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Research Paper/

Hydraulic Characterization of Unconfined Aquifers with Oscillatory Excitations: A Numerical Analysis

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1 Abstract

2 We present a synthetic hydraulic analysis of the propagation of oscillatory perturbations in a two-dimensional saturated zone bounded above by a capillary fringe. Unsaturated flows are 3 simulated in a physical model using a hysteretic form of Richards' equation parameterized 4 using the van Genuchten water retention curve and the Mualem hydraulic conductivity 5 equation for a sand, loam, and intermediate soil. Soil type affects periodic responses as a 6 7 function of their hydrodynamic and van Genuchten properties. We first analyze the effect of various hydraulic or signal properties on the oscillatory responses simulated at different 8 9 locations and depths. We then test the imaging potential of oscillatory responses recorded in the saturated zone to spatially charaterize homogeneous or heterogeneous soils, also 10 considering the effect of period of oscillation. We find that a separation of these responses 11 12 into amplitude/phase couples permits to dissociate the characterization of different hydraulic properties. Periodic amplitudes decay with distance mainly as a function of hydraulic 13 conductivity and phase lags decrease with frequency due to storage in the capillary fringe. 14 Thus, responses amplitude appears to be especially sensitive to conductivity K, which allows 15 to isolate this property from the others. Phases can then be used to better characterize the 16 17 vertical flows effect, through the Van Genuchten parameters α and n. Higher periods will tend to accentuate the unsaturated flows effect on the responses and can therefore be adopted 18 for a better characterization of α and n. However, using low-period responses can also be 19 useful, as they provide better estimates of conductivity values in media with low 20 heterogeneities. We consider this work as a useful preliminary analysis for future sandbox or 21 22 field real cases applications and provide advices for such applications in the discussion.

23 **1. Introduction**

In hydraulic characterization of unconfined aquifers by pumping tests, identifying the impact 24 25 of the capillary fringe on saturated flows remains a non-trivial task. Indeed, the unsaturated 26 zone can contribute substantially to the flows in the saturated zone through vertical fluxes (Neuman 1972; Mishra et al. 2012; Lin et al. 2017). Therefore, a rigorous interpretation of 27 these tests requires a quantification of these vertical fluxes and a characterization of the 28 29 hydraulic properties of the unsaturated zone. In addition, a spatial characterization of the hydraulic properties (such as hydraulic conductivity) of unconfined aquifer including its cover 30 31 can substantially improve our comprehension of the processes of recharge and contaminant transport in the critical zone. This can be performed with a hydraulic tomography approach in 32 which a physical numerical model is used in an inversion process to retrieve the hydraulic 33 34 properties by fitting hydraulic head measurements. Usually, in such approach, these hydraulic heads are measured simultaneously in multiple wells and at multiple depths in response to 35 cross-wells perturbations (Yeh and Lee 2007; Yeh et al. 2013; Liu et al. 2002; Zhu and Yeh 36 2005). 37

In the literature, several hydraulic tomography of unconfined aquifers have already been 38 39 performed on field or laboratory applications. In particular on field cases applications, the Boise Hydrogeophysical Research Site (BHRS), has been particularly studied (Cardiff et al. 40 41 2009; Cardiff and Barrash 2011; Cardiff et al. 2012; Cardiff et al. 2013a; Rabinovich et al. 2015; Hochstetler et al. 2016; Cardiff et al. 2019). However, in these applications, the authors 42 considered that the drainage occurring during their tests was instantaneous and did not 43 generate delayed responses effect. Thus, they simulated only the saturated flows in the aquifer 44 in order to characterize the conductivity and specific storage fields. It is shown that this 45 approximation is acceptable when a specific yield value is employed for the drainage in the 46 early-time pumping (Cardiff and Barrash 2011; Cardiff et al. 2012). However, to apply this 47

method, the effective porosity must trigger instantaneous drainage at the beginning of the 48 49 pumping or the effective porosity must contribute only for a negligible vertical flux compared to the horizontal fluxes generated by pumping (Cardiff and Barrash 2011). Mao et al. (2013a) 50 have presented a theoretical analysis of the application of hydraulic tomography on an 51 unconfined aquifer also taking into account hydraulic properties related to the unsaturated 52 flows (pore-size distribution parameters and saturated water content). This approach has been 53 successfully applied theoretically and experimentally in sandboxes with an analysis of 54 temporal drawdown curves in response to constant-rate pumping (Mao et al., 2013b; Zhao et 55 al. 2015).. However to date a real field case application following this method has not been 56 57 presented. Therefore further recommendations have been provided for adapting such process in real applications in Mao et al. (2013a) and Zhao et al. (2015). The major concerns in its 58 application remains effect of noise on the data and the necessity to assess a sufficient amount 59 60 of information on both the saturated flows (rather horizontal) and the unsaturated flows (rather vertical) in the dataset. 61

62 Oscillatory pumping tests can improve the quality of hydraulic data and thus the characterization of unconfined aquifers, including the effect of the marginal capillary zone. 63 During the last decades, applications of oscillatory excitations in the identification of the 64 65 hydraulic properties of aquifers have been widely explored, both theoretically and experimentally (Black and Kipp 1981; Rasmussen et al. 2000; Rasmussen et al. 2003; Renner 66 and Messar 2006; Fokker et al. 2013; Fischer et al. 2018; Salina Borello et al. 2019; Cardiff et 67 al. 2019; Fischer et al. 2020a; Fischer et al. 2020b). The imaging potential of such data has 68 been studied in Cardiff et al. (2013b) and their advantages in field application have been 69 70 discussed in Bakhos et al. (2014) in terms of ability to easily eliminate noises from the measurements and in Cardiff and Barrash (2014) for configuring the period of oscillation in 71 72 order to investigate different flowpaths in the aquifer.

The propagation of oscillatory signals in soils under conditions of variable saturation has been 73 74 analyzed in several works with numerical data (Revil et al. 2008; Shoushtari et al. 2015) or laboratory data (Cartwright et al. 2003; Cartwright et al. 2004; Cartwright 2014). All these 75 works discuss the effect of hysteresis, existing for unsaturated flows and having an impact on 76 the oscillatory responses. This hysteresis effect is due to the wetting and dewatering processes 77 of soils that generate loops in the water content curves. These scanning loops can be modeled 78 79 with hydrodynamic-dependent unsaturated flows parameters. Effects of air entrapment during soils wetting, can also temporarily affect the saturated water content value (Kool and Parker 80 1987). 81

82 Several analytical solutions have recently been proposed for the estimation of soils hydraulic property values in unconfined aquifers from oscillatory signal responses (Dagan and 83 Rabinovich 2014; Huang et al. 2018; Huang et al. 2019; Cheng and Renner 2018). However, 84 it is still rare for spatial variability to be taken into account in characterization applications 85 considering both the saturated and unsaturated hydraulic properties. Furthermore the 86 87 information brought by oscillatory responses for the spatial characterization of unconfined aquifers still needs to be investigated. With this work our aim is to further investigate the 88 effect of oscillatory flows generated at the limit of the saturated zone in an unconfined 89 aquifer, in order to propose a preliminary analysis of this type of data for future 90 characterization application, in particular hydraulic tomography. For this purpose we 91 simulated flows associated to extraction/injection oscillations in a synthetic sandbox with a 92 physical numerical model. We first present an analysis of the effect of different soil properties 93 on the oscillatory responses. Then we focus more particularly on the effect of conductivity K 94 95 and the unsaturated Van Genuchten parameters α and n and study the possibility to spatially characterize these properties with the information carried in the oscillatory 96

97 responses. Finally we discuss our analysis and imaging results in order to provide some98 advices for future works of hydraulic tomography using this type of data.

99 **2. Presentation of the model**

We developed a physics-based model of an unconfined soils with variable saturation with 100 COMSOL Multiphysics (see Figure 1). This model represents a 2-D side-views of a synthetic 101 102 sandbox at a metric scale: 3m wide for 1m depth. We considered the initial water table to be 50 cm below the surface (thus, initially, half of the model is saturated and the other half 103 unsaturated). The modeled sandbox is equipped with a pumping/injection point (hereafter 104 noted S) and measurement axes at distances of 20, 40 and 60 cm from the pumping axis, in 105 which hydraulic pressure responses are simulated at different depths of the saturated zone (60 106 and 90 cm). 107



108

109 <u>Figure 1:</u> Schematic representation of our side-viewed models of an unconfined aquifer. 110 Surface is at Z=0 cm and the water table at Z=-50 cm. The white circles represent the 111 pressure simulations points while the black circle represents the perturbation source point 112 (also used as pressure measurement). Orange color represents the soil, light blues the 113 unsaturated fringe and blue the saturated zone of the aquifer.

In order to take into account the capillary fringe effect on the saturated responses, we simulated water flows with Richards' formulation of the continuity equation for a 2D sideviewed temporal model:

118
$$\left(C_{m} + S_{e}.S\right)\frac{\partial h}{\partial t} + \nabla \left(-K.k_{r}\left(\nabla H_{p} + \nabla z\right)\right) = q , \qquad (1)$$

where t is time (s), H_p is the hydraulic pressure (m) at a given depth Z (m), K is the 119 hydraulic conductivity (m/s), S is the storage coefficient (m⁻¹) related to the soil 120 compressibility, S_e denotes the effective saturation (-), C_m is the specific moisture capacity 121 (m^{-1}) , k_r is the relative permeability (-) and q is the Darcy's velocity at the pumping 122 locations (m/s). We consider that no vertical flows occur at the upper boundary of the 123 sandbox during the simulations. The other boundaries are impervious, implying a finite 124 125 volume of water in the sandbox (no inlet or outlet). The flows in the model are then solved within an adaptive-size triangular mesh with a finite-element method. 126

127 This model simulates, in time, the hydraulic pressures in the variably saturated soil in 128 response to a sinusoidal oscillating perturbation, injecting and extracting successively a same 129 amount of water.

130
$$Q = -Q_A \cdot sin\left(\frac{2.\pi}{Pe} \cdot t\right)$$
(2)

where Q is the extraction/injection flowrate (m^3/s), Q_A is the oscillating flowrate amplitude (m^3/s) and and Pe is the oscillating flowrate period (s).

133 S_e , C_m and k_r are calculated with the Van Genuchten equations. These equations are 134 dependent on the groundwater pressure $H_p = h - z$; i.e. if the water, at a given location (x,z)135 , is at an atmospheric pressure or not:

136
$$\begin{cases} S_{e} = \frac{1}{\left(1 + \left|\alpha.H_{p}\right|^{n}\right)^{1-1/n}} & \text{if } H_{p} < 0\\ S_{e} = 1 & \text{if } H_{p} \ge 0 \end{cases}$$
(3)

137
$$\begin{cases} C_{m} = \frac{\alpha \left(1 - \frac{1}{n}\right)}{1 + \frac{1}{n}} \cdot \left(\theta_{s} - \theta_{r}\right) \cdot S_{e}^{\frac{1}{1 - 1/n}} \cdot \left(1 - S_{e}^{\frac{1}{1 - 1/n}}\right)^{1 - 1/n} & \text{if } H_{p} < 0 \\ C_{m} = 0 & \text{if } H_{p} \ge 0 \end{cases}$$
(4)

138
$$\begin{cases} k_{r} = S_{e}^{\ell} \cdot \left(1 - \left(1 - S_{e}^{\frac{1}{1 - l/n}}\right)^{1 - l/n}\right)^{2} & \text{if } H_{p} < 0 \\ k_{r} = 1 & \text{if } H_{p} \ge 0 \end{cases}$$
(5)

139 where α (m⁻¹), n (-) and $\ell = 0.5$ (-) are the Van Genuchten parameters and θ_s , θ_r are the 140 saturated and residual water content (-).

141 A hysteretic effect occurs in unsaturated soils, inducing a difference in the dewatering and the 142 wetting of the soil. In this study, a spatial and temporal frequency-dependent hysteresis effect 143 is implemented in the model, based on the formulation of Revil et al. (2008) for periodic 144 sources and the observations made in Shoushtari et al. (2015) that hysteresis effects attenuates 145 with distance to the signal source. The hysteresis is generated by computing dynamic values 146 of α and n, following the induced periodic movement, over space and time:

147
$$\alpha(t) = \alpha_{mean} \times \left[1 - \left(M_{hyst} - min\left(\frac{|z_p - z|}{z_{hyst}}, 1 \right) \cdot M_{hyst} \right) \cdot sin\left(\frac{2\pi t}{Pe} \right) \right]$$
(6)

148 where M_{hyst} is the magnitude of the hysteresis effect (%), α_{mean} represents the mean value of 149 α (1/m), z_p is the pumping depth (m) and z_{hyst} is the distance of attenuation of the hysteresis effect (hereafter 50 cm). A similar formulation is also used to compute n(t), considering a
n_{mean} value (-).

We briefly present in Figure 2 the effects of the simulated hysteresis on the saturation level 152 and the simulated pressures in our model. After one cycle of pumping/injection the saturation 153 level will not come back to its origin when incorporating a hysteresis effect. A part of the 154 mobilized water will remain in the unsaturated zone, generating a lowering of the saturation 155 level. After several cycle, the effect generates a global decrease of the saturated/unsaturated 156 interface. In the unsaturated zone, the shape of the signal becomes deformed by the hysteresis 157 158 effect (especially observable for the period of 30 min), wherein it cannot be considered as a sinusoidal form anymore. The effect of the period of oscillation is also more important in the 159 unsaturated zone, where the oscillatory response tends to vanish faster (in terms of amplitude) 160 161 than in the saturated zone when the period of the signal is decreased. In the saturated zone, the hysteresis effect does not seem to modify the shape of the signal directly. Thus the pressure 162 responses in the saturated zone contain a sinusoidal part (h_{osc}) in response to the oscillating 163 signal that can be written: 164

165
$$\mathbf{h}_{\rm osc} = \mathbf{h}_{\rm A} \cdot \sin\left(\frac{2.\pi}{\rm Pe} \cdot \mathbf{t} - \mathbf{h}_{\rm P} \cdot \frac{\pi}{180}\right) \tag{7}$$

where h_A is the oscillating response amplitude (m) and h_P is the oscillating response phase lag to the signal source (°). These oscillatory parts can be extracted from the head responses through a Fast Fourier Transform (FFT) directly in terms of timeless amplitudes (h_A) and phases (h_P).



Figure 2: (a) Effect of simulated 25% hysteresis on the soil effective saturation and the saturation level (cyan line) during one cycle of pumping and injection. The initial saturation level is indicated as a dotted line. (b) Effect of the hysteresis on the effective saturation simulated at position (0;-0.4) in the unsaturated zone and the pressure simulated at position (0.2;-0.6) in the saturated zone after several cycles of injection/pumping and for different periods of oscillation (5 and 30 min)

We simulated and observed the oscillatory responses in the saturated zone for different types of soils, by modifying the property values inputs in the model. Hereafter in this work we principally compare these responses in sand, in loam or an intermediate soil with properties between sand and loam ones. The hydraulic property values employed for these two configurations are presented in Table 1 and were chosen mainly according to the UNsaturated SOil hydraulic DAtabase (UNSODA) in Leij et al. (1996) and to previous works in the unconfined aquifers literature.

185

	K (m/s)	Anisotropy (Kx / Kz)	α (1/m)	n (-)
'Loam' soil	1.10 ⁻⁵	4	3.2	2.4
'Intermediate' soil	5.10-5	3	4.0	2.7
'Sand' soil	1.10^{-4}	2	5.0	3.0

187 <u>Table 1:</u> Property values used in our model for the two types of soils and the intermediate soil
 188 considered.

For the hydrogeological soil properties we chose constant values, also based on what can be usually found in the literature: $\theta_r = 0.05$, $\theta_s = 0.40$ and $S = 10^{-5} \text{ m}^{-1}$. We considered a $M_{hyst} =$ 25 % magnitude hysteresis effect in the unsaturated zone, based on the recommendations in Kool and Parker (1987).

Figure 3 presents the differences between our simulated sand and loam soils in terms of unsaturated flows (i.e. effective saturation profiles, water content curves and hysteresis effects on the responses in the saturated zone). It can be noted that this hysteresis effect, shown in Figure 2, is more important in sand than in loam.



199 Figure 3: (a) Effective saturation in sand and loam between the surface and the saturated zone, 200 at 50cm depth. (b) A spatial and temporal-evolving hysteresis effect ('scanning loop') has 201 been taken into account in the water content curves during the successive pumping and 202 injection phases. (c) This hysteresis effect does not substantially affect the oscillation 203 response, but rather the mean pressure level, especially in sands (here the pressures simulated 204 at position (0.2;-0.6) with 0% and 25% hysteresis effects for a period of oscillation of 30 205 min).

206

207 3. Comparative analysis of the effect of various soil properties on the

208 oscillatory responses

By simulating flows during pumping and injection phases in sand and loam (Figure 4), we can clearly observe the different types of flows that will be mobilized in these two configurations. Vertical flows will occur in the unsaturated zone, horizontal in depths of the saturated zone, and mixed vertical/horizontal flows near the saturated/unsaturated interface. It can also be observed from the arrows sizes (proportional to the flow intensity) in the unsaturated zone in Figure 4 that vertical flows are, in proportion, more important in sand than in loam.



215

<u>Figure 4:</u> Flow velocity vectors (red arrows) in a log10 scale when pumping and injecting in
loam or in sand. Current and initial saturation levels are indicated as blue lines and dotted
lines respectively.

219

We first evaluated how oscillatory responses (i.e., amplitudes, phase lags) are affected by variations of individual parameters values for the intermediate soil (Table 1) using a pumping

amplitude of $Q_A = 1$ mL/s and period of oscillation Pe = 15 min.

In Figure 5, we present the variations induced in the amplitude and phases responses at the different locations when modifying the conductivity and anisotropy values of our 'intermediate' soil (to values corresponding rather to 'sand' soil ones or rather to 'loam' soil

ones). The absolute responses (presented for the 'intermediate' soil in the middle column of 226 the figure) globally show an amplitude decrease and phase increase with the radial distance to 227 the perturbation source point S. However the oscillation better propagates in the deep 228 229 saturated zone (below S) than near the unsaturated one, as amplitudes are higher and phases lower below S, even if these simulation points are more distant to the source than the ones 230 above S. It clearly appears that the oscillatory responses are affected by the conductivity and 231 its anisotropy, especially in terms of amplitudes. For a similar perturbation the amplitude 232 responses will be higher in loam than in sand. Oppositely, the phases will become globally 233 lower when applied in loam and higher in sand. However, in this case the conductivity seems 234 to more particularly affect the phases of responses associated to horizontal flows (below S). 235 The degree of anisotropy will have a similar but less important effect than conductivities on 236 amplitude responses, becoming more important in loam with higher anisotropy. The phase 237 238 responses are especially affected when lowering the anisotropy, generating higher phases in sand when moving away from the perturbation source. 239





<u>Figure 5:</u> Lateral columns: spatial variations (in %) of amplitudes (blue, A) and phases (green,
P) at each measurement point and for the saturated flows properties (K and anisotropy)
tending to their 'sand' soil or 'loam' soil values. Middle column: absolute amplitude (in mm)
and phase responses (in °) obtained with medium property values of the 'intermediate' soil.

Figure 6 presents a similar analysis with the Van Genuchten parameters α and n, associated 246 247 to the unsaturated flows. These parameters also affect the oscillatory responses, but in a different manner than conductivity. Parameter α appears to affect the differences in the 248 responses above and below S. In fact, its modification will generate more important variations 249 250 in terms of amplitude above S (denoting an effect on the vertical flows impacts). It will also affect the phase responses but rather reducing the vertical differences in loam, and 251 accentuating it in sand, thus, again, generating responses variations vertically. Parameter n, in 252 contrary, generates variations affecting essentially the phases of the responses, accentuating 253 them and their vertical differences in loam and lowering them in sand. The phase variations 254

remain constant with distance to S. This suggests a more local impact at the perturbation point that is then propagated to the other responses. As for the previous conductivity analysis, the effects on the responses induced by α and n are opposites when tending to one or another sand or loam property value. This already suggest that quantitatively analyzing the responses spatially and vertically could allow to assess a soil's saturated and unsaturated hydraulic property values.



261

262 <u>Figure 6:</u> Lateral columns: spatial variations (in %) of amplitudes (blue, A) and phases (green, 263 P) at each measurement point and for the unsaturated flows properties (α and n) tending to 264 their 'sand' soil or 'loam' soil values. Middle column: absolute amplitude (in mm) and phase 265 responses (in °) obtained with medium property values of the 'intermediate' soil.

266

A third similar analysis has been conducted on other parameters, not necessarily linked to the two types of soil (loam and sand) considered in this study. This analysis is presented in Figure 7 with the effect of the period of oscillation, the saturated water content of the soil and the

magnitude of hysteresis effect. The period of oscillation influences the distance of 270 propagation of the perturbation in the soil. A lower period will attenuate more rapidly with 271 distance to S. An opposite effect is observed when increasing the period. A vertical effect of 272 the period can also be observed. The period tends to accentuate the vertical difference 273 observed in the responses above and below S when it is decreased (more important horizontal 274 flows), and to reduce this difference for higher periods. The saturated water content generates 275 a similar effect, but with opposite variations. In fact, a higher saturated content will accentuate 276 277 the vertical differences in the responses, while a lower saturated content will reduce the vertical differences. The hysteresis effect occurring in the unsaturated zone does not 278 substantially affects the oscillatory responses in the considered range of periods of oscillation 279 (5 to 30 min) except a global low increase of the phase responses that can be observed for a 280 high hysteresis magnitude. Nevertheless, Figure 2 shows that this effect affects the mean 281 282 saturation level over time. However, when performing a FFT analysis on the pressure responses, this mean level can be isolated. 283





<u>Figure 7:</u> Lateral columns: spatial variations (in %) of amplitudes (blue, A) and phases (green,
 P) at each measurement point and for different parameters (oscillation period, hysteresis
 magnitude and saturated water content) tending to minimal and maximal values. Middle
 column: absolute amplitude (in mm) and phase responses (in °) obtained with medium
 parameter values between these extrema.

This first comparative analysis shows that the spatial oscillatory responses are differently affected by the different soil properties and signal parameters. One advantage of oscillatory responses is that they can be easily dissociated into amplitudes and phases, which are also differently affected by each properties. Therefore, this type of responses could be used to assess the values of different soil properties.

4. Imaging potential of the oscillatory responses in the saturated zone

4.1. Inverse problem

In order to analyze if, and how, responses to oscillatory signals may provide information in 298 order to image the spatial distribution of hydraulic properties in an aquifer, we have re-299 300 interpret generated oscillatory responses in our 'sand' or 'loam' soils models through inversion processes. The inverse problem is based on objective functions, which quantify the 301 gap between responses simulated through a physical model for given property values and a set 302 303 of observed responses that one wants to interpret. These objective functions also incorporate a priori information on the property values in order to overcome the issue of non-unicity of the 304 solution. 305

We use our model presented in section 2 to generate oscillatory responses for different values of conductivities K and Van Genuchten parameters α and n. This operation can be mathematically written:

309

$$\mathbf{d} = f\left(\mathbf{p}\right) \tag{8}$$

where **d** is a $(n \times 1)$ vector containing the amplitude and phase responses simulated at each measurement location, f is the solver of the numerical model and **p** is a $(m \times 1)$ vector containing distributed values of K, α and n in logarithmic scale. Using logarithmic values permits avoiding negative values during the optimization process.

314 A simultaneous optimization of different properties in the iterative inversion process can lead 315 to a divergence of the process. Furthermore, as shown in previous section, the amplitude responses appear to be especially sensitive to conductivity. Therefore, we decided to perform our inversion process sequentially, with two different objective functions Ψ_{K} and $\Psi_{\alpha,n}$, that are conceived to successively optimize the hydraulic conductivity K, only with the amplitude responses, and then the Van Genuchten parameters α and n by adding the phase responses in the process:

321
$$\Psi_{K} = \left(\mathbf{d}_{amp}^{obs} - \mathbf{d}_{amp}\right)^{T} \cdot \mathbf{R}_{amp}^{-1} \cdot \left(\mathbf{d}_{amp}^{obs} - \mathbf{d}_{amp}\right) + \left(\mathbf{p}_{K}^{prior} - \mathbf{p}_{K}\right)^{T} \cdot \mathbf{C}_{K}^{-1} \cdot \left(\mathbf{p}_{K}^{prior} - \mathbf{p}_{K}\right)$$
(9)

322
$$\Psi_{\alpha,n} = \left(\mathbf{d}^{\text{obs}} - \mathbf{d}\right)^{\text{T}} \cdot \mathbf{R}^{-1} \cdot \left(\mathbf{d}^{\text{obs}} - \mathbf{d}\right) + \left(\mathbf{p}_{\alpha,n}^{\text{prior}} - \mathbf{p}_{\alpha,n}\right)^{\text{T}} \cdot \mathbf{C}_{\alpha,n}^{-1} \cdot \left(\mathbf{p}_{\alpha,n}^{\text{prior}} - \mathbf{p}_{\alpha,n}\right)$$
(10)

where Ψ designates the objective functions for determining K or α and n from the 323 information carried by the amplitude and phase responses contained in a *n*-vector \mathbf{d}^{obs} . 324 $\mathbf{R} = \sigma^2 Id(n)$ is a $n \times n$ diagonal matrix holding variances σ^2 on the amplitude ($\sigma^2 = 0.1$ 325 cm) and phase responses ($\sigma^2 = 1^\circ$). \mathbf{d}_{amp}^{obs} and \mathbf{R}_{amp} designate the sub-vector and sub-matrix 326 associated only to the amplitude responses. $\mathbf{p}^{\text{prior}}$ is a *m*-vector containing a priori values of 327 K (in sub-vector $\mathbf{p}_{K}^{\text{prior}}$) and α and n (in sub-vector $\mathbf{p}_{\alpha,n}^{\text{prior}}$). C is a $m \times m$ matrix holding 328 covariances constraining the hydraulic property values and their distribution. \mathbf{p}_{K} , $\mathbf{p}_{\alpha,n}$, \mathbf{C}_{K} 329 and $C_{\alpha,n}$ designate the sub-vectors and sub-matrices associated to K or α and n. 330

The inversion process consists in an iterative process aiming to minimize the values of these objectives function successively, by updating deterministically the property values in the model via the computation of a Jacobian matrix (Tarantola and Valette 1982):

334
$$\mathbf{F}_{i} = \frac{f_{i} \left(\mathbf{p}_{j} + \Delta \mathbf{p} \right) - f_{i} \left(\mathbf{p}_{j} \right)}{\Delta \mathbf{p}}$$
(11)

where \mathbf{F}_i represents the sensitivity of a data i to modification $\Delta p = 10^{-2}$ on the property value j.

337 During the first inversion sequence, the update of the conductivity values from an iteration 338 k-1 to k is given by:

339
$$\mathbf{p}_{K}^{k} = \mathbf{p}_{K}^{k-1} + \left(\mathbf{F}_{K}^{T}.\mathbf{R}_{amp}^{-1}.\mathbf{F}_{K} + \mathbf{C}_{K}^{-1}\right)^{-1} \cdot \left(\mathbf{F}_{K}^{T}.\mathbf{R}_{amp}^{-1}.\left(\mathbf{d}_{amp}^{obs} - \mathbf{d}_{amp}\right) + \mathbf{C}_{K}^{-1}.\left(\mathbf{p}_{K}^{prior} - \mathbf{p}_{K}\right)\right)$$
(12)

340 where \mathbf{F}_{K} is the Jacobian matrix described in Eq. 11, performing the sensibility analysis 341 between the K values and amplitude responses.

342 During the second inversion sequence, the update of the Van Genuchten parameters values 343 from an iteration k-1 to k is given by:

344
$$\mathbf{p}_{\alpha,n}^{k} = \mathbf{p}_{\alpha,n}^{k-1} + \left(\mathbf{F}_{\alpha,n}^{T} \cdot \mathbf{R}^{-1} \cdot \mathbf{F}_{\alpha,n} + \mathbf{C}_{\alpha,n}^{-1}\right)^{-1} \cdot \left(\mathbf{F}_{\alpha,n}^{T} \cdot \mathbf{R}^{-1} \cdot \left(\mathbf{d}^{obs} - \mathbf{d}\right) + \mathbf{C}_{\alpha,n}^{-1} \cdot \left(\mathbf{p}_{\alpha,n}^{prior} - \mathbf{p}_{\alpha,n}\right)\right)$$
(13)

where $\mathbf{F}_{\alpha,n}$ is the Jacobian matrix described in Eq. 11, performing the sensibility analysis between the α and n values and amplitude and phase responses.

At the end of the inversion, the standard deviations on the inverted property values can be obtained from the square-roots values of the diagonal entries of matrix \mathbf{C}^{post} , using the last iterations Jacobian matrices:

350
$$\mathbf{C}^{\text{post}} = \left(\mathbf{F}^{\mathrm{T}} \cdot \mathbf{R}^{-1} \cdot \mathbf{F} + \mathbf{C}^{-1}\right)^{-1}$$
(14)

Performing an inversion in this way, by isolating the K values in the process, we could improve the stability of the inversion and accelerate its convergence to more realistic solutions. In fact, the results presented hereafter show that the amplitude responses can be closely reproduced by optimizing the K field, regardless of the Van Genuchten parameters. The remaining amplitude and phase differences can then be adjusted by optimizing the Van For all inversion applications presented hereafter we did not consider any hysteresis effect on the responses simulated in the inversions, even if the observed data were generated with a 25% hysteresis magnitude.

362 4.2

4.2. Homogeneous cases applications

Inversions have been performed with oscillatory responses generated in homogeneous loams or sands (using property values presented in Table 1). For this generation we applied an injection/extraction rate aiming to generate similar pressure amplitudes (10 cm) at the perturbation point in both type of soil (i.e. $Q_A = 1$ mL/s in loam and $Q_A = 10$ mL/s in sand). The generated responses have been noised (2% added noise) for the imaging applications.

The hydraulic properties were optimized within two blocks (one 'superficial' block between 0 368 and 65 cm depth and one 'deep' block between 65 and 100 cm depth). Thus, in our inversions 369 the number of property values to be inverted was m = 6 (2 distributed values for each 370 property) for a dataset composed of n = 7 amplitude/phase responses couples. We considered 371 372 a diagonal covariance matrix for C with a 0.01 variance on each property value. We initialized our inversions with the 'medium' soil properties (see Table 1) so that we would be 373 able to estimate if the information carried by the oscillatory responses would permit to 374 partially or totally recover the loam and sand properties used for their generation. The 375 anisotropy of the medium was considered as known. 376

Figure 8 and Figure 9 present the inversion results obtained with oscillatory responsesgenerated with different oscillation periods (5 and 30 min) respectively in loam and in sand.



Figure 8: Inversion results obtained with responses simulated in a homogeneous loam with
 different periods of oscillations (5 and 30 min). Conductivities are firstly inverted only with
 the amplitude responses, then the Van Genuchten coefficients are inverted with both
 amplitude/phase responses.



386 <u>Figure 9:</u> Inversion results obtained from responses simulated in a homogeneous sand with 387 different periods of oscillations (5 and 30 min). Conductivities are firstly inverted only with 388 the amplitude responses, then the Van Genuchten coefficients are inverted with both 389 amplitude/phase responses.

385

Accurate conductivity values can be obtained from the amplitude responses alone, for both 391 type of soils and any oscillation period. A slightly more accurate result is obtained with lower 392 393 periods. Thus, most of the amplitude responses can be reconstructed by optimizing the conductivities. Then, the remaining responses differences, in terms of amplitudes and phases, 394 can be essentially linked the unsaturated flows and the Van Genuchten parameters. 395 Unsurprisingly, these properties were optimized only in the upper blocks of the models, 396 associated to the unsaturated zone. For α , the accuracy of the characterization seems more 397 period-dependent, better assumptions being systematically obtained with the 30 min periodic 398 399 responses (i.e. a lower frequency). Regarding n, the accuracy appears to be more related to 400 the soil, with better quantifications obtained in sands rather than in loams.

Globally, we observe that the oscillatory responses measured in the saturated zone provide sufficient information to distinguish the type of soil type in the medium. They can also allow the quantification of accurate properties values associated to the saturated and the unsaturated flows without necessarily having to simulate a hysteresis effect.

405

4.3. Simplified applications for heterogeneous cases

406 We have then performed inversions with oscillatory responses simulated in simplistic heterogeneous cases (see Figure 10) in a wider sandbox (3.6 m width). These cases consisted 407 in 3 perturbations points (black dots in Figure 10) in a 'medium' soil (as described in Table 408 1), surrounded by sand or loam areas in the saturated or unsaturated zones. The velocity 409 vectors simulated at each observation point (white dots in Figure 10) show that the generated 410 flows are differently affected in each areas of the model. Most important velocities are 411 observed in the sand areas, both in saturated and unsaturated zones. Therefore, in order to 412 efficiently characterize the whole heterogeneity, it is necessary to cross-interpret data 413 414 generated by signal sources located at different locations (hydraulic tomography principle).



416 <u>Figure 10:</u> Flow velocity vectors (red arrows) in a log100 scale when pumping at different 417 locations (X=-0.8, X=0 and X=+0.8) in the heterogeneous model (shown in the upper left 418 corner). Current and initial saturation levels are indicated as blue lines and dotted lines 419 respectively.

420

Thus, for the inversions we have simultaneously inverted the responses generated with each 421 422 of the three perturbation sources. These responses have been noised (2% added noise) for the imaging applications. We considered the anisotropy of the medium and also the properties of 423 the soil at the perturbation locations to be known. We have performed two types of inversions. 424 425 In a first inversion we have considered having a certain prior knowledge on the existing contrast in the soil, and therefore invert properties within delineated zones. In a second 426 inversion, we did not consider this knowledge and inverted the properties within a grid 427 regularly distributed in 2D in the saturated zone and in 1D in the unsaturated zone (see dotted 428 429 lines delineations in Figure 12).

For our zoned inversions the number of property values to be inverted was m = 12 (4 zoned values for each property) for a dataset composed of n = 45 amplitude/phase responses couples (15 responses obtained for each perturbation). We considered a diagonal covariance matrix for **C** with a 0.01 variance on each property value. We have tested different combinations of responses generated with lower or higher periods of oscillation (5, 15 or 30 min) in terms of imaging efficiency, and for different heterogeneity configurations (3/4 sand, 3/4 loam and half sand/half loam). The best imaging results obtained are presented in Figure 11.



Figure 11: Results obtained for the best inversion configurations with responses simulated in
 heterogeneous soils with different periods of oscillations (5, 15 and 30 min). Conductivities
 are inverted only with the amplitude responses, while the Van Genuchten coefficients are
 inverted with both amplitude/phase responses.

437

Here again, amplitude responses alone are sufficient to reconstruct the heterogeneous contrast 443 444 in the conductivity field for each period of oscillation tested. The inverted conductivity values, however do not always exactly match the true ones. It appears that a contrasted soil 445 (half sand/half loam zones) is better characterized with higher periods of oscillation, while a 446 less contrasted medium is better characterized with lower periods. Concerning the Van 447 Genuchten parameters, optimized with the remaining differences in the amplitude and phase 448 responses that could not be reproduced with conductivity alone, they are better characterized 449 with the higher period of oscillation in each case. As for the homogeneous cases, they can be 450 characterized only in the unsaturated zone of the soil and do not image heterogeneities in the 451

saturated zone. Parameter α appears to be more reliable than n for the interpretation of heterogeneity in the capillary fringe. In fact, in our results, inverted n values are good for the upper left zone, but not always for the upper right one, while α values are always coherent in both corners.

For our distributed inversions the number of property values to be inverted was m = 123 (41 distributed values for each property). We constrained the spatial distribution of the inverted property values with an exponential variogram model with a range of 2 to compute the covariance values in matrix **C**. We inverted the responses generated in the half sand/half loam heterogeneous configuration with a period of oscillation of 30 min (according to the best result configuration in the zoned inversions). The inverted property fields and their associated normalized standard deviations are presented in Figure 12.



464 <u>Figure 12:</u> Property values and their associated normalized standard deviations obtained from 465 the inversion of amplitudes (for K) and amplitudes/phases (for α and n) responses generated 466 in an heterogeneous soil (true properties) solicited with 30 min period oscillations. The 467 inversion grid is delineated with dotted lines.

The inverted property values globally do not match the true ones, they are mostly 469 underestimated. This can be explained by the lack of spatial constraints in this inversion that 470 471 allows optimization process to generate local equivalent property values for the reproduction of the data, especially for K, which is optimized first. However, the trends and localizations 472 of the heterogeneous contrasts can be imaged in both the saturated and unsaturated areas in 473 the conductivity field. The conductivity field is mainly sensible to the sand zones in the 474 475 saturated area, according to the distribution of its uncertainties. On the other hand, again unsurprisingly, the Van Genuchten parameters image only the heterogeneities in the 476

477 unsaturated area. However, in this distributed inversion it appears that α rather image the 478 loam areas, while n rather image the sand areas. The uncertainty analysis shows a globally 479 higher local sensitivity, near the perturbation sources for n, and a more homogeneous 480 sensitivity among the whole unsaturated area for α .

481 **5. Discussion**

482 **5.1.Effects of hydraulic properties on the saturated responses**

Our hydraulic analysis, presented in this article, tends to indicate that the different hydraulic properties considered K, α and n affect differently the measured oscillatory responses in the saturated zone and that their relation to such type of responses is also conditioned to different factors, such as the depth of the source or the measurement locations.

The conductivity K globally appears as the most interesting hydraulic property to be characterized with oscillatory responses. In fact, it is highly linked to the amplitude of the responses, more than the other studied properties, and, thus, can be easily isolated from these other properties when analyzing the responses. Basing our inversions of K on the amplitudes alone resulted, indeed, in good characterizations of its distributions in each configuration,

even without considering accurate Van Genuchten parameters. This observation is in 492 493 agreement with other works on unconfined media. Huang et al. (2019) analyzed the sensitivity of oscillatory responses in unconfined aquifers through an analytic solution and noted the 494 same high sensibility of the responses to K. However this observation does not seem specific 495 to oscillatory data. In fact, in their hydraulic tomography applications taking account 496 unsaturated flows, Mao et al. (2013b) and Zhao et al. (2015) also observed that the contrasts 497 in conductivity fields could be globally well imaged with responses to constant-rates 498 pumping. Mao et al. (2013b) even noticed the same fact that saturated flows properties could 499 be well characterized even without accurate guesses on the unsaturated ones. 500

501 Concerning the Van Genuchten parameters, there is currently no previous studies taking them into account in a characterization of an unconfined aquifer with oscillatory signals. Mao et al. 502 (2013b) and Zhao et al. (2015) employed the Gardner-Russo's model to simulate the 503 unsaturated flows and found that its parameters could be well characterized only in the 504 unsaturated area. In our study we observed that the oscillatory responses in the saturated zone 505 506 are affected by both α and n, with various intensities depending on the period of oscillation, the type of soil and the type of flows generated. The effect of n appears to be more related to 507 508 the local response at the perturbation source (local fluxes), while α generates a more distributed effect on the responses (vertical flows affecting the whole capillary fringe). The 509 510 imaging potential of α , therefore, appears as more reliable at the scale considered in our results (metric scale). Trying to link this hydraulic behavior to geological explanations is a 511 complex topic that is discussed in the literature. It is mainly accepted that α is related to the 512 513 air entry suction of the soil and n to the distribution of the pore size. Benson et al. (2014) observed that, for a uniform sand, the breadth of the particle size influenced n, while α was 514 more linked to a median value of the particle size, indicating a more integrative effect. 515 516 Porebska et al. (2006) noted that n was directly dependent to their soil composition (sand,

clay, silt), which we also observe in our results, while parameter α appeared to be more 517 related to the granulometry of the sample. 518

519

5.2. Advantages of oscillatory signals and period-dependent effects

Separating the responses signals into amplitude and phase allow for a better separation of the 520 information contained in the data. Absolute amplitudes can be used to specifically 521 characterize the conductivity K and appear to carry already a sufficient amount of 522 information to interpret its variations around the perturbation points, which can then be used 523 to guide the characterization of the unsaturated flows parameters. This possibility of 524 separating the responses into amplitudes and phases in real cases can be achieved only if the 525 responses reach a simple harmonic motion, mainly after several periods. The conditions 526 allowing to reach this conditions are described in Bakhos et al. (2014) and in Huang et al. 527 (2019). Oscillatory signals also offers the possibility to be easily extractable from other 528 sources of signals or noises. Techniques to efficiently process field oscillatory responses are 529 530 proposed in Bakhos et al. (2014). It can also be noted that oscillatory responses generated 531 with wetting/dewatering of an unsaturated soil potentially allow to assess mean values of α 532 and n in the water content curves, while responses associated to constant pumping would characterize only the Van Genuchten values associated to the dewatering part of the curve due 533 to the hysteresis 'scanning loops' effect. 534

The effect of the period of oscillation on the flows generated in an aquifer has been discussed 535 in previous works (Rabinovich et al. 2015; Cardiff et al. 2013b; Fischer et al. 2018; Fischer et 536 537 al. 2020b). Globally, according to these works, decreasing the period of oscillation accentuate flows in the most conductive and mobilizable areas of the field and in the vicinity of the 538 pumping/injection location. As water in the unsaturated zone represents a less mobilizable 539 540 source of water than the volume in the saturated area, it appears as logical that a lower period

of oscillation accentuate the horizontal flows and does not allow for a good characterization 541 542 of the unsaturated area. In their field applications, Rasmussen et al. (2003) observed, in fact, that with a very low period of oscillation, the responses generated in an unconfined aquifer 543 could be assimilated to confined-medium responses. Therefore, low periods of oscillations 544 may be employed with care for unconfined aquifers according to several previous works on 545 this topic (Rasmussen et al. 2003, Rabinovich et al. 2015; Cardiff et al. 2019). Cardiff et al. 546 547 (2019) also suggested that, for high frequencies (period < 1 min), the existing models such as the Richards-based may become inaccurate. 548

According to our results, if lower periods provided better imaging results for K when the 549 medium was homogeneous or with lowly contrasted heterogeneities, a higher period of 550 oscillation should be adopted if one wants to characterize draining effects parameters, 551 552 especially for α (n being more related to local responses seems less dependent to the period). However, when dealing with higher period signals, hysteresis effects should be considered 553 with unsaturated flows. In our results, for periods between 5 and 30 min and at a metric scale, 554 we show that we can neglect its effects on the responses (only for the responses in the 555 saturated zone). Experiments made in Cartwright (2014) and Shoushtari et al. (2015) are in 556 agreement with this observation when the period of oscillation remain relatively low. 557 However the authors noted that for high periods of oscillations reaching several hours or 558 559 more, the hysteresis effect could become important even on the responses in the saturated 560 zone and should be taken into account.

561 **5.3.Toward real cases**

The analysis proposed in this article represents a preliminary work for future real cases tomographic applications. It remains theoretical and real cases applications would face other problematics not considered in our models, such as the impact of environmental noise on the data. However, it provides some information and methods that may be helpful for a bettersetup of oscillatory data interpretation in an unconfined aquifer.

A first adaptation for a field application would be to consider 3-D flows with boundary 567 568 conditions often not affecting the perturbed volume. Therefore we have also simulated flows in a cylindrical homogeneous model with a similar geometry but a constant head boundary 569 condition located far away from the perturbation source point S (50 m away). This 570 571 configuration thus considers volumetric effects and a theoretical infinite volume (as water can enter or leave the model through the constant head boundary). These consideration are more 572 realistic for a field case. We compare the responses simulated in this way in sand and loam to 573 574 our 2-D model previously discussed in Figure 13. In order to generate a signal of similar amplitude at the perturbation source it is necessary to increase its flowrate amplitude (40 575 times in loam, 30 times in sand). However, the spatial responses simulated in this way will be 576 different from the ones obtained in the 2-D finite-volume model: the attenuation of amplitude 577 responses and the phase lags increase with distance become more important in the cylindrical 578 579 infinite-volume model. In order to generate responses in the cylindrical model that are closer to the 2-D ones, it is necessary to also increase the period of oscillation and the signal source 580 depth (relatively more in loam than in sand). If the adopted cylindrical model remains very 581 582 simplistic compared to real field, it permits to provide insights on what configuration parameters should be especially considered for fields applications (i.e. flowrate amplitude, 583 signal source depth and oscillation period) and how to adapt to different type of soils. 584



586 <u>Figure 13:</u> Observed amplitude (A in cm) and phase (P in $^{\circ}$) responses and simulated 587 saturated interface during pumping phase in homogeneous sand or loam considering either 2D 588 flows in a finite volume or cylindrical flows in an infinite volume and different signal 589 amplitudes (Q_A), depths (S) and periods (Pe).

590

591 **5.4.Imaging potential in tomographic applications**

According to the results presented in this work, having measurements and perturbation 592 locations distributed spatially and also at different depths of the aquifer might provide 593 different information on the different hydraulic properties. Horizontal flows effects might be 594 595 better characterized by deeper responses or perturbation, while the vertical flows effects can be better characterized by perturbation and measurements near the unsaturated zone. This 596 accumulation of distributed perturbations and information is, furthermore, a well-known and 597 widely used technique for the characterization of aquifers in hydraulic tomography. 598 599 Furthermore, we could observe that the localization of the signal source in depth was crucial for the characterization of the unsaturated area. It is, in fact, necessary to generate a 600 601 movement of the saturated/unsaturated interface, in order to generate vertical flows, mainly with a source close to this interface, or at this interface directly (such as tide periodic sources). 602 603 Mao et al. (2013a) provided several conditions on the dataset to perform accurate hydraulic tomography of unconfined aquifers. In particular they recommend to measure fluxes in 604 addition to pressure data and to couple different type of data in order to better characterize the 605 606 heterogeneity of the medium. Ideally, the different data should also identify flow processes in 607 the saturated and the unsaturated zone separately. Coupling geophysical data, allowing to image water content variations in the soil and heterogeneity contrasts, could greatly improve 608 the imaging results. Indeed, our inversions constrained with zones (that can be typically 609 delineated from geophysical interpretations) showed better results than the regularly 610 distributed ones. 611

In the method and the imaging applications presented in this work, we consider prerequisites knowledges on the properties. In particular we assume the storage coefficient, the anisotropy, and the saturated and residual water content of the medium to be known. Therefore, for a real application case using the inversion method proposed in this paper, one would need to estimate these values. For this purpose, Cheng and Renner (2018) proposed analytical

solutions comparing pressures amplitude and phase responses measured above and below an 617 618 oscillatory source to its flow-rate signal allowing to estimate the anisotropy and storage coefficient at the perturbation location. These solutions provide local estimates that can then 619 be used for the imaging application. However, even if the storage coefficient remains 620 unknown it is possible to image diffusivity ($D = K/S_s$), thus inverting K and S_s together. 621 Estimations of water contents constants would be more complicate in field applications, but 622 623 important impacts on the oscillatory responses can be observed only for large variations in their values, according to our analysis in section 3. Thus, an average guess may be sufficient 624 for an imaging application. 625

626 **6. Summary and conclusion**

This article presents a numerical analysis for the hydraulic interpretation of oscillatory responses measured in an unconfined media at a metric scale and including the effect of the capillary fringe. It represents a useful preliminary work for future real cases tomographic applications in unconfined media (sandbox or field cases), as it permits to point out several comments concerning the characterization of the hydraulic properties K, α and n with such data:

633 1) Conductivity K is highly correlated to the amplitude of the oscillatory responses compared
634 to the other hydraulic properties. Thus, a good characterization of the conductivity
635 distribution in an unsaturated media can be obtained separately with the amplitudes of the
636 responses alone and independently from the unsaturated properties;

637 2) The Van Genuchten parameters α and n, related to unsaturated flows, also affect the 638 responses in the saturated zone. They can be assessed, in a second step, from the amplitude 639 and phase responses that could not be reproduced by the previously reconstructed 640 conductivity; 641 3) In a heterogeneous soil, interpreting oscillatory responses in the aforementioned way 642 allows for a coherent reconstruction of the K field (that can then be used to guide the Van 643 Genuchten parameters characterization). The α and n values can be characterized only in the 644 unsaturated zone, and α appears to better image the heterogeneities than n at this scale;

4) The period of oscillation of the signal tends to accentuate rather horizontal flows for low periods and generate more vertical flows effects on the responses for high periods. Low periods signals are useful to an accurate assessment of the conductivity values in the saturated area. However, for the characterization of the unsaturated area, high periods of oscillations provide more information but may also be subject to more important hysteresis effects. Nevertheless, for the periods considered in this study (5 to 30 min), these effects could be neglected.

652 These comments may represent interesting advices for real cases applications. However, other problematics not taken into account in this work, might also be considered. Real cases 653 654 applications are naturally more complex than the model studied in this work, and effect of noise on the measurements also represents a common problematic in such cases. A commonly 655 employed and efficient technique that reduce uncertainties in real field applications is 656 hydraulic tomography. This technique, based on a crossed interpretation of responses to 657 perturbations obtained at several locations and depths, should therefore be considered in 658 association with periodic signals for the spatial characterization of unconfined aquifers 659 properties in future field applications. Addition of other types of data, such as geophysical 660 information could also greatly improve the inversion results in real-cases applications. 661

662

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