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Modeling unsaturated flow in a layered formation under quasi-steady state conditions using geophysical data constraints

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Abstract

The identification of vadose zone flow parameters and solute travel time from the surface to the water table are key issues for the assessment of groundwater vulnerability. In this paper we use the results of time-lapse monitoring of the vadose zone in a UK consolidated sandstone aquifer using cross-hole zero-offset radar to assess and calibrate models of water flow in the vadose zone. The site under investigation is characterized by a layered structure, with permeable medium sandstone intercalated by finer, less permeable, laminated sandstone. Information on this structure is available from borehole geophysical (gamma-ray) logs. Monthly cross-hole radar monitoring was performed from August 1999 to February 2001, and shows small changes of moisture content over time and fairly large spatial variability with depth. One-dimensional Richards' equation modeling of the infiltration process was performed under spatially heterogeneous, steady state conditions. Both layer structure and Richards' equation parameters were simulated using a nested Monte Carlo approach, constrained via geostatistical analysis on the gamma-ray logs and on a priori information regarding the possible range of hydraulic parameters. The results of the Monte Carlo analysis show that, in order to match the radar-derived moisture content profiles, it is necessary to take into account the vertical scale of measurements, with an averaging window size of the order of the antenna length and the Fresnel zone width. Flow parameters cannot be uniquely identified, showing that the system is over parameterized with respect to the information content of the (nearly stationary) radar profiles. Estimates of travel time of water across the vadose zone are derived from the simulation results.

Keywords: Cross-hole radar; Richards' equation; Monte Carlo simulations; Gamma logs; Sherwood Sandstone

1. Introduction

The characterization of vadose zone dynamics is of key importance to assess groundwater vulnerability to pollution. However, the unsaturated zone beyond a few meters from the surface is difficult to study using traditional hydrologic techniques (pore water sampling and hydraulic testing). Boreholes, the traditional method for accessing the subsurface, are of limited use for vadose zone characterization. As a consequence, non-conventional techniques are gaining popularity. Among these, a key role is played by geophysical methods since they provide information on the characteristics of the subsurface spatial structure ("static", or geological information) as well as on the fluid presence and motion ("dynamic", or hydrologic information). The most commonly applied techniques are: ground penetrating radar (GPR), both from the surface (e.g. [17,18]) and in boreholes (e.g. [14,29]); and electrical resistivity tomography (ERT), again in surface [19] and borehole [13] applications. Other techniques, such as high resolution seismics (e.g. [21,1]) are especially useful to investigate the subsurface geometry.

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In order to translate the geophysical data into information of hydrological use, two approaches can be adopted:

1. empirical relationships are sometimes used to link measurable geophysical quantities (e.g. electrical resistivity or permittivity) to hydrological parameters (e.g. hydraulic conductivity);
2. geophysical quantities are translated into hydrological quantities (e.g. moisture content or solute concentration) that are used in turn to calibrate hydrological models and determine hydrological parameters.

The first approach found early applications in the 1980s (e.g. [20]) with mixed results. Indeed, some of these early studies may have induced some hydrogeologists to be skeptical about the usefulness of geophysical methods, since the approach may be somewhat limiting due to the necessary assumptions [8].

The second approach is, in our view, conceptually and practically more robust and has the potential to provide quantitative hydrologic information. The "model calibration" approach recognizes that hydrological parameters are inherently defined by hydrological constitutive models (consider hydraulic conductivity and its link to Darcy's law) and cannot be measured, albeit indirectly, via techniques that are not based on the same physical–mathematical equations. On the other hand, hydrological quantities such as moisture contents are defined only in terms of mass and volume, and are more likely to find geophysical "proxys" based on the same elementary physical quantities. For example, dielectric properties depend directly on the soil moisture content (e.g. [28,25]).

The model calibration approach requires that parameters of the hydrologic model are inferred from geophysically derived hydrological quantities, i.e. from the values of the dependent variables. This is equivalent to saying that an "inversion" must be performed. Inversion requires (a) a forward model—that solves the relevant initial boundary value problem governing the physical phenomenon, and (b) an algorithm that explores the parameter space and either finds the "best" set of parameters and/or assesses how well such optimal parameters are identified. Note that it is not uncommon that many parameter sets can lead to fitting the data equally well ("equifinality" problem—see [2]).

The principal objectives of the work presented here are:

(1) To demonstrate the strengths and limitations of geophysical–hydrological data inversion for vadose zone characterization in a layered formation and under quasi-steady state infiltration conditions. This approach is applied to a well-characterized sandstone site (UK Sherwood Sandstone) where vertical layering is the prevailing feature controlling the vadose zone hydrological dynamics. The geophysical data used for this purpose are time-lapse cross-hole radar measurements and down-hole gamma logs.

(2) To investigate the spatial resolution of cross-hole radar measurements—the scale issue—in a layered formation. The layered structure observed at this site makes it an ideal environment for this assessment, since strong moisture content variations are expected across small vertical distances, unlike in other more homogeneous environments [3].

2. Site description

The field site discussed in this paper is located near Eggborough, North Yorkshire, UK, adjacent to a small sand quarry (UK National Grid Reference SE 570 232). The field site is one of two selected for detailed study of the vadose zone in the Sherwood Sandstone using cross-borehole geophysics. Recent papers [4–6] describe other elements of the research program which aims to utilize cross-borehole geophysical methods to improve models of vadose zone recharge dynamics.

Eleven boreholes were drilled at the Eggborough site during June 1999. The boreholes were drilled using 127 mm diameter tip rotary air-flush to a depth below the water table (≈17 m). Six of the boreholes (labeled R1, R2, R3, R4, A, B) were drilled for deployment of borehole radar. The other boreholes (E1, E2, E3, E4, C) were installed for DC resistivity measurements in both cross-hole and single-hole mode. In March 2000, a further radar borehole (labeled D) was drilled and cored by colleagues at Leeds University. Another borehole (R5) was cored in May 2003. Fig. 1 shows the layout of the boreholes at the site.

Hydraulic and geophysical analyses of core samples have been the focus of West et al. [31] and Pokar et al. [23]. From analyses of the cores, the sandstone sequence

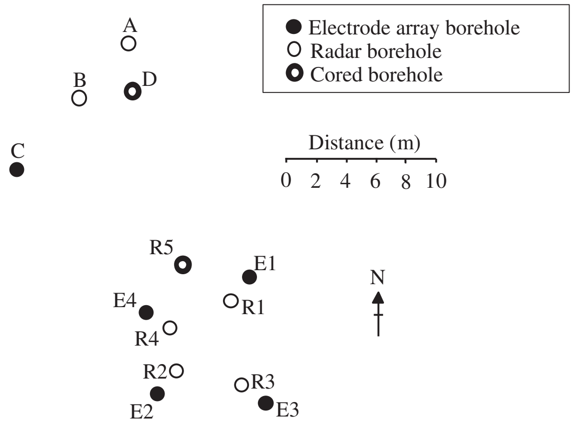

Fig. 1. Layout of borehole arrays at the Eggborough site.

at the site consists of fluvially derived fining upwards sequences 1–3 m thick, grading from medium grained to fine grained sandstone. The glacial drift cover (mainly gravels and cobbles in fine matrix) at the site is typically 1–2 m thick. Fig. 2 shows profiles of particle size characteristics derived from samples taken from core R5.

In each of the radar boreholes, a 76 mm diameter PVC casing was installed, surrounded by a sand/cement backfill. All boreholes (except E1 due to weakness of the borehole wall and thus possible collapse) were geophysically logged (using Mount Sopris natural gamma and 39 kHz electromagnetic conductivity sondes) prior to final completion. The layered sequence at the site is clearly evident from the cores and from the well logs.

3. Methodology

3.1. Geostatistical analysis of well logs

The natural gamma logs show further evidence of the layering in the sandstone. Fig. 3 shows examples of these logs from E3, R3, R4, E4 from which considerable horizontal correlation is apparent. The gamma logs show similar behavior to the particle size logs in Fig. 2: distinct layers (at least locally) are seen at depths of 4 m, 5.5 m, 8.5 m, 12 m and 14.5 m.

The high spatial density of boreholes within the plot permit analysis of spatial characteristics of the logged parameters, thus giving insight into the horizontal and vertical extent of lithological features. This geostatistical analysis is aimed at obtaining a stochastic description of the layering at the site. In order to perform such analysis the semi-variograms in the horizontal and vertical direction were computed, using logs from eleven boreholes. The gamma log semi-variograms of gamma log counts per second (cps) are shown in Fig. 4a. They show a geostatistical stationary (spatially homogeneous) behavior, with a well defined sill, particularly evident in the vertical semi-variogram for lags up to 8 meters. The horizontal semi-variogram is based on a considerably smaller dataset (11 boreholes), but the same large-scale sill as the vertical semi-variogram (roughly 80 cps^2) seems to be reached within the observed distance range (Fig. 4b). The experimental semi-variograms of gamma counts were matched with a semi-variogram model built with two nested structures: (1) a small scale exponential model with vertical correlation length equal to 0.35 m and sill equal to 55 cps^2; (2) a large scale Gaussian model with vertical correlation length equal to 1.5 m and sill equal to 22 cps^2. A horizontal/vertical anisotropy ratio equal to 8 was used to match both vertical and horizontal semi-variograms with the same nested model. A weak periodicity in the vertical semi-variogram ("hole" effect) is consistent with observations of a number of fining upwards sequences in the sandstone.

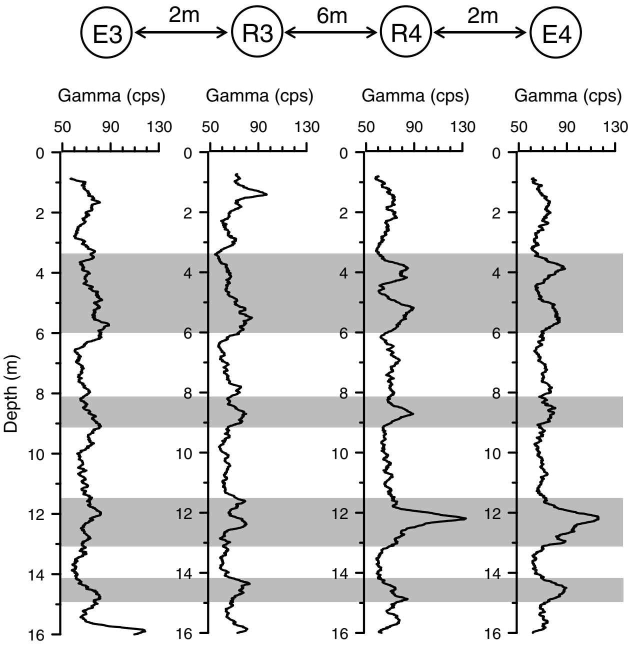

Fig. 3. Natural gamma logs from boreholes E3, R3, R4, E4 (surveys carried out June 1999). The horizontal bands indicate zones of relatively high gamma count (inferred layers of finer sandstone/siltstone).

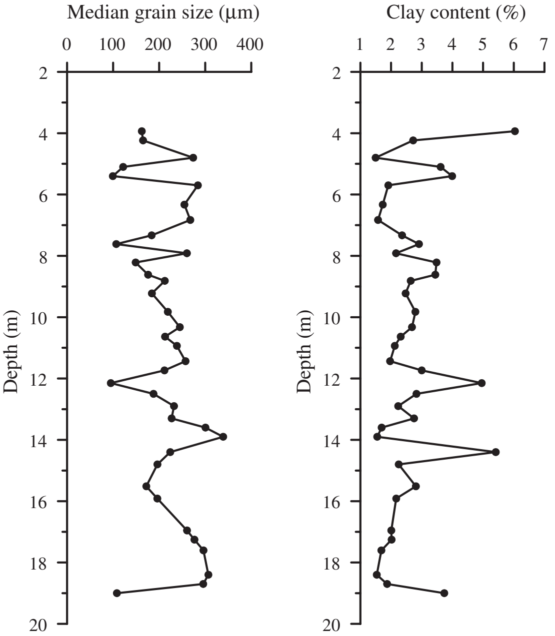

Fig. 2. Median particle size and clay fraction profiles for core R5.

3.2. Cross-hole radar

Hydrological dynamics at the Eggborough site has been monitored via time-lapse cross-hole ERT and

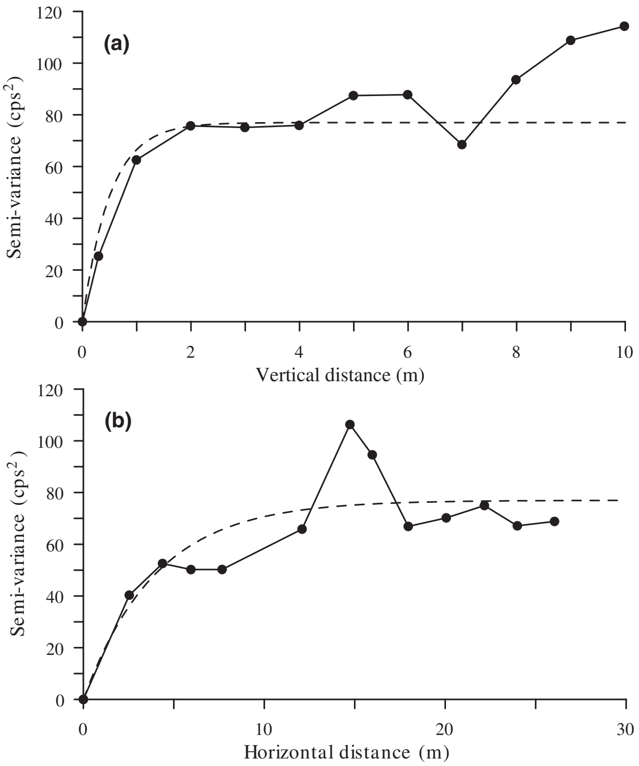

Fig. 4. Vertical and horizontal semi-variograms of natural gamma logs: solid lines with dots represent experimental data; dashed lines are model semi-variograms.

GPR. For this study, we focus on the use of radar data, since they are uniquely related to soil moisture content (see Section 3.3).

In order to determine changes in bulk dielectric properties at the Eggborough site, borehole-to-borehole radar surveys were conducted in a zero-offset transmission mode. This is achieved by keeping the transmitter and receiver at equal depth. By systematically lowering or raising the pair of antennae in the two boreholes it is possible to build up a one-dimensional profile of travel time over the entire borehole length. This type of borehole data acquisition is suitable for situations where the variations of physical properties in the subsurface are mainly in the vertical direction. Such is the case for infiltration-dominated moisture content distribution, as in the case presented herewith. In low loss materials and at high frequency, the relative permittivity, or bulk dielectric constant, κ [–] is derived from:

$$\sqrt{\kappa} = \frac{c}{v} \tag{1}$$

where c is the radar wave velocity in air ($\cong$0.3 m/ns), and v is the radar wave velocity in the medium.

Care must be taken to ensure that critical refraction at the soil/air interface does not produce the first arrival of energy at the receiver antenna. If such first arrival is mistaken for a direct wave through the soil, serious errors can be made in the estimation of soil dielectric properties [27]. In our case, first arrivals of the radar pulse were considered only at a depth greater than 3 meters below ground, were the occurrence of critically refracted first arrivals is unlikely. However, critical refractions could still occur at the interface between high and low velocity layers in the sequence [26].

3.3. Link between geophysical data and hydrologic quantities

The research site at Eggborough was developed to monitor changes in moisture content in the unsaturated zone and ultimately develop improved models of vadose zone flow dynamics. Cross-borehole radar measurements may be used to compute moisture content profiles as demonstrated by Binley et al. [4,6]. Such estimates are made on a much larger and more representative support volume, in comparison to conventional techniques, such as neutron probes and time domain reflectometry.

In order to describe the relationship between bulk dielectric constant (κ) and volumetric moisture content (θ) the complex refractive index method (CRIM) was used [25]. The CRIM model can be stated as

$$\sqrt{\kappa} = (1-\phi)\sqrt{\kappa_s} + \theta\sqrt{\kappa_w} + (\phi-\theta)\sqrt{\kappa_a} \tag{2}$$

where κ_s is the dielectric constant of the sediment grains, κ_w is the dielectric constant of water (assumed to be equal to 81), κ_a is the dielectric constant of air (assumed to be 1) and ϕ is porosity. West et al. [31] carried out measurements of dielectric properties at different levels of water saturation in cores samples extracted from this site. Based on these measurements we assume that $\kappa_s = 5$ and $\phi = 0.32$.

At the Eggborough site cross-borehole zero-offset radar profiles were measured on borehole pairs (R1, R2), (R3, R4) and (A, B) between 3 August 1999 and 20 February 2001 on 15 occasions at roughly regular intervals. The range of variation in moisture content over this period was approximately 0.05 [L^3/L^3] between 3 m and 5 m depth and less than 0.02 at depths beyond 5 m. Mean standard deviation over time is 0.69% (in moisture content), while mean standard deviation over space is 2.04% (in moisture content). Given such a low degree of variation over time (Fig. 5), a steady state vadose zone flow model was adopted. The steady state form of Richards' equation that governs flow in unsaturated porous media is

$$\frac{\partial}{\partial z}\left[K(h)\frac{\partial(h+z)}{\partial z}\right] = 0 \tag{3}$$

where z is elevation, h is pressure head and $K(h)$ is the unsaturated hydraulic conductivity.

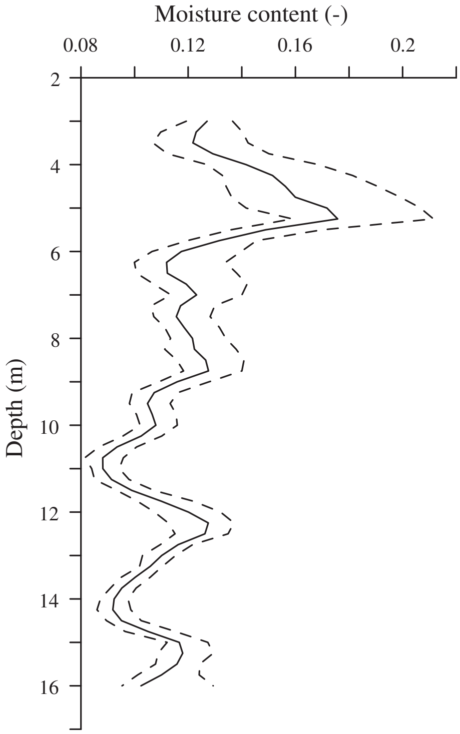

Fig. 5. Moisture content data derived from radar profiles at Eggborough between August 1999 and February 2001. Solid line indicates average profile, dashed lines show range.

The relationships $\theta(h)$ and $K(h)$ are commonly described by van Genuchten [30] and Mualem [22] parameterization:

$$\theta(h) = \theta_r + \frac{\theta_s - \theta_r}{[1 + |\alpha h|^n]^m} \tag{4}$$

$$K(h) = K_s S_e^{0.5}[1 - (1 - S_e^{1/m})^m]^2 \tag{5}$$

where θ_r [L^3/L^3] is the residual moisture content, θ_s [L^3/L^3] is the saturated moisture content, K_s is the saturated hydraulic conductivity [L/T], S_e is effective saturation [L^3/L^3] (=$(\theta - \theta_r)/(\theta_s - \theta_r)$), α [L^{-1}], m [–] and n [–] are parameters and it is often assumed that $m = 1 - 1/n$. Using such formulation, solution of Eq. (4) thus requires estimates of five parameters $(\theta_r, \theta_s, K_s, \alpha, n)$ for each soil type.

3.4. Richards' equation numerical model

By using the relationships described in the previous section, one can derive a profile of moisture content directly from a radar velocity profile. However, the interpretation of the derived moisture content profile requires further analysis to yield useful hydrological information. A rigorous approach requires that the radar-derived data are compared with the values predicted in space and time by a mathematical model based on Richards' equation. As previously discussed, the small variation of moisture content over time at Eggborough leads to simplifying the problem by solving a steady state model. At the upper boundary of the soil column we imposed a second type condition, corresponding to a net infiltration rate equal to 3.5×10^{-4} m/d, based on rainfall data and actual evapotranspiration estimates over the period of monitoring at the site. The lower boundary has been set at 17 m below ground level, with a first type condition corresponding to the water table.

The layer structure of the Eggborough site requires that the steady state model be capable of solving Eq. (3) in a heterogeneous domain, with sharp boundaries between material types, a non-trivial task. Two steady state models have been adopted, and the results compared:

(a) a model based on a finite difference discretization of Eq. (3) with line-search Newton–Raphson non-linear solver, developed in-house;
(b) the semi-analytical model (*ss_infil*) described by Rockhold et al. [24] that implements an integral solution for 1-D steady vertical water flow in layered soils with arbitrary hydraulic properties. For this model, the adopted $\ln K(h)$ function must be discretized in a number of piecewise-linear curve segments.

For both models a vertical discretization of 0.01 m was adopted (even though *ss_infil* could have adopted a variable space discretization, based on the material layering). The comparison of the model results, for a number of cases in the range of parameters adopted for the Eggborough site, has demonstrated the following:

- the finite difference code shows numerical oscillations in pressure head and moisture content around the material boundaries, especially in cases of strong parameter contrasts; this problem can be reduced by using a finer space discretization around those edges, at the price of an increased computational burden; the difficulties associated with solving the Richards' equation numerically are well known (e.g. [16]);
- the semi-analytical code does not show any numerical oscillation. However, the results are sensitive to the number of piecewise-linear curve segments used to discretize the $\ln K(h)$ function. If the number of segments is too small, the computed moisture content distribution with depth is substantially biased towards smaller values, as compared to the finite difference solution. The number of segments suggested by Rockhold et al. [24]—in the 1000 to 10,000 range—proved insufficient for the Eggborough case. The code had to be modified to handle 50,000

segments. Given this modification, the code proved to be robust, and much faster to run than the equivalent finite difference solution.

3.5. Monte Carlo simulations

The vertical layering observed at the Eggborough site requires that parameters for different materials be hypothesized, and that the spatial distribution of layers be inferred. Potentially both factors could be crucial when trying to match the observed moisture content profiles. At this stage a parsimonious approach was adopted, defining a small number of different materials, each characterized by a set of model parameters. Based on observations of cores from the site, the 17 m unsaturated profile was parameterized into two geometrical units: a top layer, 2 m thick, representing surface soil and drift cover and a 15 m thick sandstone unit. Observations at the site (consider Figs. 2, 3 and 5) show that modeling the sandstone as a uniform unit is inappropriate. Distinct layering is present, with fine sandstone intercalated in the medium sandstone. An attempt to run a steady state Richards' equation model under the assumption of a uniform sandstone unit produced results that clearly contradict observed behavior (Fig. 6).

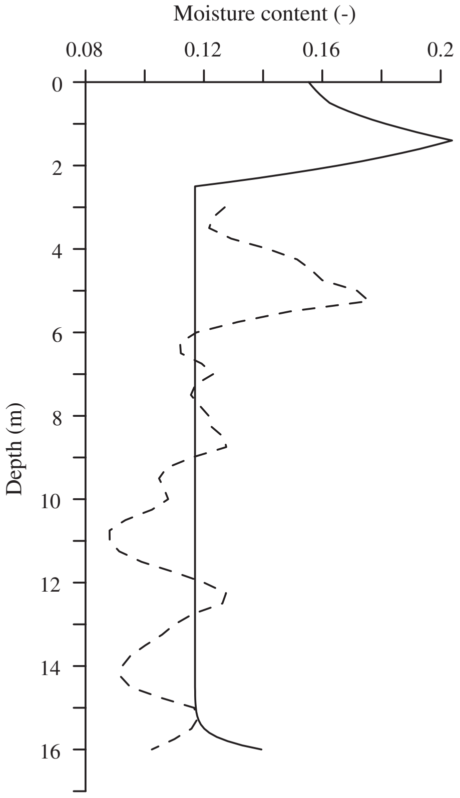

Fig. 6. Best simulation (solid line) assuming no layering and measured average moisture content profile (dashed line).

In order to incorporate layering within the Richards' equation model, we adopted the approach sketched in Fig. 7. The details of each step are:

Step 1: Adopting the sequential Gaussian geostatistical simulator (SGSIM from GSLIB—[15]) and the spatial correlation structure of the gamma logs (Section 3.1) a number of equally probable realizations of gamma counts in a soil column corresponding to the R3–R4 interwell location were generated.

Step 2: Based on a designated threshold (75 cps), the 17 m unsaturated sandstone was parameterized into layers of fine sandstone and medium sandstone. Such a threshold has been designated using core sample physical characteristics shown in Fig. 2. The soil column was thus discretized into three material types, one with fixed geometry representing the drift cover down to 2 m below ground level, the other two representing layers of medium and fine sandstone. Fig. 8 illustrates a sample of five geological realizations generated using the procedure above.

Step 3: For a given realization of 'geology', a series of Monte Carlo realizations of the five parameters in Eqs. (4) and (5) were created for each material. The parameters were selected randomly from a wide range of values consistent with observations in soils [11], UK Triassic sandstone [7] and a limited number of measurements made on core samples. The ranges used for the three material types were identical (Table 1).

Step 4: For each realization of geology and unsaturated flow parameters, a steady state Richards' equation simulation was run using *ss_infil*. The output from this model was then compared with the average moisture content profile observed between R3 and R4 using radar data over the 19 month period (Fig. 5). The goodness of fit was quantified using the efficiency measure:

$$\text{efficiency} = 1 - \frac{\sigma^2_{\text{error}}}{\sigma^2_{\text{data}}} \tag{6}$$

where σ^2_{error} is the error of fit variance, and σ^2_{data} is the overall data variance.

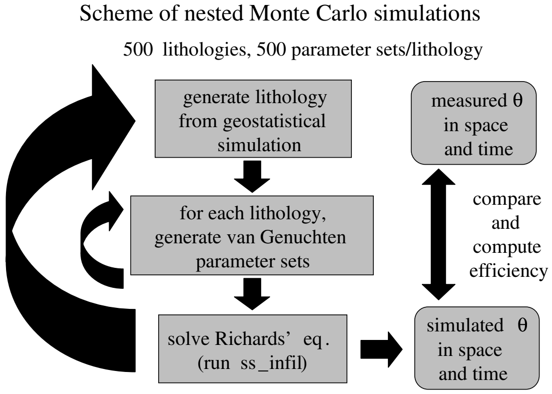

Fig. 7. Schematic of nested Monte Carlo procedure.

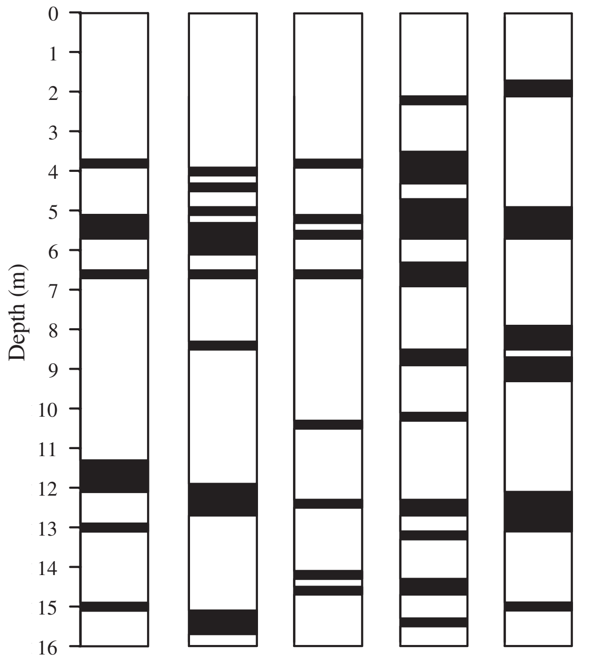

Fig. 8. A sample of five realizations of geological structure generated for the region between boreholes R3 and R4. The black zones represent gamma counts above the designated threshold and are used to zone the fine sandstone layers within the medium sandstone unit.

Table 1
Parameter ranges selected for the three material types

Parameter	Minimum	Maximum
K_s (m/d)	0.01	2.0
n (–)	1.5	2.5
α (m^{-1})	0.1	2.0
θ_s (–)	0.25	0.35
θ_r (–)	0.03	0.1

In principle, the net infiltration rate could have been varied within the Monte Carlo analysis. However, the net infiltration value is derived from field measurements and is much better constrained than the subsurface flow parameters. Consequently the net infiltration rate at the soil surface was maintained equal to 3.5×10^{-4} m/d for all simulations. Nevertheless it must be noted that some uncertainty in this rate may have marginally impacted the identification of saturated hydraulic conductivity of the subsurface layers.

The nested Monte Carlo search was conducted with 500 hydrological parameter realizations for each of 500 geological realizations.

4. Results and discussion

The Monte Carlo modeling helps identify both the value and the limitations of the data derived from cross-hole radar measurements. The most important issues are described below.

4.1. Scale of measurement

An obvious scale issue is inherent to the measurement of moisture content by using cross-borehole radar. Three factors must be considered:

(a) the borehole radar antenna have a finite size; for the 50 MHz measurements at the Eggborough site, the antenna length is approximately 2 m. It is reasonable to expect that the size of the measurement support volume is conditioned by the antenna size;

(b) the spatial resolution of cross-hole methods based on wave propagation is defined by the Fresnel volume [12,9]; this defines the averaging volume from which energy arrives in-phase to the receiver antenna; the paraxial approximation for Fresnel volume gives a maximal radius of the Fresnel volume equal to

$$r_{\max} = \frac{\sqrt{vL/f}}{2} \tag{7}$$

where v is the propagation velocity, L is the interwell distance and f is the signal central frequency. For the Eggborough dataset, v is on average 0.1 m/ns, L is about 6 m (R3–R4 distance), f is 50 MHz. Consequently, $r_{\max} \approx 1.7$ m, and the lowest resolution, midway between the boreholes, is two times such radius, i.e. 3.4 m;

(c) the propagation of radar energy does not occur necessarily along straight lines: refraction of energy occurs at interfaces between fast (dry) and slow (wet) zones, thus smearing the first arrival times and making the detection of sharp contrasts practically impossible. This phenomenon may cause some underestimation of the total moisture content along the profile [26].

In order to compare simulated and measured profiles of moisture content, these averaging factors must be accounted for. With no provision for such scale problem, the "best" simulated result has efficiency no better than 51%—see Eq. (6)—and the predicted moisture content variability, induced by layering, is much larger than observed in the field data (Fig. 9a). The simulated profiles have much sharper changes in moisture content than the field data seem to indicate. In order to reconcile field and model results, the scale of radar measurement was investigated by averaging the simulated data over moving windows of increasing vertical size. This is a simplified approach, but that lumps together at least the averaging factors (a) and (b) described above. Note that the method proposed by Rucker and Ferré [26] to correct for the phenomenon (c) is applicable only in presence of layers having a uniform moisture content. On the basis of the simulation results, this is not the case at the Eggborough site (Fig. 9a).

Window averaging has a strong impact on the simulated moisture content profiles, as shown in Fig. 9. The most striking consequence is dependence of the maximum efficiency value on the window size (Fig. 10). The maximum efficiency reaches a plateau between window sizes of 1 to 3 m, and decreases sharply for smaller and larger windows. This range of optimal window averaging is fully consistent with the measurement scales identified by antenna length (2 m) and Fresnel volume (⩽3.4 m).

4.2. Unsaturated flow parameter identification

The use of a stochastic (Monte Carlo) approach for the "inversion" of the moisture content data has an obvious advantage over more commonly adopted optimization techniques, such as ridge regression or least squares: the parameter space is fully explored and the equifinality issue made explicit.

In this study, all the unsaturated flow parameters of the three materials considered (15 parameters overall) are poorly identified. We present a few examples of plots of efficiency—computed according to Eq. (6)—versus parameter value in Fig. 11, where the efficiencies are computed with 2 m averaging windows (the cases of 1 m and 3 m are no different). The upper envelope of the dots cloud can be viewed as the 2 D projection of the objective function of an equivalent parameter identification based on optimization. Flatness of this objective function is an index of poor parameter identification, in that many different parameter combinations lead to nearly equivalent efficiency value. All 15 unsaturated flow parameters have very flat plots. Note that fairly high efficiency values (70% or higher) are reached, but this does not warrant a proper identification of parameters. Even parameter ratios (e.g. Fig. 11c) are not well identified.

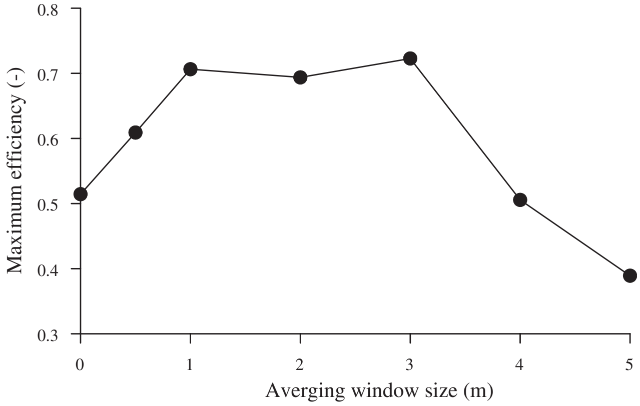

Fig. 10. Maximum efficiency versus averaging window size on simulated data.

The most likely reasons for this behavior are:

1. the quasi-steady state behavior of the moisture content profile does not induce sufficient hydraulic stress on the system to define the parameters: the most

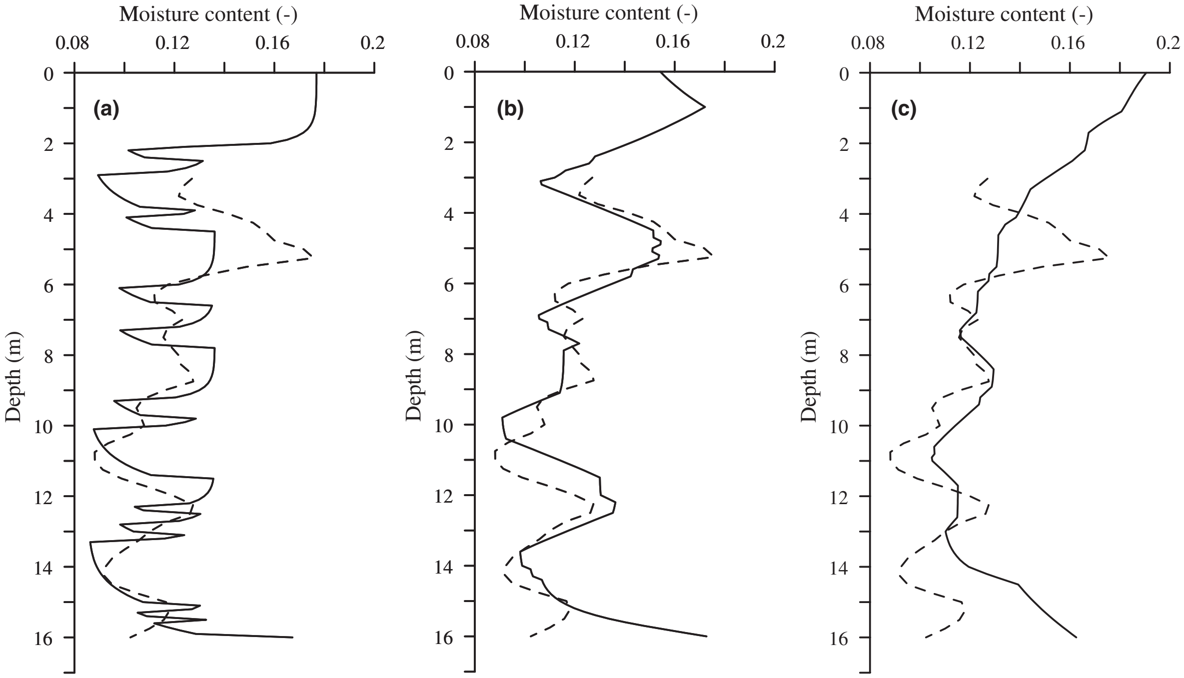

Fig. 9. (a) Best simulation with no window averaging and comparison with time-averaged data, (b) best simulation with vertical averaging window = 2 m, (c) best simulation with vertical averaging window = 5 m.

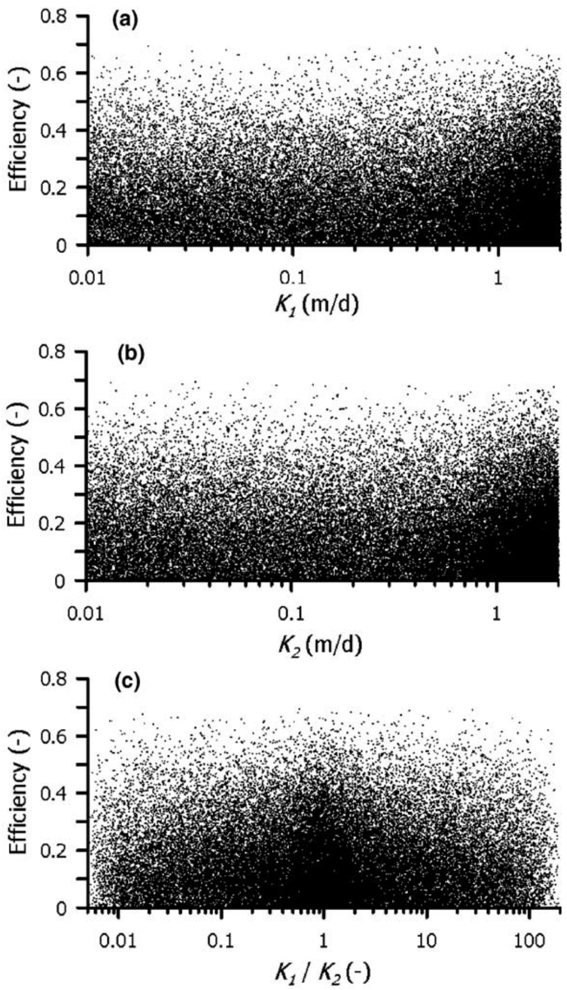

Fig. 11. (a) Efficiency of simulation results versus hydraulic conductivity of medium sandstone (K_1), (b) efficiency of simulation results versus hydraulic conductivity of fine sandstone (K_2), (c) efficiency of simulation results versus ratio of hydraulic conductivities of medium and fine sandstone (K_1/K_2). All results are plotted for the case with averaging window = 2 m.

obvious example is that the saturated moisture content (porosity) is not identifiable in a system that never reaches full saturation;

2. the strong stratification can easily lead to trade-offs between unsaturated flow parameters; for instance, a layer can have high moisture content because either (a) the layer itself has low hydraulic conductivity; or (b) the layer below has low hydraulic conductivity; or (c) the layer has high residual water saturation; or (d) the layer has a low α value or a low *n* value (i.e. high capillary rise), etc.;
3. the number of parameters is too high as compared to the information content of the data. To investigate this aspect, a Monte Carlo simulation limited to hydraulic conductivities only has been attempted (500 hydrological parameter realizations for each of 500 geological realizations), but the efficiency values obtained are far lower, thus demonstrating that a good fit with field data requires combinations of governing parameters.

We recognize that even with 250,000 realizations our search in the parameter space is somewhat limited. Furthermore, each set of hydraulic parameters for each of the three material types were generated from uncorrelated uniform distributions. It is likely that correlation between parameters is significant but no a priori information is available on samples from this site.

4.3. Analysis of vertical travel time

One of the goals of this project was to assess the travel time of water, and consequently of dissolved pollutants, across the Sherwood Sandstone to the water table. This travel time is an important parameter for describing aquifer vulnerability to pollution. Given the time-averaged moisture content profile $\theta(z)$ assessed via cross-hole radar measurements for depth z between 0 and $z_{\max}$, and given an estimate of the net mean annual precipitation q, it is straightforward to compute the corresponding travel time as

$$t_{\text{travel}} = \frac{1}{q}\int_0^{z_{\max}} \theta(z)\,\mathrm{d}z \qquad (8)$$

However, this approach assumes that $\theta(z)$ is the actual moisture content profile, while the estimate of $\theta(z)$ derived from cross-hole radar is a spatially averaged version of the actual profile, as previously discussed.

In order to evaluate the impact that scale effects have on the estimation of travel time, the results of Monte Carlo Richards' equation modeling were used. Fig. 12 shows the plot of efficiency (computed using an averaging window of 2 m) versus travel time (computed on the corresponding non-averaged simulated moisture content profiles) across the Sherwood Sandstone (from 3 m to

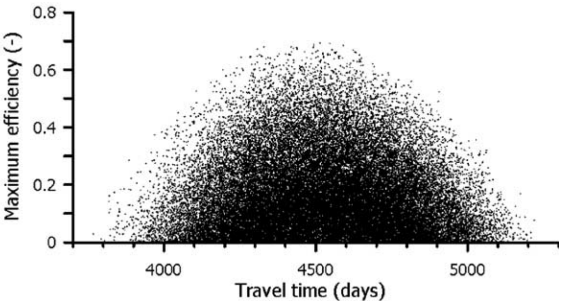

Fig. 12. Efficiency versus travel times across the unsaturated Sherwood Sandstone at the Eggborough site (from 3 m to 17 m below ground level). Travel times are computed on the simulated non-averaged moisture content profiles, while efficiency values have been obtained using a vertical averaging window size equal to 2 m.

17 m below ground level, i.e. to the water table). Very similar plots are obtained using averaging windows of 1 m and 3 m. According to the results in Fig. 12, an estimate of the average water infiltration velocity across the 17 m of unsaturated Sherwood Sandstone at the site is roughly 300 d/m.

5. Conclusions

The analysis presented in this paper aims at demonstrating strengths and weaknesses of zero-offset cross-borehole radar profiles as a means to derive moisture content information in the deep unsaturated zone, and understand its dynamics. The specific application scenario is that of a weakly consolidated sandstone (Sherwood Sandstone) from the UK.

The principal tool applied in the analysis is numerical modeling in a stochastic (Monte Carlo) fashion. The quasi-stationary nature of the data derived from the site under investigation allowed us to utilize steady state models; however, the procedure can be generalized to transient Richards' equation models.

We generated conditional stochastic realizations of possible lithology sequences (derived from well logs) and random sets of unsaturated flow parameters for the materials considered. Comparison between simulated and measured moisture content profiles is the key to the analysis. We purposely decided not to adopt an optimization approach that could have led to identifying a single ''best'' set of parameters to fit the moisture content data. In fact, the full investigation of the parameter space is necessary in order to assess properly the limitations of the method.

A few key aspects have been identified:

1. In order to compare measured and simulated moisture content data, it is essential to assess properly the scale of radar measurements. This is governed by (a) the antennae size, (b) the Fresnel volume, and (c) the refraction of radar energy into faster (dry) zones. We demonstrated that, for our purposes, a simple window averaging of simulated data is sufficient to homogenize field data and simulations. The optimal averaging window size is in the range expected from theory.
2. The unsaturated flow parameters are not individually constrained by the quasi-stationary data at hand. Under dynamic conditions (for instance induced by an artificial tracer injection) the same approach could lead to a meaningful parameter estimation [10].
3. The identification of flow parameters is, however, not necessary in order to derive an estimate of travel time across the model or across the formation of interest; the value derived for the unsaturated Sherwood Sandstone is roughly 300 d/m.
4. The importance of acquiring independent information on the geology of the subsurface (here from well logs) cannot be overstressed. No meaningful analysis could have been conducted at the site under consideration without knowledge of the characteristics of its layered structure.

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