Inverse upscaling of hydraulic parameters during constant flux infiltration using borehole radar

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ABSTRACT

Modeling unsaturated flow in porous media requires constitutive relations that describe the soil water retention and soil hydraulic conductivity as a function of either potential or water content. Often, the hydraulic parameters that describe these relations are directly measured on small soil cores, and many cores are needed to upscale to the entire heterogeneous flow field. An alternative to the forward upscaling method using small samples are inverse upscaling methods that incorporate soft data from geophysical measurements observed directly on the larger flow field. In this paper, we demonstrate that the hydraulic parameters can be obtained from cross borehole ground penetrating radar by measuring the first arrival travel time of electromagnetic waves (represented by raypaths) from stationary antennae during a constant flux infiltration experiment. The formulation and coupling of the hydrological and geophysical models rely on a constant velocity wetting front that causes critical refraction at the edge of the front as it passes by the antennae. During this critical refraction period, the slope of the first arrival data can be used to calculate (1) the wetting velocity and (2) the hydraulic conductivity of the wet (or saturated) soil. If the soil is undersaturated during infiltration, then an estimate of the saturated water content is needed before calculating the saturated hydraulic conductivity. The hydraulic conductivity value is then used in a nonlinear global optimization scheme to estimate the remaining two parameters of a Broadbridge and White soil.

1. Introduction

Inverse methods to obtain hydraulic parameters that describe the soil water retention and soil hydraulic conductivity functions of unsaturated soils are often more desirable than direct methods. Direct methods traditionally rely on making a series of laboratory measurements at different equilibria established between a small soil sample in direct contact with a body of water at a known potential. Direct methods are based on steady state procedures that make direct use of Darcy’s law with some simplifying assumptions [43]. Inverse methods, on the other hand, involve more complex formulations through the coupling of: (1) a transient flow experiment with prescribed boundary and initial conditions and measured flow variables; (2) a mathematical model that describes transient water flow; and (3) an optimization algorithm that estimates the unknown parameters of the hydraulic functions [17]. Previous investigators have used time-lapse measurements of the cumulative outflow volume of water [24,54,49], cumulative inflow volume [1,39], the position of the wetting front [6,42], or multi-step pressure pulses [52] to estimate these hydraulic parameters.

Many of the transient flow experiments reported in the literature have been conducted on extracted soil cores, either disturbed (e.g., [9,58]) or undisturbed [29,12]. A soil core represents only a small volume within the larger flow field. Forward upscaling methods must then be used to derive local or field scale effective hydraulic properties, given some information about spatial structure and variability of the properties [53].

An alternative to the forward upscaling methods on small samples are inverse upscaling methods that incorporate soft data from geophysical measurements observed directly on the larger flow field, as described in Vereecken et al. [53]. In this approach, the parameter estimation procedures still require a transient mathematical flow model with appropriate boundary and initial conditions that describe the circumstances under which the hydrogeophysical data were collected. In addition, petrophysical models that relate the geophysical measurement to a hydrologic variable are needed. Examples of inverse upscaling include electrical resistivity tomography [59,21], ground penetrating radar tomography [2,8,10], and acoustic tomography [3]. Tomography itself is an inverse procedure by which the geophysical property of either electrical resistivity or velocity (including electromagnetic and acoustic wave velocity) are estimated based on energy measurements of voltage potential or first arrival time of acoustic or EM waves. The inverse methods for tomography should not be
confused with the inverse methods for hydraulic parameter determination.

Tomographic methods for geophysical data processing can produce an inaccurate depiction of the subsurface due to the ill-posedness of the inverse problem and the additional constraints needed to formulate a unique solution. Tomographic results may create an artificially smooth representation of the subsurface, particularly at the boundaries between material types, or it may produce distortions in the depiction of the flow regime [20,26,34]. To compound the problem, the tomographic results are then used in the conversion from the geophysical property to a hydrological property, such as water content, using petrophysical relationships. Although the petrophysical relationships were derived on core samples, whereby all of the parameters that compose the relationships are measured at the same scale, many have adopted them to convert field-scale values [32]. Singha and Gorelick [44] summarize the complications from this approach, including the mismatch in scale between measurements and the decreased sensitivity of measurements in the far field.

One can minimize the issues surrounding tomographic inversion by taking advantage of direct observations of the measured geophysical data without the artifacts introduced from tomographic methods. In this situation, the temporal measurements of voltage data during an electrical resistivity survey [31] or ray-based electromagnetic wave travel time data from cross-borehole radar [20,35] can be incorporated directly into a coupled hydrological-geophysical modeling scheme. To demonstrate this methodology, we extend the work by Rucker and Ferré [35] by incorporating field data from a zero-offset profiling, cross-borehole ground penetrating radar (z-BGPR) survey made during infiltration into an initially drained soil profile. The previous work (ibid) stopped short of providing actual data and presented only synthetic examples for a prescribed head boundary condition. Here, an analytical solution to the vertical, 1D, water content-based Richard’s equation (or diffusivity equation) with a gravity term is used to model the unsaturated water flow. To accommodate the boundary conditions of the field experiment, a constant flux formulation is used, along with a Broadbridge and White-type (BW) soil [4]. A ray-tracing routine is then used to model both direct and critically refracted z-BGPR raypaths during infiltration. The raypath model inherently assumes infinite frequency, and resolution issues surrounding the use of finite frequencies and ray scattering within the Fresnel zone are ignored. It is shown that due to critical refraction, the position of the wetting front can be tracked, allowing an accurate estimation of the hydraulic conductivity of the wet soil. Additionally, since the relative hydraulic conductivity function for the BW soil is reliant on a single hydraulic parameter, the entire function can be described without the need for ancillary head or outflow information provided that easily obtainable soil data (saturated water content) is available. These results present a major advance in using geophysical data to constrain hydrological models because there are less unresolved hydraulic parameters to estimate.

2. Theory

2.1. Unsaturated flow in porous media

The vertical, 1D, \( \theta \)-based, Richards’ equation is:

\[
\frac{\partial h}{\partial t} + \frac{\partial}{\partial z} \left(D(h) \frac{\partial h}{\partial z} - \frac{dK(h)}{dh} \frac{\partial h}{\partial z} \right) = 0
\]

where \( h \) is the volumetric water content as a function of depth and time, \( z \) is depth (positive downwards), \( K \) is hydraulic conductivity as a function of \( \theta \), and \( D \) is the soil water diffusivity as a function of \( \theta \) [56]. No sources or sinks are considered. Philip [27] and Clothier et al. [5] presented early solutions to Eq. (1) using Burger’s equation. Broadbridge and White [4] and Warrick et al. [57] also presented solutions to Eq. (1) in a slightly different form assuming a constant flux top boundary condition of

\[
t = 0, \quad z = 0 : K(\theta) - D(\theta) \frac{\partial \theta}{\partial z} = R
\]

with the other boundary and initial conditions of

\[
t = 0, \quad z > 0 : \theta = \theta_0
\]

and

\[
t \geq 0, \quad z \to -\infty : \theta = \theta_0
\]

where \( \theta_0 \) is the antecedent moisture content. A dimensionless form of Eq. (1) can be solved by applying transformations, which convert the nonlinear equation to a linear diffusion equation. The solution requires Fujita [14] functions for the diffusivity and hydraulic conductivity:

\[
D(\theta) = \frac{a}{(b - \theta)^c}
\]

and

\[
K(\theta) = \beta + \gamma(b - \theta) + \frac{\chi}{2(b - \theta)^2}
\]

where \( a, b, \beta, \gamma, \) and \( \chi \) are constants. Furthermore, assuming that \( K(\theta_0) = 0 \) and the introduction of a dimensionless hydraulic parameter \( C \) and the sorptivity \( S \) reduces the five hydraulic parameters to a manageable two parameters. These two parameters completely describe the Broadbridge and White (BW) soil. The hydraulic conductivity function reduces to a function of \( C \):

\[
K(\theta) = K_0 \left[ \theta^2 \frac{C - 1}{C - \theta} \right]
\]

where \( \theta \) is the relative saturation

\[
\theta = \frac{\theta - \theta_0}{\theta_s - \theta_0}
\]

\( \theta_0 \) and \( \theta_s \) are the irreducible and saturated water content, respectively, and

\[
C = \frac{b - \theta_0}{\theta_s - \theta_0}
\]

Eq. (6) assumes that the initial soil profile is dry so that both \( K(\theta_0) \) and \( \theta_0 \) are very small in comparison to \( K_0 \).

As an example of the properties that would describe a common soil type, the hydraulic parameters for a Brindabella silt clay loam are a saturated hydraulic conductivity \( K_s = 3.27 \times 10^{-3} \text{ m/s} \), \( S = 1.335 \times 10^{-3} \text{ m/s}^{1/2} \), \( C = 1.02 \), \( \theta_r = 0.11 \), and \( \theta_s = 0.485 \) (see [57] for soil properties). Admittedly, the BW soil functions are not common, but many researchers use this soil model in analytical solutions of a constant flux upper boundary condition, including infiltration and evaporation. Table 1 shows a short list of works that include the BW soil. Of prominence are a series of studies that uses the model WAVES [60], which is a physically-based ecohydrological model that allows the simulation of land system behavior under alternative vegetation management scenarios and climatic variation. The WAVES model uses the BW soil for calculating the soil moisture content and potential and the effects on transpiration from plants. Furthermore, Triadis and Broadbridge [48] show similarities between the parameters that describe a BW soil and a van Genuchten–Mualem (VG) soil [23,50]. The relation shows that for a Yolo light clay, the BW model can be parameterized with \( C = 1.13 \) and \( S = 1.254 \times 10^{-4} \text{ m/s}^{1/2} \), and the VG model can be parameterized with \( n = 1.77 \) and \( a = 2.43 \text{ l/m} \), where the effective saturation \( S_e \) is redefined as
and the soil moisture characteristic curve as a function of soil potential ($\Psi$) and hydraulic conductivity functions are, respectively:

\[
S_e = \frac{\theta - \theta_f + \Theta(\theta_i - \theta_f)}{\theta_i - \theta_f},
\]

and

\[
K = K_s S_e^{1/2} \left[1 - \left(1 - S_e^{(n-1)}\right)^{1-1/n}\right].
\]

Fig. 1A demonstrates the solution for a water content profile at two times during infiltration into a drained silt clay loam with properties described above. The initial water content is $\theta_0 = 0.11$ and the infiltration rate is $R = 4.58 \times 10^{-2}$ m/s (where $R/K_s = 0.14$). This is the same problem presented in Fig. 3 of Warrick et al. [57] and is tested here to ensure that the set of equations were properly coded. When comparing against the original work, Fig. 1A is shown to have identical results.

Broadbridge and White [4] reported that the wetting front will move with an approximate vertical velocity of

\[
\frac{dz_f}{dt} = \frac{2(C - 1)K_s}{\Delta \theta} \left[1 + \frac{4eC(C-1)}{(C-1)^{1/2} - 1}\right]^{-1/2},
\]

where $z_f$ is the position of the wetting front and $dz_f/dt$ is the vertical velocity of the wetting front. Applying Eq. (12) to the properties of the silt clay loam gives a wetting front velocity of $1.352 \times 10^{-2}$ m/s. Direct calculation of the wetting front velocity in Fig. 1 provides a value of $1.404 \times 10^{-2}$ m/s.

2.2. Ray tracing radar model

The travel paths of electromagnetic energy in a layered earth structure can be described using ray tracing methods. This approach assumes that the energy travels as straight rays through a medium that reflects or refracts at boundaries of differing dielectric properties according to Snell's Law. Additionally, ray theory assumes ideally that waves propagate at infinite frequency [18]. Inasmuch, resolution limits based on scattering theory, which takes the finite-frequency effect of waves into account, are not con-

Table 1

<table>
<thead>
<tr>
<th>Citation</th>
<th>Research highlights</th>
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<td>Fuentes et al. [13]</td>
<td>Examined the parameters of the BW soil (termed the Fujita model) in addition to four other closed-form soil models during infiltration</td>
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<td>Parkin et al. [25]</td>
<td>Used time-domain reflectometers to estimate the BW soil properties</td>
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<td>Short et al. [41]</td>
<td>Used the BW soil in an analytical model to compare to numerical results</td>
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<td>Grifoll and Cohen [16]</td>
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sidered. Ray tracing methods are prone to less error if the inhomogeneity is larger than the width of the Fresnel zone [46]. Accordingly, it is justified to use ray theory in modeling of sufficiently smooth media.

Tracing the paths of first arriving rays traveling from the transmitter to the receiver is critical in the accurate calculation of the dielectric permittivity, and hence water content, using z-BGPR. Rucker and Ferré [33–38] have shown that the direct and critically refracted travel paths must be considered when analyzing z-BGPR radargrams.

The travel time of a direct wave through a high water content, low velocity ($v_{low}$) layer is:

$$t_{direct} = \frac{x}{v_{low}},$$

(13)

where $x$ is the antennae separation distance. The travel time of a critically refracted wave is:

$$t_{refr} = \frac{x}{v_{high}} + z_{f} \left[ \frac{2}{v_{low} \cos k} - \frac{2 \tan k}{v_{high}} \right],$$

(14)

where

$$k = \sin^{-1} \left( \frac{v_{low}}{v_{high}} \right).$$

$z_{f}$ is the distance to the refracting (wetting front) boundary, and $v_{high}$ is the high velocity layer where refraction occurs. When the antennae are located within the low velocity layer, near the boundary with the high velocity layer, the critically refracted wave will have the lowest travel time (i.e., first arrival time), otherwise the direct wave will be the first. During a transient flow experiment, it has been shown that the electromagnetic waves from radar measure-

$$\text{ments will refract critically at the edge of the wetting front [35]. This refraction will continue until the wetting front has moved beyond a distance that no longer gives rise to first arriving critically refracted waves. This depth is known as the refraction termination depth [30,33].}$$

Consider the infiltration event similar to that of Fig. 1, but conducted for a much longer time period such that the wetting front passes a depth of 4 m in a little over two days. Fig. 1B shows the water content profile again at two separate times, and the wetting front can be seen to pass a set of z-BGPR antennae placed at a depth of 1.5 m. For this synthetic case, travel time measurements are reported approximately every 0.25 h. At early time, when the wetting front is above the antennae, the travel path is direct. As the wetting front passes the antennae, the waves refract critically at its edge. The time series of first arrival travel time during critical refraction is a function of the velocity of the wetting front, which is manifest in the slope of the time series curve of first arrivals. For comparison, the arrival time of the direct wave is also shown, which has the typical appearance of data obtained from stationary water content sensors, such as time domain reflectometers, TDRs, (e.g., [42,35]). When the front has moved well beyond the antennae, the travel path returns to this direct path for the remainder of the active infiltration. The differences in travel time between the two curves are clear, allowing an obvious distinction in z-BGPR data whether critical refraction actually occurs in the subsurface.

2.3. Parameter estimation

The wetting front (or the refracting boundary) position can be related to the position of the stationary borehole antennae as a function of infiltration time. The first arrival travel time of the critically refracted wave can also be expressed as a function of infiltration time. Using the reciprocal of velocity (slowness, or $s$) and the proper trigonometric identities, Eq. (14) can be rewritten as

$$t_{refr}(t) = x s_{high} + 2z_{f}(t) \sqrt{s_{low}^2 - s_{high}^2}.$$  

(16)

The derivative of Eq. (16) with time yields

$$\frac{dt_{refr}}{dt} = 2 \sqrt{s_{low}^2 - s_{high}^2} \frac{dz_{f}}{dt}.  

(17)$$

At long times, Broadbridge and White [4] demonstrated that a steady convection of the soil water profile emerges, and the velocity of the wetting front becomes constant at:

$$\frac{dz_{f}}{dt} = \frac{K_{wet}}{\Delta \theta}.$$  

(18)

where $K_{wet}$ is the hydraulic conductivity of the wet soil (not necessarily at $K_{s}$) provided that $K_{wet} \gg K(\theta_{s})$. Substituting Eq. (17) into Eq. (18) gives

$$K_{wet} = \frac{dt_{refr}}{\Delta \theta} \left( \theta_{w} - \theta_{0} \right).$$  

(19)
Eq. (19) shows that the slope of the z-BGPR first arrival travel time curve in Fig. 2A can be used to estimate the effective upscaled $K_{wet}$. Using linear regression, the slope of the linear travel time is $0.000448$ (ns/s). The slowness values at the beginning ($s_{high}$) and end ($s_{low}$) are calculated for the antennae separation of 3 m as: $s_{low} = 17.92$ ns/m and $s_{high} = 8.33$ ns/m. The calculated $K_{wet}$ using Eq. (19) is $4.8 \times 10^{-3}$ m/s, which shows good agreement with the value used in the forward model, $4.58 \times 10^{-3}$ m/s. The 5% difference between the calculated and modeled $K_{wet}$ is likely due to the approximation of the wetting front velocity in Eq. (18), which was shown above to have a 4% difference.

Fig. 2B shows a second series of z-BGPR first arrival travel time curves that covers a range of relative flux ($R/K_s$) from 0.05 to 1. For reference, the preceding Figs. 1A and B, and 2A used a value of 0.14, which is highlighted in Fig. 2B by a dashed line. The infiltration time scale has been compressed to log space to incorporate all curves together for a relative comparison. As such, the displayed curves cannot be used directly to estimate the hydraulic conductivity. However, the figure does demonstrate the limits under which the first arrival travel time will be due to critical refraction. Specifically, for the Brindabella loam, the relative flux limit appears to be near a value of 0.14, with lower relative flux values having some or all direct arrivals as the first arrival. The figure shows a marked change in the character of the two curves represented by the lower relative flux.

To determine whether an inverse procedure can be used to uniquely estimate the BW soil hydraulic parameters of $C$ and $S$, we examined the error surface of $S$ vs. $C$ space in a manner similar to that used by Hopmans et al. [17]. The first arriving travel time as a function of infiltration time was calculated for many combinations of $S$ and $C$ with a single value on the function of $K(\Theta)$ using the forward water flow and z-BGPR models. The error for each parameter combination was defined as the root mean square error (RMSE) between the first arrival travel time series for a synthetic case with $S$ and $C$ of 0.001335 and 1.02, and the series determined for the different parameter combinations:

$$RMSE = \sqrt{\frac{1}{N} \sum_{j=1}^{N} [\tau_p(t_j) - \tau_m(t_j, \beta)]^2}, \quad (20)$$

where $\tau_p$ is the measured first arrival travel time from path $p$ (either direct or critically refracted) at time $t_j$, $\tau_m$ is the modeled first arrival travel time from path $p$ at time $t_j$ subject to the soil hydraulic parameters $\beta = \{K_s, C, S\}$ (e.g., $K_s$, $C$, and $S$). The error surface (presented as the logarithm of RMSE) in Fig. 3A indicates that the method is very sensitive to the parameter $C$, based on the steep gradient near the actual value of 1.02. However, uniquely determining $S$ is more difficult, due to an elongated valley of low error values that may impede the process of searching for the global minimum, depending on how the stopping criteria is set during the iterative optimization procedure. Additionally, most locally-based optimization procedures would likely estimate the optimal parameter set based on the starting guess [35], the degree of measurement error, and how well the models represent the hydrogeological and geophysical systems (i.e., model error).

As a comparison, Fig. 3B shows the error surface for $S$ vs. $C$ for water content measurements made during the same infiltration experiment. The surface is extracted assuming the $K(\Theta)$ is known beforehand. Surprisingly, the shape of the surface is similar, especially near the actual values and the parameter $C$ is extremely sensitive to these measurements. It should be noted that a measure of $K$ is not attainable from the water content data alone, and that it too would have to be estimated in the optimization procedure adding another dimension of uncertainty.

At this point, it may be of interest to discuss the moisture characteristic curve and the relationship between saturation and potential, $\Psi$. Broadbridge and White [4] showed that when $K(\Theta_0)$ is negligibly small relative to $K_s$, the potential can be written as:

$$\Psi(\Theta) = \Psi(\Theta_0) + \frac{(\Theta - 1)}{\Theta} \frac{1}{C} \ln \left[ \frac{C - \Theta}{\Theta(C - 1)} \right], \quad (21)$$

where $\lambda$ is the macroscopic capillary length that acts as a natural scaling factor for $\Psi(\Theta)$.
\[ \lambda_s = \frac{S^2 h/\Delta t}{K_0} \]

and the approximation of \( h \):

\[ h = h(C) = C(C - 1) \frac{\pi(C - 1) + B}{4(C - 1) + 2\pi} \]

with \( B = 1.46147 \). Now, using the same methodology as with the moisture content, it is assumed that potential measurements can be made during an infiltration event and the error surface computed for a range of \( C \) and \( S \) values. The results are presented in Fig. 3C, and it is clear that the head is more sensitive to both \( C \) and \( S \), but much less so to \( C \) compared to either the error surface computed from data acquired with water content or z-BGPR refracted travel time. These differences in sensitivity between the water content-based measurements and potential-based measurements are basically due to the fact that the hydraulic conductivity function is exclusively a function of \( C \), and \( S \) is only incorporated when forming the dimensionless parameters of depth and time, which are scaled to \( \lambda_s \) according to Warrick et al. [57]. The scaling
at least creates a low sensitivity for the parameter $S$. The potential, on the other hand, is a function of both $S^2$ and $C$, and the results are manifest in a global minimum that should be easily found with any optimization procedure. It is noted again, that a measure of $K$ cannot be obtained alone and the hydraulic conductivity will also need to be included in the optimization.

2.4. Limitation of the methodology

Up to this point, we have only considered one dimensional steady flow in a homogeneous earth. This idealized case provides an accurate depiction of the hydraulic conductivity using z-BGPR first arrival travel time data, and error surfaces show that the parameter $C$ to describe the complete relative hydraulic conductivity function can likely be obtained without much difficulty, provided a reasonable first guess is submitted for any optimization method employed to find it. Deviating from the ideal case, where the earth is heterogeneous and the flow not steady, one would expect that the error in estimation due to model uncertainty could be significant. Complications, such as an uneven wetting front, preferential flow, instability due to fingering, or even hydrophobic soils, may prove the idealized model completely inadequate. To test model uncertainty, however, would require numerical modeling of both the Richards’ equation for flow and Maxwell’s equations for radar wave propagation, as analytic solutions do not lend themselves well to the degree of heterogeneity expected for truly natural systems. Modeling subsurface heterogeneity may show in some instances that critical refractions do not occur at the wetting front interface as suggested, but instead reflect at lateral interfaces along the raypath. A test of model uncertainty is certainly warranted, but beyond the scope of this work. It is mentioned here only to alert the reader that the methodology presented herein may not be suitable for their particular case and other analyses may need to be considered.

3. Global optimization with simulated annealing

To effectively search the error space for the optimum set of hydraulic parameters that minimizes Eq. (20), the global optimization method of simulated annealing was chosen. Rucker and Ferré [34] demonstrated that simulated annealing is an effective method to discern the spatial patterns of subsurface layers with z-BGPR data. It’s use here is an extension of that work to replicate the temporal patterns of z-BGPR data. A full description of the simulated annealing method can be found there (ibid).

To simulate the annealing process for our optimization problem, a random-walk model was devised so that the hydraulic parameters were perturbed in a random direction by a random amount. A model that improves the fit from is accepted, while a parameter set that worsens the fit is accepted according to the Metropolis algorithm [40]:

$$\text{Pr} (\text{accept } +1) = \begin{cases} 1, & \text{if } E(i+1) \leq E(i), \\ e^{-\frac{c_i}{c_0}}, & \text{if } E(i+1) > E(i). \end{cases}$$

(24)

where $\Delta E$ is the difference between the new energy state and the current energy state, $c_i$ is the control parameter, and $e^{-\frac{c_i}{c_0}}$ is the Metropolis criterion. The control parameter plays the role of the temperature and is reduced during the course of the simulation following a cooling schedule. A simple cooling schedule is an exponential reduction in the control parameter by:

$$c_i = \frac{c_i}{c_0},$$

(25)

where $\alpha$ usually ranges between 0.85 and 0.99 and $c_0$ is the initial temperature.

To implement the simulated annealing algorithm, an initial guess is made by choosing a random value for each $C$ and $S$ between a set of user-defined limits. These limits are also used in constraining the algorithm during its search. Then both parameters are perturbed and the coupled hydrological-geophysical forward model is run to compare against the measured z-GPR data. The process is repeated until an acceptable parameter set is found that minimizes Eq. (20).

Fig. 4 shows a set of results for the simulated annealing algorithm when estimating hydraulic parameters that give rise to the travel time data of Fig. 2A. Three tests were run by changing the cooling schedule from 0.9 to 0.99. Fig. 4A shows the improvement in RMSE for three example runs versus the iteration number; the three example runs correspond to different values of $\alpha$. The optimi-
zation procedure generally finished within 30–50 iterations by attaining the desired RMSE of 0.451. The RMSE is based on the expected measurement error as presented in Rucker and Ferré [34] from a series of radar shot in air during calibration. At the beginning of each example run, the RMSE starts high but drops quickly for about the first 20 iterations. During this early period, improvement to the estimation of C and S are made easily. Fig. 4B and C show the progression of the individual parameters during the optimization process. The large improvement at the beginning of the optimization is generally attributed to the improvement in C. Occasionally, a worse fit for C and S is accepted, as shown in the increase in RMSE for later iterations. The probability of accepting worse fits decreases during optimization, but is counter balanced with the fact that finding a better fit becomes more difficult. Final improvements to the minimization of the objective function occurred by honing in on parameter C. Fig. 4D shows a track of the hydraulic parameters in error space for $x = 0.99$. Towards the end of the optimization, the parameters track along the valley shown in Fig. 3. The target is not actually reached for this simulation because of the error requirements taken from the measurement error. However, Fig. 4E shows that the fit to the target travel time is quite good.

4. Experimental method: travel time measurements with z-BGPR

To demonstrate the inverse upscaling procedure on field data, an infiltration experiment was conducted at a site located in Tucson, AZ. The soil profile was characterized by inspection of continuous cores obtained during drilling of the boreholes [38], and Fig. 5 shows a cut-away geological profile of the site along with the original gravimetric moisture content prior to any infiltration experiment. The experiment presented herein is the third within 1.5 years. The top 0.15 m of soil consists of dry, unconsolidated loose sand and silt. A thick (~3.3 m) coarse sandy layer with inter-spersed lenses of organic material and clay underlies the surface material. A black, peat-like organic layer is located approximately one meter below surface. The sand changes to a gravelly sand to about 6 m, which turns to cobbles, gravel, and sand to 8.5 m. From 8.5 to 13 m the medium varies from a 1.5 m-thick clay lens to a rich clayey sand. The remainder of the profile to 15 m is comprised of fine sand with small amounts of clay.

Water was applied within a bermed infiltration gallery of 5 m per side through a manifold that distributed water evenly over the area at a constant flow rate of $9.44 \times 10^{-2} \text{ m}^3/\text{s}$ for 66 h. The
infiltration experiment has been described elsewhere [33,34], but is presented here for completeness. This rate was chosen to minimize water ponding at the surface. The field was instrumented with sensors, such as advanced tensiometers [45] and two-pronged TDR probes, to measure pressure head and volumetric water content, respectively. The sensors were placed at various depths within hand-augered 15 cm diameter holes. The depth profiles for the sensors are shown in Fig. 5. For tensiometer placement and borehole completion, 0.3 m of diatomaceous earth was used to surround the ceramic cup and bentonite plugs above the diatomaceous earth prevented short-circuiting of the advancing wetting front during infiltration. The procedure for TDR placement and completion was similar except that native material was used to backfill around the sensor instead of diatomaceous earth.

Fig. 6 shows the time series data of the tensiometer and TDR data during the infiltration. The tensiometer data in Fig. 6A and B show dramatic pressure increases as the wetting front reaches and eventually passes the sensor. These data were then used to estimate the velocity of the wetting front by differentiating the time of arrival between sensors. The calculated velocities are presented in Table 2, with the definition of each velocity measurement in the subplots of Fig. 6. The same was repeated for the TDR data, with the location of the wetting front defined as the midpoint point between the high and low water content. Based on all of the data in Table 2, the arithmetic average for the velocity measurements was 22 $\mu$m/s with a range from 13 to 34 $\mu$m/s. The large range is primarily caused by TDR instrument R2. However, when looking specifically at instruments separated the furthest in each borehole ($v^2$), the velocity range is much more narrow with values of 19.9, 20.1, 20.6, and 23.4 $\mu$m/s. This would suggest a fairly steady wetting front over vertical distances appropriate for z-BGPR measurements. The smaller scale variability could be due to localized conditions around the instrument or small scale heterogeneities.

A PulseEkko100 system with 100 MHz antennae (Sensors and Software, Mississauga, ON) was used for all z-BGPR measurements during infiltration. Post-processing of first-arrival picking was accomplished through automated picking software, ‘Picker’ (Sensors and Software) and Fig. 7 shows a series of traces during the infiltration period from which these first-arrival travel time picks were made. The traces show clear arrivals that were not significantly attenuated during the experiment. The z-BGPR profiles were collected in two-inch, PVC-cased boreholes that were completed to 15 m within the infiltration gallery. The borehole separation was 3.25 m and first arrival travel time measurements were recorded approximately every 0.5 h while the antennae remained at a fixed depth of 2.25 m bgs. The depth equates to the position of the center of the antennae, which are approximately 1 m in length. Travel time profiles collected before infiltration showed that there was not a refracting boundary near this depth (these data are presented in [33,34]). As a result, the travel time at the beginning and end of the experiment (i.e., before the wetting front arrives and after it has passed the refraction termination depth) can be considered to be from first arriving direct waves.

The time series of z-BGPR first-arrival travel time data (Fig. 8A) exhibited a nearly flat, albeit sinusoidal, appearance up to about $9 \times 10^4$ s. The periodicity of the beginning portion of the curve is approximately equivalent to one day, suggesting that maybe diurnal heating effects on the black cables comprising the PulseEkko100 system could be playing some role in the noise. From approximately $9 \times 10^4$ to $15 \times 10^4$ s, a linear increase is seen as the advancing wetting front moves past the antennae. This portion of the curve is explicitly identified as critical refraction in Fig. 8A. When the wetting front moves beyond the refraction termination depth, the first arrival travel time returns to a direct wave. Unfortunately there is a missing section of time series data due to early termination of the z-BGPR readings before realizing the wetting front had not moved as far as originally anticipated. One last reading was obtained at 66 h, before cessation of the infiltration experiment. The values for the missing first arrival travel time is assumed to be constant at 35.8 ns. For comparison, data from a nearby tensiometer and TDR are plotted to demonstrate, alongside z-BGPR, the differences in these different types of data. It is obvious that the z-BGPR data are similar to the hypothesized critical refraction curve shown in Fig. 2A.

The first-arrival travel times at the beginning and end of the infiltration experiment were converted to volumetric water content using an empirical calibration equation [11]:

![Fig. 7. Traces from z-BGPR survey conducted during the infiltration test to show strong first arrivals. Numerical values atop every other trace relates to the infiltration time in seconds when they were collected (values are divided by 10,000).](image-url)
\[
\theta = 0.1181 \frac{v_{\text{air}} t_{\text{direct}}}{x} - 0.1841, \tag{26}
\]

where \(v_{\text{air}}\) is the velocity of propagation in air (0.3 m/ns), \(x\) is the antennae separation, and \(t_{\text{direct}}\) is the first arrival travel time assuming a direct wave. Based on this petrophysical relationship, volumetric water content values at the beginning and end of the experiment were 0.085 and 0.206, respectively. Eq. (19) was then used to calculate the velocity of the wetting front (11 l/m/s) based on the slope of the travel time data (0.00173 ns/s). The velocity calculated with z-BGPR is below the range of that measured with the buried sensors. The overestimation by the buried sensors could be due to a number of factors, such as preferential flow within the disturbed boreholes or an insufficient number of sensors to properly characterize the flow field. Alternatively, the underestimation of the velocity by z-BGPR could be due to inaccurate petrophysical relationships, model error (1D vs 2D flow), or first-arrival travel time measurement errors.

The wetting front velocity was used to calculate the unsaturated hydraulic conductivity of the wet soil, \(K_{\text{wet}}(\theta = 0.206)\). The value, \(K_{\text{wet}} = 1.34 \times 10^{-6} \text{ m/s}\), was then used to estimate the remaining parameters. Within 24 iterations, the simulated annealing algorithm yielded 1.011 and 0.00045 m/s\(^{1/2}\) for \(C\) and \(S\), respectively. The stopping criteria for RMSE was set to 0.451 based on the expected measurement error presented in Rucker and Ferré [35], and the final RMSE value was 0.405. Fig. 8B shows the travel time model results using these estimated parameters, which are overlain on the original measured data. The curve fits quite well, both quantitatively and qualitatively, to the measured data.

It is clear from the soil water potential data in Figs. 6 and 8 that the hydraulic conductivity obtained from the z-BGPR data is not \(K_s\) due to the buried tensiometers recording soil water potential values less than 0 cbar during the course of the infiltration experiment. Since \(C\) is now known, however, we at least have a means to calculate the relative hydraulic conductivity function \((K(\theta)/K_s)\). Fig. 9A shows the relative hydraulic function (Eq. (6)) for the infiltration experiment, using \(C = 1.011\). Additionally, the flow model implicitly assumes an unit gradient condition for the lower boundary in Eq. (3) with \(\theta = \theta_0\) at \(z = \infty\), allowing us to fix one value on the full hydraulic conductivity curve: \(K_{\text{wet}}(\theta = 0.206) = 1.34 \times 10^{-6} \text{ m/s}\). An advantage of a lower unit boundary condition is that the flux is the unsaturated hydraulic conductivity at that measured water content. To obtain the full description of the hydraulic conductivity function, a value of \(K_s\) is needed, which may be obtained...
An analytical unsaturated flow model coupled with an analytical z-BGPR ray-tracing model were used to evaluate the inversion of hydraulic parameters based on first arrival time measurements made during infiltration into a drained soil. The hydrogeophysically coupled model relied on the Broadbridge and White (BW) description of soil hydraulic functions and a steady wetting front of constant velocity. The use of a BW soil makes the solution for the Richards' equation tractable for a known constant-flux boundary condition, and the soil can be described by the two main hydraulic parameters of $C$ (dimensionless fitting parameter) and $S$ (sorptivity in m/s$^{1/2}$) as well as the saturated hydraulic conductivity.

The z-BGPR ray tracing routine simulated both direct and critically refracted waves. The first-arrival travel time was obtained by taking the minimum travel time for either mode of travel. For the experimental procedure, the z-BGPR antennae were fixed at a constant depth while the wetting front passed by the antennae's position. It was found that before the wetting front arrived at the antennae's depth and long after it had passed, the first arrival travel time was from the direct wave. There was an intermediate wetting front depth that caused critical refraction at the edge of the wetting front. The time during which critical refraction occurred was shown to have a linear slope for the curve of first-arrival travel time data, which was proportional to the hydraulic conductivity. If the soil happens to be saturated during the infiltration, then the estimated hydraulic conductivity will be the saturated hydraulic conductivity. If the soil is unsaturated, then the hydraulic conductivity will be a point on the hydraulic conductivity function. This value along with the parameter $C$ and saturated water content can then be used to obtain the full hydraulic conductivity function.

The inverse procedure for estimating the two hydraulic parameters ($C$ and $S$) relied on the global optimization routine of simulated annealing. The inverse routine was demonstrated on both synthetic and field z-BGPR travel time data made during an infiltration experiment. While the synthetic case primarily established the methodology, the field example helped show the practicality of the inverse procedure to real data. The ease by which the inversion procedure can obtain the hydraulic parameters was demonstrated through the error surface, which showed that the parameter $C$ is quite sensitive to the synthetically-derived first-arrival travel time data, and that $S$ can be obtained with reasonable confidence. For the field experiment, the antennae were fixed at 2.25 m bgs and the time series of first-arrival travel time data in Fig. 8 showed that there is a time during which critically refracted waves were the first to arrive. The linear increase in first arrivals during a brief segment of the experiment is similar to the model presented in Fig. 2A. Had critical refraction not occurred, the time series of first arrivals would look more like that of a buried point sensor measuring the water content (such as TDR). Furthermore, the z-BGPR has an advantage over point sensors by explicitly measuring the wetting front velocity with critical refraction. The linear slope of this portion of the curve produced a wetting front velocity of $1.1 \times 10^{-5}$ m/s, which was about one half of that observed on several nearby buried tensiometers and TDRs. The overestimation by the buried sensors could be due to a number of factors, such as preferential flow within the disturbed boreholes or an insufficient number of sensors to properly characterize the flow field. Alternatively, the underestimation of the velocity by z-BGPR could be due to inaccurate petrophysical relationships, model error (1D vs. 2D flow), or first-arrival travel time measurement errors. The wetting front velocity along with the water content before and after infiltration were used to obtain the wet hydraulic conductivity.

Finally, the z-BGPR data were used to help constrain the inversion model to obtain field values for $C = 1.011$ and $S = 0.00045 m/s^{1/2}$. A plot of modeled first arrival travel time overlain on measured first-arrival travel time shows that the two curves match quite well, with an error between the two curves defined by a root mean square error of 0.405. With $C$ defined, the relative hydraulic conductivity was plotted over a range of effective saturation values. To obtain the full description of the hydraulic conductivity function, a value of $K_s$ is needed, which may be obtained easily if the porosity (or saturated water content) is known beforehand. With a point on the hydraulic conductivity function defined by the slope of the first-arrival travel time data, the two parameters were shown to be related through a simple second order polynomial.