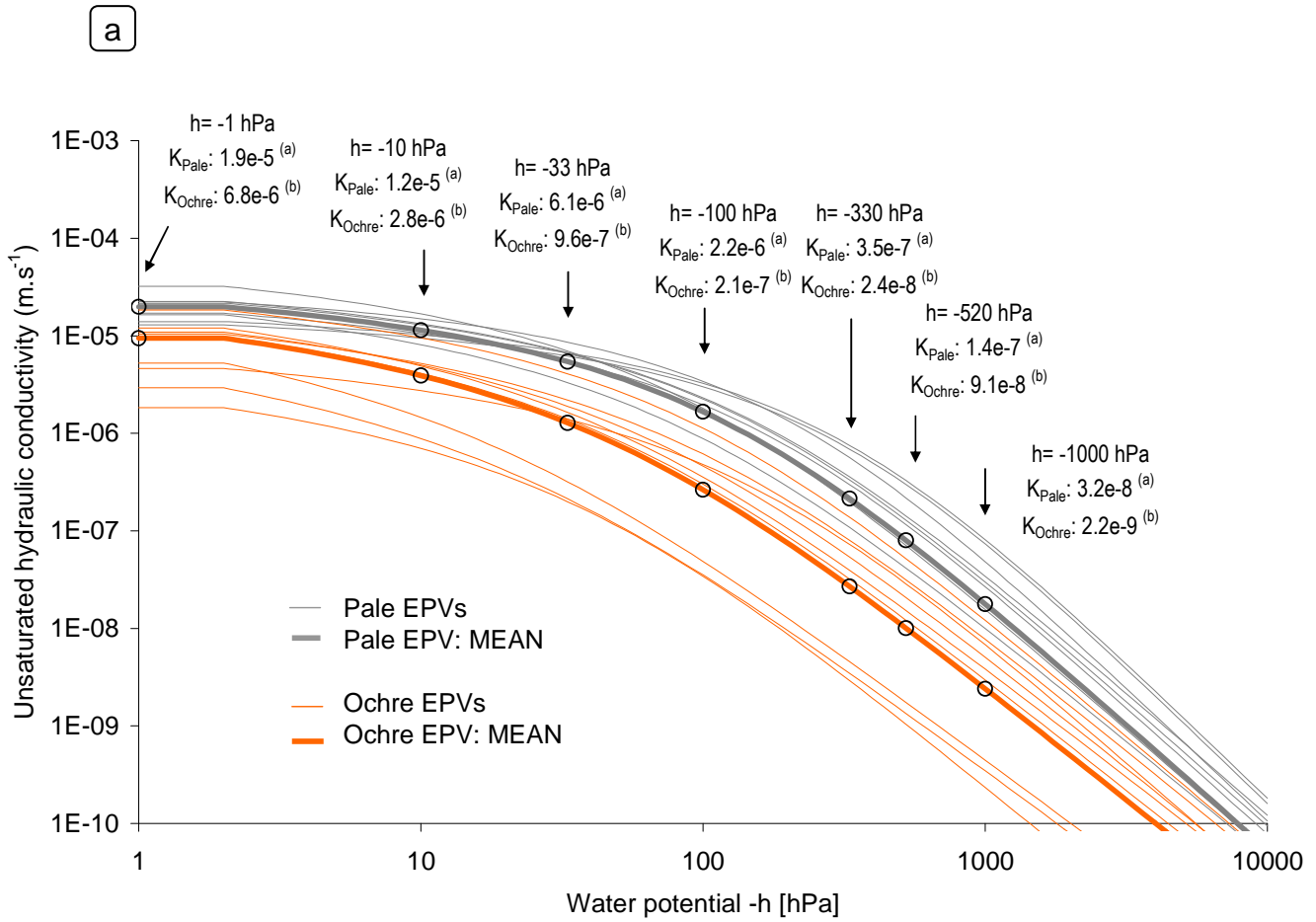


Figure 3

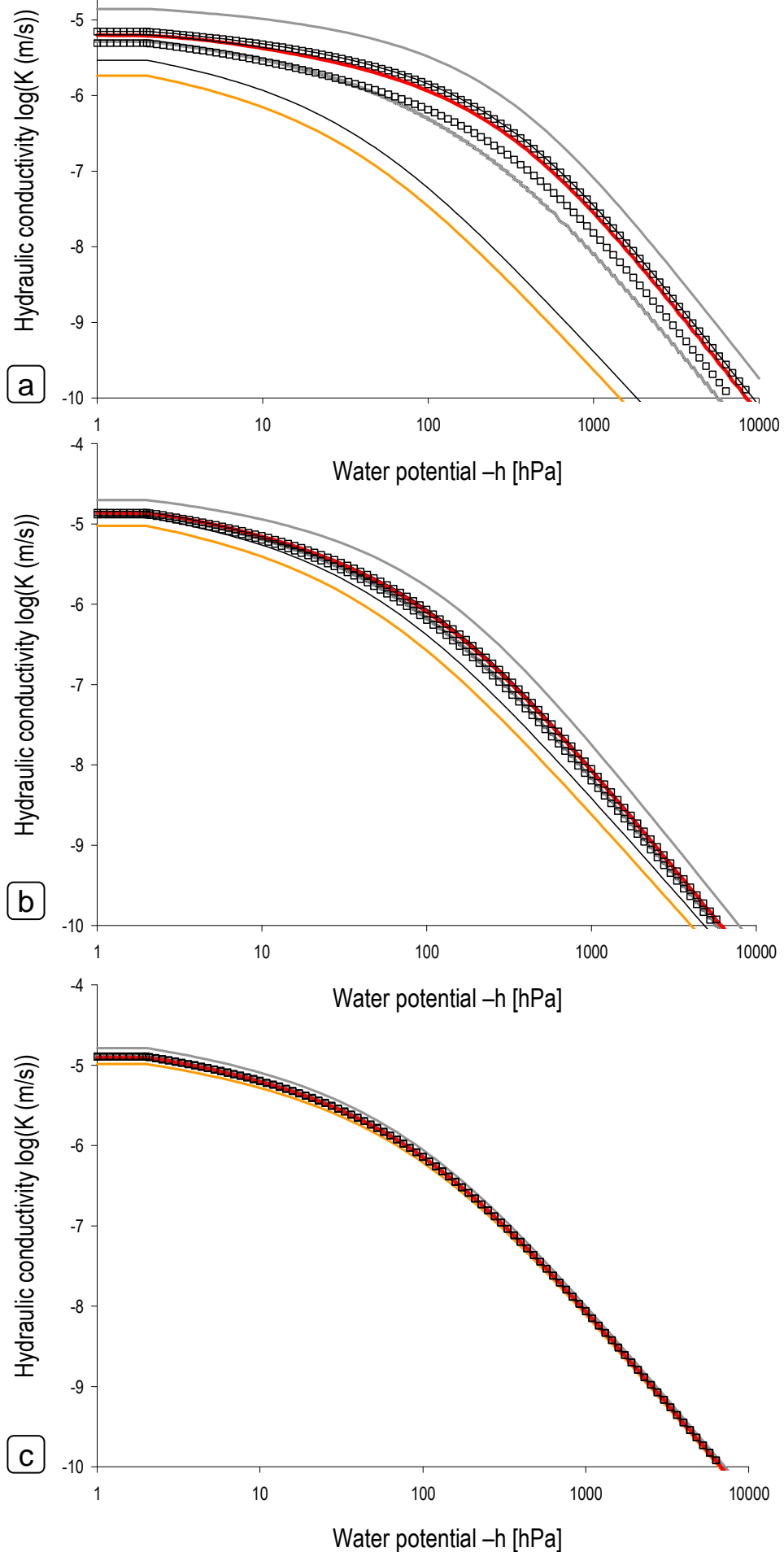


Figure 4

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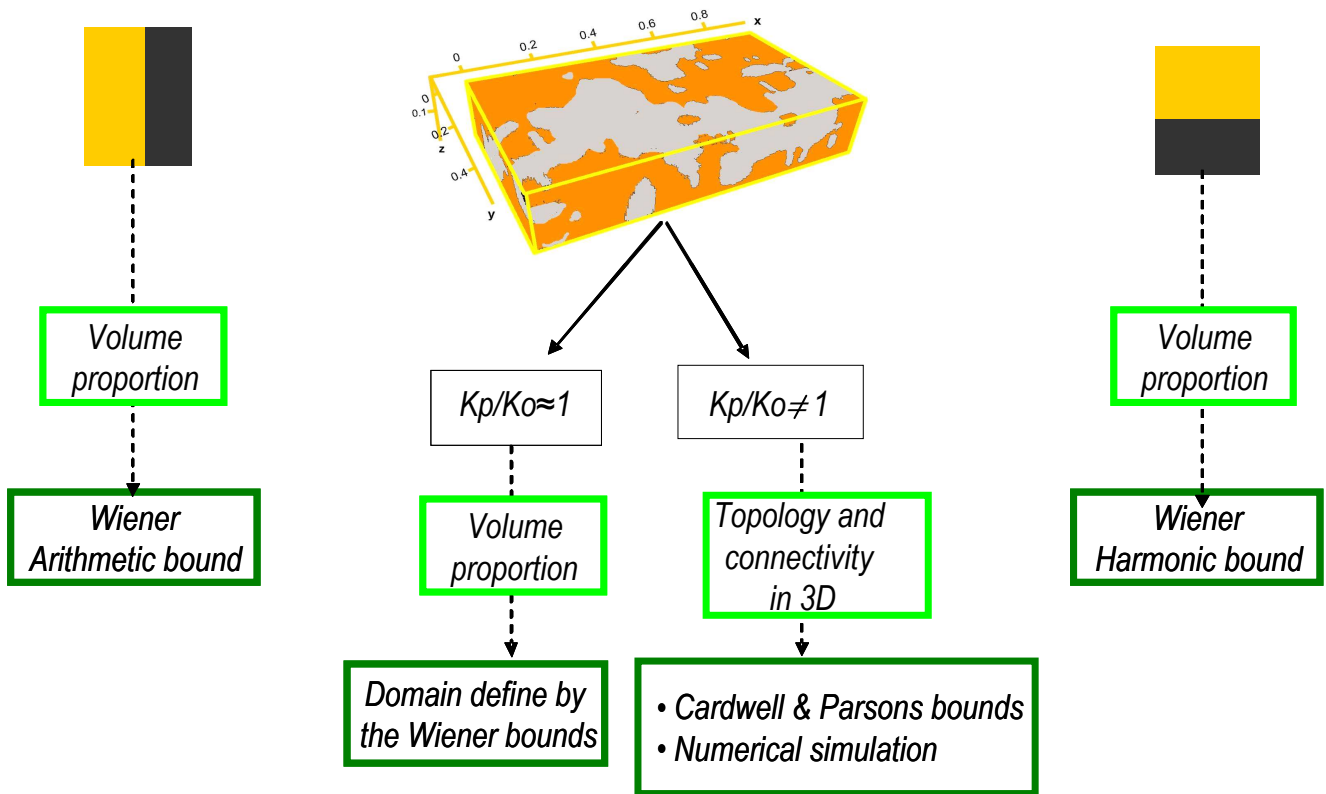


Figure 5

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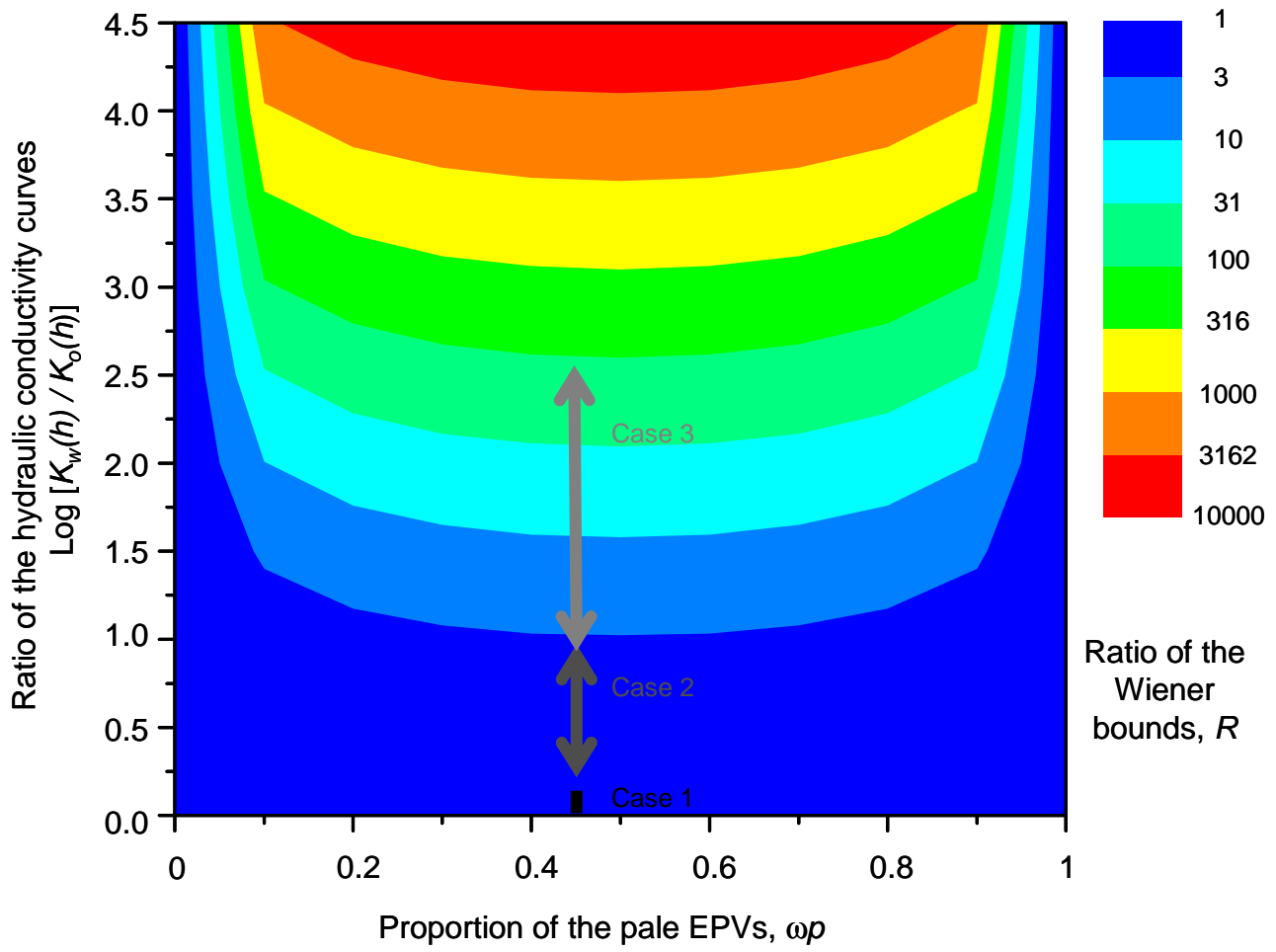


Figure 6

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

.p: pale EPV  
 .o: ochre EPV

Table 1

	Nb (-)	Mean bulk density (g cm <sup>3</sup> )	Mean saturated water content (cm <sup>3</sup> cm <sup>-3</sup> )	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
$\alpha / \text{m}^{-1}$	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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