A model for flow in the Chalk unsaturated zone incorporating progressive weathering

A. M. Ireson * S. A. Mathias H. S. Wheater A. P. Butler

Department of Civil and Environmental Engineering, Imperial College London, UK

J. Finch

Centre for Ecology and hydrology, Wallingford, UK

Abstract

Groundwater from unconfined chalk aquifers constitutes a major water resource in the UK. The unsaturated zone in such systems plays a crucial role in the hydrological cycle, determining the timing and magnitude of recharge, and the transport and fate of nutrients. However, despite more than three decades of study, our physical understanding of this system is incomplete. In this research, state of the art instrumentation provided high temporal resolution readings of soil moisture status, rainfall and actual evaporation from two sites in the Pang and Lambourn catchments (Berkshire, UK), for a continuous two year period (2004/5). A parsimonious, physically based model for the flow of water through the Chalk unsaturated zone, including a novel representation of the soil and weathered chalk layers, was developed. The parameters were identified by inverse modelling using field measurements of water content and matric potential. The model was driven by rainfall and evaporation data, and simulated fluxes throughout the profile (including the discrete matrix and fracture components), down to the water table (but not the water table response). Results showed that the model was able to reproduce closely the observed changes in soil moisture status. Recharge was predominantly through the matrix, and the recharge response was strongly attenuated with depth. However, the activation of fast recharge pathways through fractures in the Chalk unsaturated zone was highly sensitive to rainfall intensity. Relatively modest increases in rainfall led to dramatically different recharge patterns, with potentially important implications for groundwater flooding. The development and migration of zero flux planes with time and depth were simulated. The simulations also provided strong evidence that, for water table depths greater than 5 m, recharge fluxes persist throughout the entire year, even during drought conditions, with important implications for the calculation of specific yield from baseflow estimates and the representation of recharge in groundwater models.

Key words: Chalk; Groundwater recharge; Richards equation; Unsaturated zone; Weathered rock; Zero flux plane

---

Nomenclature

C	specific capacity, [m^{-1}]
h	hydraulic head, [m]
K	hydraulic conductivity, [m/d]
K_r	relative hydraulic conductivity, [-]
K_s	saturated hydraulic conductivity, [m/d]
L	Conductivity exponent parameter, [-]
L_{rd}	depth above which 63 % of root density is located, [m]

* Corresponding author. E-mail address: andrew.ireson@imperial.ac.uk. Telephone: +44 (0)20 75946120

OF_1 objective function for calibration of $\theta(\psi, z)$ relationship, [-]

OF_2 objective function for calibration of $K(\psi)$ parameters, [-]

q Darcian velocity, [m/d]

r pore radius, [m]

r_d root distribution function, [-]

r_s Feddes root stress function, [-]

S sink term in Richards' equation, [d^{-1}]

S_s specific storage, [m^{-1}]

S_e effective saturation, [-]

$S_{e,1}$ effective saturation related to parameter ψ_1, [-]

$S_{e,2}$ effective saturation related to parameter ψ_2, [-]

t time, [d]

w_f fracture domain volume fraction, [-]

$w_{f,0}$ fracture domain volume fraction at the ground surface, [-]

$w_{f,\infty}$ fracture domain volume fraction in the deep Chalk, [-]

z depth below groundlevel, [m]

Z_α CUZ model shape parameter, [m^{-1}]

Z_β CUZ model shape parameter, [m]

α general relative hydraulic conductivity model parameter, [-]

β general relative hydraulic conductivity model parameter, [-]

θ volumetric moisture content, [m^3/m^3]

θ_s saturated water content, [m^3/m^3]

θ_r residual water content, [-]

σ Kosugi parameter, [m]

ψ pressure head, [m]

ψ_0 Kosugi parameter, [m]

ψ_1 modified Kosugi model parameter, [m]

ψ_2 modified Kosugi model parameter, [m]

$\psi_{1,\infty}$ modified Kosugi model parameter in the deep Chalk, [m]

$\psi_{0,\infty}$ modified Kosugi model parameter at the ground surface, [m]

ψ_{an} matric potential threshold for anaerobiosis , [m]

ψ_d matric potential below which plant water stress begins, [m]

ψ_w wilting point, expressed as a matric potential, [m]

1 Introduction

The importance of Chalk aquifers as a water resource in north west Europe (specifically in the UK, northern France, northern Germany and Belgium, Downing et al., 1993; Kloppmann et al., 1998; Brouyère et al., 2004; Pinault et al., 2005) and as a potentially significant hydrological pathway for contaminants in Israel (Nativ and Nissim, 1992; Nativ et al., 1995; Dahan et al., 1998, 1999) is well established. This paper focuses on a Chalk catchment in south east England where Chalk aquifers represent approximately 80% of total water supply (Downing, 1998). In this region much of the Chalk is overlain by a thick unsaturated zone which can be in excess of 100 m (Jackson et al., 2006).

The need for a good hydrological understanding of the Chalk unsaturated zone (CUZ) is well recognised, as it is the main control for aquifer recharge (Ragab et al., 1997; Bradford et al., 2002; Ireson et al., 2006; Lee et al., 2006), contaminant transport (Haria et al., 2003; Jackson et al., 2006, 2007; Mathias et al., 2005, 2006, 2007; Gooddy et al., 2007) and groundwater flooding (Jacobs, 2006; Pinault et al., 2005). Chalk comprises a fine-grained porous matrix (high porosity 20-45%, low permeability $< 10^{-2}$ m/day) intersected by a fracture network (low porosity <2%, higher permeability $> 10^{-2}$ m/day) (Price et al., 1993). Conceptual models of how water and solutes move through the CUZ have evolved over past decades (Smith et al., 1970; Wellings and Bell, 1980; Price et al., 1993, 2000). In unsaturated conditions pore water pressure is sub-atmospheric. Hence the fractures and matrix may be partially saturated and hydraulic pathways within and between these may be restricted/discontinuous. Wellings and Bell (1980) suggested that the fractures become activated when the matric potential exceeds a threshold of -0.5 m. Price et al. (2000) proposed that, in addition to providing a flow pathway, water held by capillary tension on fracture walls could be an important means of storing and supplying water to groundwater. Such conceptual models can be tested using mathematical models to reproduce field observations. The first mathematical models of the CUZ focused on solute transport and assumed steady state flow (Young et al., 1976; Oakes, 1977; Oakes et al., 1981; Barker and Foster, 1981). More recently, there has been an increased interest in transient flow models based on Richards' equation (Mathias et al., 2006; Brouyère, 2006; Van den Daele et al., 2007).

Mathias et al. (2006) considered a flow and transport model comprising of a 1D fracture coupled to a 2D matrix block. Flow in the fractures and matrix was described by Richards' equation. Parameters describing the matrix were obtained from the mercury intrusion data (Price et al., 2000). Fracture parameters were inferred from hydraulic conductivity – matric potential relationships observed in the field (Wellings, 1984; Hodnett and Bell, 1990; Cooper et al., 1990; Mahamood-ul-Hassan and Gregory, 2002). In order to reproduce solute profiles which were consistent with previous experimental observations (Smith et al., 1970; Oakes et al., 1981; Barraclough et al., 1994) it was necessary to attentuate the input of rainfall, by means of a soil layer. The importance of the soil layer as a control on flow in the CUZ had previously been postulated by Cooper et al. (1990).

Mathias (2005, p. 87) demonstrated that if the temporal resolution of the driving rainfall data is daily or coarser, the time for pressure equilibrium between the fractures and matrix becomes negligible. Consequently, if solute transport is not considered, flow in the unsaturated Chalk can be represented using the equivalent composite medium (ECM) approach of Peters and Klavetter (1988). Richards' equation is solved as for a single porous medium, but the hydraulic properties (i.e. relationships of water content, θ, hydraulic conductivity, K, and specific storage, C, with matric potential, ψ) are defined for both domains. The same approach was applied to the CUZ of the Hesbaye region in Belgium by Brouyère (2006). The main difference was that whereas Mathias (following Peters and Klavetter, 1988), obtained composite hydraulic properties by summing the volume averaged characteristics for each domain, Brouyère defined a threshold matric potential, ψ_j, below which the medium is defined by matrix properties, and above which it is defined by fracture properties. This difference is merely practical – both models could be used to obtain an identical result, albeit with different parameter values.

Van den Daele et al. (2007) used a modelling package called MACRO (Larsbo et al., 2005), under the assumption that chalk fractures are analogous to soil macropores and the chalk matrix is analogous to the soil matrix. Flow in the matrix was controlled by Richards' equation, whereas flow in the fractures was represented by the kinematic wave equation; thus assuming that capillary effects in the fracture domain are negligible. Van den Daele et al. (2007) applied this model to the Fleam Dyke lysimeter in Cambridgeshire. The 5 m deep lysimeter contained a 20 cm soil layer overlying weathered chalk which gradually blended into undisturbed chalk at the base. To accommodate this vertical heterogeneity, 5 discrete layers were considered, including a soil layer, weathered chalk layers and an undisturbed chalk layer. The model was calibrated against two years of θ, ψ and drainage flux data. However, the range of $\theta(\psi)$ data for the undisturbed chalk (see their Figure 2) appears to be unsuitable to adequately parameterise a soil moisture characteristic relationship (a problem explicitly acknowledged by Cassiani and Binley, 2005, see their discussion of unsaturated flow parameter identification). It was noted that the weathered chalk layers were even harder to characterise. The model was unable to simulate the observed matric potential data (see their Figure 4) although it did exhibit good correspondence with the observed water content and drainage flux data.

The use of a kinematic wave in this context essentially represents a simplifying assumption, which is made because of the general problem of a lack of information concerning the hydraulic properties of the fractures/macropores close to saturation (Larsbo et al., 2005). However, this assumption is deemed unnecessary in this study where a high quality field dataset is available to parameterise the fracture properties. Furthermore, there is a well established precedent for using Richards' equation to represent unsaturated fracture flow in fractured rocks as a whole (Wang and Narasimhan, 1985; Peters and Klavetter, 1988; Kwicklis and Healy, 1993; Gerke and van Genuchten, 1993, 1996; Liu et al., 1998, 2003; Doughty, 1999).

The three studies described above illustrate an increasingly more sophisticated representation of near surface properties: a decoupled soil layer (Mathias et al., 2006); a coupled discrete soil layer (Brouyère, 2006); a multi-layered approach which represents both soil and weathered Chalk (Van den Daele et al., 2007). We seek to improve on these by accounting for soil and weathered chalk overlying consolidated rock using continuous functions to describe the vertical variations in physical and hydraulic properties, using the ECM approach (Mathias, 2005; Peters and Klavetter, 1988). The model will be conditioned and tested against observed field hydrological data, and techniques to assess parameter identifiability and model uncertainty (similar to those used by Cassiani and Binley, 2005) will be applied.

2 The field monitoring scheme

In this study, we exploit data from an extensive set of instrumentation installed in the Pang and Lambourn catchments (Berkshire, UK) during the LOCAR programme (an overview of which is given by Wheater et al., 2006). In particular, we focus on data from two field sites where there is a deep CUZ above the unconfined Chalk aquifer: West Ilsley (WI) and Warren Farm (WF) (see Ireson et al., 2006, for detailed site descriptions). These sites are located on the Seaford Chalk formation, where marl bands are rare, but flint nodules may be present, and this is overlain by a very shallow soil layer. Frequent measurements of soil moisture status (θ and ψ) were taken over a range of depths down to 3 m, along with measurements of water table response, rainfall and actual evaporation. Discussion of the instrumentation was provided by Ireson et al. (2005) and the data were analysed in detail by Ireson et al. (2006). In this study, we focus on the following aspects of the data:

- Coincident (in time and depth) readings of θ and ψ are used to construct observed soil moisture characteristic relationships at four depths (0.2, 0.4, 0.6 and 1.0 m), which are then used to optimise a number of model parameters;
- Rainfall and actual evaporation data are used to drive the model, applied at the upper boundary and over the rooting depth, respectively;
- Time series of observed θ and ψ data at various depths ($\leq$3 m) are used to optimise the remaining model parameters (data from 2004), and to gauge the model performance (data from 2005).

The water table response is influenced by both drainage from the unsaturated zone and lateral flow processes in the saturated zone. Therefore the observed water table response cannot by reproduced by a one-dimensional model, but can be used to draw inferences about model performance and system behaviour.

3 CUZ model development

3.1 Conceptualisation of the profile

Figure 1 shows photographs of the upper 2.4 m of the unsaturated zone at West Ilsley. These show major changes in the structure and composition of material in the profile over this depth. In the upper 0.2 m is a soil layer, below which there is chalk which becomes progressively less weathered with increasing depth. The objective of this study is to develop a physically realistic representation of these changing properties in a continuous, progressive and parsimonious manner. The progressive nature of these changes is evident from the statistical properties of the neutron probe θ data in Figure 2. Plant water uptake will strongly affect the water content in the upper 0.2 m. Below this it is reasonable to associate the degree of variation of θ at each depth with the volume of the fracture domain, under the assumption that since the matrix will generally remain saturated by capillary forces (Price et al., 1993), any changes in water content occur in the fractures. Similarly, the trend in the minimum water content can be associated with the volume of the matrix, assuming that under these conditions the matric potential would be too low for the fractures to hold water, yet higher than the air entry pressure of the matrix (i.e. the matrix is saturated). On this basis it is assumed that as we approach the surface the proportion of rock which is comprised of matrix will reduce, whilst that which is fractures will increase.

As well as the changes in the relative proportions of each domain, if we are to represent the soil layer using properties which are scaled as a function of depth, the hydraulic properties of one or both of the domains must also be modified. Weathering of the Chalk is conceptualised here as enhanced fracturing of the matrix, with the properties of the intact matrix blocks remaining unchanged. Therefore, it is proposed that the fracture pore size distribution should be progressively modified as a function of depth, whilst the matrix pore size distribution be kept constant. In this way, the material in the near surface comprises relatively small, porous matrix blocks, surrounded by fractures and soil macropores which constitute the fracture domain. In the consolidated Chalk the fracture domain is made up of a number of discrete and visible fractures (with fracture apertures of the order of 30 μm, Wellings, 1984). In summary, the qualitative conceptualisation of the CUZ profile is characterised by the following changes as we approach the surface:

(1) A reduction in the proportion of the domain taken up by the matrix
(2) An increase in the proportion of the domain taken up by the fractures
(3) The fracture pore size distribution is modified such that there are more fractures, with a wider range of apertures
(4) The matrix pore size distribution is unchanged

It is intended that this conceptualisation be applied to the entire unsaturated chalk profile, from the water table up to the ground surface, including the soil layer in the top 0.2 m. The physical basis for the extrapolation beyond the weathered chalk and into the soil is questionable. However, the advantages of doing this are considerable, including the elimination of a sharp, artificial discontinuity in the hydraulic properties where the soil meets the chalk, and a potentially significant reduction in the number of parameters required to characterise the entire profile. It is further assumed that there are no significant lithological features (such as marl bands) or karst features (such as those described by Allshorn et al., 2007) in the CUZ, which would significantly complicate the recharge processes. This assumption is not unreasonable at the chosen field sites.

3.2 Quantitative representation of the profile

The CUZ model requires parametric relationships for $\theta(\psi)$, $C(\psi)$ and $K(\psi)$ for both the matrix and the fracture domains, which can be modified as a function of depth in order to achieve the four characteristics identified above. Formulae have been proposed (Kosugi, 1994, 1996) which explicitly relate hydraulic properties to pore size distributions, based on the assumption that the pore radii are lognormally distributed and inversely proportional to the negative pore capillary pressure. In this study the two parameter Kosugi model (Kosugi, 1996) (hereafter referred to as the KS model) is adopted, as defined by items 5 to 8 in Table 1, where θ_r [-] and θ_s [-] are the residual and saturated water content, respectively, ψ_0 [L] is the mode pore capillary pressure, σ [L] is the standard deviation of the $\ln(\psi)$ distribution, K_s [LT^{-1}] is the saturated hydraulic conductivity and L [-] is a free parameter, referred to here as the conductivity exponent, whose value may be positive or negative (Mualem, 1976; Schaap and Leij, 2000). An investigation of different possible forms of the hydraulic conductivity relationship was performed, which is described in Appendix A. Based on the results, a non-conventional form of the general relationship for hydraulic conductivity (Hoffmann-Reim et al., 1999; Kosugi, 1999) was adopted (given by item 8 in Table 1, which can be compared to the Mualem form presented by Kosugi, 1996).

A useful feature of the KS model is that the parameters (ψ_0 and σ) can be obtained analytically from any two known points on the $S_e(\psi)$ curve. Hence the model can be defined by arbitrarily selecting two effective saturation values, $S_{e,1}$ and $S_{e,2}$, and defining the pore capillary pressure at these points, ψ_1 and ψ_2, which are treated as the new model parameters. Given that $S_{e,1} = 0.5 + 0.5\text{erf}(-x_1/\sqrt{2})$ (Equation 5 in Table 1), it follows that $x_1 = -\sqrt{2}(\text{erf}^{-1}[2S_{e,1} - 1]) = \ln(\psi_1/\psi_0)/\sigma - \sigma$ (and likewise for $S_{e,2}$ and x_2). After some further manipulation it can be shown that σ and ψ_0 can be found from items 3 and 4 of Table 1.

Both the matrix and the fracture domains require six parameters. Bulk properties are obtained by summing the volume averaged properties of each domain, as in items 9 to 11 of Table 1, where w_f is the fracture domain volume fraction (i.e. the volume of the fracture domain over the total volume, after Gerke and van Genuchten, 1993) and the superscripts f and m refer the fracture and matrix domains respectively. The fracture domain porosity is taken to be 100 % (i.e. the fracture domain is a void), so $\theta_s^f = 1.0$. The matrix domain volume fraction is given by $1 - w_f$. Therefore, the basic model structure consists of 13 parameters (6 KS parameters for each domain, plus w_f). The next step is to introduce vertical heterogeneity into the model, by scaling some of the parameters as a function of depth, consistent with the qualitative conceptualisation of the profile, developed above.

In order to scale the size of each domain as a function of depth, z, (the first two scaling objectives above), a relationship for $w_f(z)$ must be established. It is proposed to use an s-shaped curve to achieve this, as shown in Figure 3a, which is defined by item 2 of Table 1, and requires four parameters: w_f as $z \to 0$, w_f as $z \to \infty$ and two 'shape' parameters (Z_α and Z_β).

The modification of the fracture pore size distribution with depth (the third scaling objective above), can be achieved by scaling either or both of the parameters ψ_1^f and ψ_2^f. It was decided that ψ_2^f, the matric potential at which the fracture domain is 95% saturated (i.e $S_{e,2} = 0.95$), would be uniform with depth, and ψ_1^f, the matric potential at which the fracture domain is 5% saturated (i.e $S_{e,2} = 0.05$), would reduce with increasing depth (see Figure 4). The effect on the fracture aperture size distribution is that larger fracture apertures remain uniform with depth, whilst the number of smaller apertures (caused by weathering) increases nearer to the surface. Thus in the consolidated Chalk the fractures are not active until a certain (relatively high) matric potential threshold is reached (as in the conceptualisation of Wellings, 1984), whilst in the near surface, the fractures can play a significant role (representing the macroporous structure of the soil) at lower matric potentials. ψ_1^f was scaled as a function of depth in the same manner as w_f, that is, using a four parameter s-shaped curve, given in item 1 of Table 1, and demonstrated in Figure 3b. The parameters include ψ_1^f as $z \to 0$, ψ_1^f as $z \to \infty$ and, to minimise the total number of parameters, the same two 'shape' parameters, Z_α and Z_β, as above.

The scaling of w_f and ψ_1^f requires an additional 4 parameters, which means that the model now requires the specification of 17 parameters. Although this appears substantial, it is worth noting that an equivalent model, which treats the soil/weathered chalk as a single discrete layer overlying homogeneous consolidated chalk would require significantly more parameters. For example, the model of Mathias et al. (2006) employs 20 parameters for the Chalk, 6 parameters to describe the soil and one additional parameter to specify the soil depth, i.e. 27 parameters in total.

3.3 Additional model details

The movement of water in unsaturated porous materials, due to gravitational and capillary forces, can be described using Richards' equation (Richards, 1931). In order to achieve good numerical stability for a range of unsaturated and saturated conditions, the form of Richards' equation advocated by Tocci et al. (1997) was selected as the governing equation:

$$\left(C(\psi) + S_s S_e(\psi)\right)\frac{\partial \psi}{\partial t} = \frac{\partial}{\partial z}\left(K(\psi)\left(\frac{\partial \psi}{\partial z} - 1\right)\right) + S \tag{1}$$

subject to initial and boundary conditions:

$$\begin{aligned}
&\psi = \psi_i(z), && 0 \le z \le z_N, && t = 0 \\
&K(\psi)\left(\frac{\partial \psi}{\partial z} - 1\right) = q_0(t), && z = 0, && t \ge 0 \\
&\psi = 0, && z = z_N, && t \ge 0
\end{aligned} \tag{2}$$

where the soil hydraulic properties are found using the system of equations in Table 1, S is the sink term which accounts for transpiration losses in the root zone (described below), and S_s [L^{-1}] is the specific storage. Strictly speaking parameter values of S_s should be defined separately for the fracture and matrix domains. However, taking base values of $S_s^f = 10^{-5}$ m^{-1} and $S_s^m = 10^{-6}$ m^{-1} (Mathias et al., 2006), a sensitivity study varing these parameters over two orders of magnitude found them to be insensitive, and therefore the base values were taken. The governing equation is applied to a one dimensional profile extending from the ground surface ($z = 0$) to just below the water table ($z = z_N$). It is solved numerically using the method of lines, with a block centred finite difference grid in space, integrated in time using the ordinary differential equation solver, ODE15s, available in MATLAB. Initial conditions, $\psi_i(z)$, were obtained from observations in the top 4 m, and assuming that below this ψ increases linearly with depth to a value of zero at the water table. As it is not possible to reproduce the water table response with a one-dimensional model of the unsaturated zone, a fixed water table boundary condition was used at the lower boundary, which was located just below the lowest observed water table level. A sensitivity study indicated that over a range of water table depths from 40 to 75 m, the simulated flux above the water table was insensitive to the fixed water table elevation, which gives us some degree of confidence in the use of this assumption when using the CUZ model to simulate recharge patterns.

For the Chalk, it is typically assumed that there is no surface runoff, due to the high infiltration capacity of the medium (Smith et al., 1970; Foster, 1975). Therefore, we can disregard the potential for ponding to occur during high intensity rainfall, and hence deal with rainfall as a straightforward specified flux boundary condition at the top of the profile.

Actual evaporation, AE, was calculated as the residual of the surface energy balance using measurements of sensible heat flux by eddy correlation, net radiation and soil heat flux over grass, at Warren Farm (a similar procedure was applied by Roberts et al., 2005). There is no way to partition the AE between evaporation (from the soil surface or interception) and transpiration, so it was assumed that all AE comes from transpiration (i.e. all rainfall enters the soil, and all AE is extracted from the soil via the plant roots). The distribution of uptake from the soil was determined using a modified version of the Feddes et al. (1976) root extraction function. The method is based on the root distribution over depth, $r_d(z)$ and a plant water stress function, $r_s(\psi)$, given by (Feddes et al., 1976)

$$r_s(\psi) = \begin{cases} 0, & \psi > \psi_{an} \\ 1, & \psi_{an} \geq \psi > \psi_d \\ 1 - \dfrac{\psi - \psi_d}{\psi_w - \psi_d}, & \psi_d \geq \psi > \psi_w \\ 0, & \psi_w \geq \psi \end{cases} \tag{3}$$

where ψ_{an}, ψ_d and ψ_w are water stress thresholds, assumed to have values of -0.5 m, -4 m and -150 m respectively. It is assumed here that the plant roots are exponentially distributed with depth, such that

$$r_d(z) = \frac{\exp(-z/L_{rd})}{L_{rd}} \tag{4}$$

where L_{rd} is the depth above which 63% of plant root density is located, and is taken to be 0.2 m. To ensure the total volume of AE was removed from the soil, the water stress function was normalised, and hence the sink term at a given depth and matric potential, $S(\psi, z)$, is found from:

$$S(\psi, z) = \frac{r_s(\psi) r_d(z)}{\int_0^{L_r} r_s(\psi) r_d(z) dz} .AE \tag{5}$$

3.4 Parameter identification

Of the 17 model parameters, some are amenable to laboratory investigation (e.g. parameters associated with the chalk matrix, which can be obtained from core samples) and some are insensitive. The remaining parameters are associated with the fracture aperture distribution and the nature of the soil and weathering at a particular site and hence require optimisation. Table 2 summarises how each parameter value was identified.

Parameters requiring optimisation were identified in two stages. The first stage applies to those parameters associated with the $\theta(\psi, z)$ relationship, for which observations are available at four discrete depths in the top 1.0 m of the profile. The second stage only involves parameters strictly associated with the $K(\psi)$ relationship, and can only be identified by inverse modelling. The basic calibration strategy was similar to that applied by Cassiani and Binley (2005), that is, a simple Monte Carlo approach whereby a number of parameter realisations are generated by randomly selecting parameter values from a uniformly distributed range, specified *a-priori*. A set of model outputs are generated for each realisation, and an objective function (the normalised root mean squared error) is used to judge the model performance against some observed data. A subset of the realisations are classed as having good performance, and these were ranked in terms of performance to establish 5 and 95% uncertainty bounds on the model output. Because the first stage simply involves fitting parametric relationship to some data points, a large number of realisations are possible. The second stage, however, requires solving Richards' equation, and as such is computationally intensive. Consequently, fewer realisations are possible due to time constraints.

3.4.1 Model calibration stage one

For the two sites studied, simultaneous, frequent measurements of water content, θ^{obs}, and matric potential, ψ^{obs}, were available at 4 depths: 0.2, 0.4, 0.6 and 1.0 m. To quantify the performance of the modelled water content, θ^{mod} for a given parameter set, the root mean squared error (RMSE) was used as an objective function, such that

$$OF_1 = \sum_{j=1}^{4} \sqrt{\left(\frac{1}{N_j} \sum_{i=1}^{N_j} (\theta_{i,j}^{mod} - \theta_{i,j}^{obs})^2 \right)} \tag{6}$$

where N_j is the number of $\theta - \psi$ observations for depth j, and OF_1 has units of water content [-]. Due to there being scatter in the observed data (thought to be caused by drift in the profile probe calibration) a subset of data was selected, which defines the primary drying curve, by selecting the maximum observed water content in each of a number of discrete ranges of matric potential.

There is some variability in the matrix porosity at different depths (indicated by the variation in mean water content with depth in Figure 2), which is largely attributed to the presence of flints. Although this has an effect on the total water content, its effect on flow processes is assumed to be minimal, due to the fact that the matrix generally remains close to or fully saturated, hence the portion of the pore space that may actually dewater is small. For simplicity, a constant effective porosity for the matrix domain, $(\theta_s - \theta_r)$, is assumed to apply throughout the profile (however, note that the matrix domain fraction, $1 - w_f$, is reduced in the near surface), and a value of 35 % was assumed, based on ranges presented by Price et al. (1993). However, in order to correct for the apparent random variation, $\theta^m_{s,j}$, was also treated as a free parameter for each depth during the optimisation. This effectively normalises the observed water content, such that the final matrix residual and saturated water content θ_r and θ_s are 0 and 35 % respectively.

In situ measurements of hydraulic conductivity have generally indicated the onset of fracture flow to occur at a matric potential of around -0.5 m H_2O (Wellings, 1984; Hodnett and Bell, 1990; Cooper et al., 1990; Mahamood-ul-Hassan and Gregory, 2002). To be consistent with this it is necessary to set $\psi^f_2 \geq -0.5 \geq \psi^f_{1,\infty}$. Following some sensitivity analysis, it was decided that the value of ψ^f_2 should be set arbitrarily to -0.1 m (which means in practice that it is assumed that the fractures are 95 % saturated at $\psi = -0.1$ m). This reduces the number of parameters in the optimisation from 10 to 9, which significantly reduces the number of model realisations required to accurately describe the objective function surface. To identify the remaining 9 parameters a 100,000 realisation Monte Carlo analysis was performed. The results for both of the sites studied, in terms of model performance, uncertainty and parameter identifiability are shown in Figures 5 and 6 (note, for brevity we do not show the dotty plots for the four $\theta^m_{s,j}$ normalising parameters, as these do not feature in the final model).

Plots of each parameter value against objective function, for the five optimised model parameters are shown, for the best 1% of all model realisations. The parameters are somewhat more strongly identifiable at WF than at WI. However, in both cases the optimum parameter set is rather isolated, indicating that potentially a larger number of realisations could be beneficial.

The optimised $\theta(\psi, z)$ curves agree well with the observations at both sites, and at all depths, with the exception of the dry range at 0.2 m and 1.0 m depth for Warren Farm, where some observations fall outside the model 5-95% confidence interval.

The optimal parameter set identified for each site determines the nature of the fracture pore size distribution as a function of depth. These are plotted (as probability distribution functions and cumulative distribution functions at various depths) in Figures 5 and 6. At WF, the parameters imply that the weathered Chalk layers are distributed over 4 m depth, whilst at WI they are distributed over only 1 m. As a result of this, we might expect there to be more attenuation of infiltrating rainfall at WF.

3.4.2 Model calibration stage two

The remaining model parameters that require optimisation are the matrix and fracture saturated hydraulic conductivities, K_s^m and K_s^f, and the fracture conductivity exponent, L^f. These parameters were identified by inverse modelling, using the numerical CUZ model driven by observed rainfall and measured actual evaporation to reproduce observed time series of θ and ψ in the top 3 m of the profile, at the two sites. The normalised RMSE was used for the objective function, such that

$$OF_2 = \sum_{j=1}^{6} \sqrt{\left(\frac{1}{N_j} \sum_{i=1}^{N_j} \left[\frac{\psi_{i,j}^{mod} - \psi_{i,j}^{obs}}{\min(\psi_{i=1\rightarrow N_j,j}^{obs})} \right]^2 \right)} + \sum_{j=1}^{4} \sqrt{\left(\frac{1}{N_j} \sum_{i=1}^{N_j} \left[\frac{\theta_{i,j}^{mod} - \theta_{i,j}^{obs}}{\max(\theta_{i=1\rightarrow N_j,j}^{obs})} \right]^2 \right)} \quad (7)$$

where j and i are indices in depth and time respectively and N_j is the number of data points at each depth, and OF_2 is dimensionless. Frequently logged observations of ψ are available at $z = 0.2$, 0.4, 0.6, 1.0, 2.0 and 3.0 m and of θ at $z = 0.2$, 0.4, 0.6 and 1.0 m.

Using variations of the instantaneous profile method, values of saturated matrix hydraulic conductivity, ranging from 0.001 to 0.006 m/day and saturated fracture hydraulic conductivities, ranging from 0.05 to 0.5 m/day have been observed at various Chalk sites across the UK (e.g. Wellings, 1984; Cooper et al., 1990; Hodnett and Bell, 1990; Mahamood-ul-Hassan and Gregory, 2002). Values of saturated fracture hydraulic conductivities observed from packer testing in the saturated zone range from 0.01 to 100 m/day (Allen et al., 1997, p. 53 and 59). This significant increase is believed to be for two reasons: firstly there is uncertainty about whether the instantaneous profile method ever observed fully saturated fractures; secondly, fractures in the saturated zone are likely to be enlarged due to continuous exposure to flowing water.

The above values apply to the bulk fracture-matrix system, so the fracture hydraulic conductivities need to be divided by w_f and the matrix hydraulic conductivities by $1-w_f$ to be compatible with item 11 of Table 1. Assuming a 1% fracture porosity, a bulk hydraulic conductivity of 100 m/day requires a fracture hydraulic conductivity of 10,000 m/day. Considering this, the following *a priori* ranges were assumed for the Monte Carlo simulations: $2 \times 10^{-4} \leq K_s^m \leq 2 \times 10^{-3}$ m/day and $1.5 \leq K_s^f \leq 1500$ m/day. For both K_s^m and K_s^f parameters were randomly sampled from a log-uniform distribution, because the parameter ranges span one or more order of magnitude. Finally, L^f is an empirical parameter. It was established that in this case, negative values for L^f performed poorly, and therefore the parameter was varied uniformly over an arbitrary range from 0 to 5.

We focus initially on WF, where two complete years of field data are available (2004 and 2005). Only data from 2004 were used in the model calibration, so that data from 2005 could be used for model verification. A 2500 realisation Monte Carlo simulation was performed for the above parameter ranges. The results are shown in Figure 7. The model is most sensitive to the value of K_s^m, but there is also some sensitivity to K_s^f, with better performance for values at the low end of the specified range. L^f appeared insensitive for values greater than around 2. Therefore, a further 1000 realisation Monte Carlo simulation was performed for a refined parameter range in terms of K_s^f, which was now varied from 1.5 to 15 m/day. These results simulation are also shown in Figure 7. Similar results were found for K_s^m (optimum value 5.3×10^{-4} m/day) and L^f (optimum value 4.1), albeit with an improved optimum objective function value. This time K_s^f appeared to be largely insensitive, though there was a slight preference for lower values, and an optimum value of 2.8 m/day was found. Both of these analyses demonstrate that the model performance is largely determined by K_s^m, for which the optimum value is around 0.5 mm/day.

The model performance with the optimum parameter set is plotted in Figure 8. The model generally reproduces well the temporal pattern of ψ at all depths, although it tends to underestimate the magnitude of the peaks at 0.2 m depth. In terms of the cumulative change in water content (*cum.* Δθ), again, the model generally performs well in reproducing the general patterns. It is also able to reproduce the wetting events. The main weakness appears to be that during dry periods the modelled Δθ tends to be more responsive than the observations, particularly at depths of 0.2 and 0.4 m.

For WI, observed data were only available for the first part of 2004, so model simulations were only run for this year, and the calibration was performed for the refined parameter range identified from the previous calibration exercises for WF. Figure 9 shows the model performance plotted against parameter values. Again, the dotty plots indicate that K_s^f and L^f are relatively insensitive, whereas K_s^m is strongly identifiable, and hence largely determines the model performance. The optimum value of K_s^m at WI was approximately 1 mm/day, i.e. double that at WF. Figure 10 shows the performance of the optimum solution. For the data that are available, the model performs well in terms of matric potential. In terms of water content, the model performance is somewhat limited at 1.0 m depth, where it tends to underestimate the changes in θ. There is no response in the observed data to the large event on 9 July, which causes a perturbation in the simulated data. This simulated response was caused by a single, high intensity, rainfall event, observed at WF, which saw 48 mm of rain in a 12 hour period. This suggests that the rainfall event recorded at WF did not occur at WI (at least not with the same magnitude). Despite the fact that limited data were available, and concerns about the use of input rainfall data from WF, the overall model performance at WI was considered to be reasonable.

4 CUZ Model application

The CUZ model was conditioned to two field sites, and was seen to perform well in reproducing the soil water dynamics in the top 3 m of the profile. Both configurations were run with two years of driving data (rainfall and actual evaporation), from 1 January 2004 to 1 January 2006, which were cycled three times to eliminate effects of the initial conditions. The results from the final cycles were analysed to gain insights into the hydrological processes occurring throughout the chalk profiles.

It was noted above that the first stage of the calibration resulted in different patterns of soil/weathered chalk layers at each of the two sites. Figure 11 shows how these differences impact upon the changes in water content throughout the near surface profile. The changes in water content with depth essentially match the pattern of fracture porosity with depth. At WF, the changes are gradual, over a depth of about 2 m, whereas at WI the changes occurs rapidly in the top 1 m. In both cases, the profiles of matrix and fracture water content show that, in the consolidated chalk, on average the matrix is close to saturation and the fractures are close to being empty. In the soil and weathered chalk layers, the fractures fill up to absorb the high intensity infiltrating fluxes, whilst the matrix desaturates to satisfy evaporative demand.

Since the model includes a fully coupled plant, the development and migration of zero flux planes (ZFPs) throughout the profile over time can be constructed from the high spatial and temporal resolution simulated ψ data. The simulations indicated very similar ZFP patterns for both sites, so the result is only plotted for WF, in Figure 12, against the observed water table elevation. The result is entirely consistent with the schematic pattern originally proposed by Wellings and Bell (1980). During the summer months, ZFPs were developed to significant depths - down to 4.85 m and 4.29 m in 2004, and 6.97 m and 6.25 m in 2005, at WF and WI respectively. The plant roots have access to large amounts of storage in the Chalk matrix, and are hence unlikely to become water stressed. This is supported by recent field measurements of actual evaporation, which have shown that Chalk outcrops almost always satisfy potential evaporation (Roberts et al., 2005, in particular see their comparison of potential and actual evaporation at Bridgets Farm, which is the same site as Warren Farm, in their Figure 3). Below the ZFP water moves downwards to water table, and in this study it was seen that the recharge fluxes were constant over time, despite the fact that there was a significant drought. Traditionally, recharge in groundwater models has been calculated using variations of the Grindley (1969) method (such as MORECS, Thompson et al., 1981), which fails to recognise the presence of a ZFP. This method predicts recharge only when the soil moisture deficit is zero, and in some cases also assuming a bypass of precipitation to the aquifer (e.g. Rushton et al., 1989; Ragab et al., 1997; Andrews et al., 1997; Bradford et al., 2002). The findings of this study indicate that these methods are inappropriate for unconfined Chalk aquifers. Such groundwater models are often calibrated against observed groundwater elevation data, by modifying the aquifer parameters (i.e. transmissivity and specific storage). However, if the recharge is represented erroneously, the aquifer parameters obtained may be wrong. Similarly, estimates of specific yield made on the basis that during a period of sustained groundwater recession there is no recharge are also liable to be wrong (as was found in the study by Lewis et al., 1993a,b, and cited by Price et al., 2000). As such, our understanding of how the aquifer will behave under different conditions (for example floods, droughts, climate change scenarios, new pumping wells, and so on) may be ill founded. The capacity of the Chalk unsaturated zone to perennially supply water to the saturated zone will have particularly important consequences for the catchment during periods of drought, potentially maintaining groundwater levels and river flows at a higher level than would previously have been predicted.

A debate which has persisted in the literature, at least since the study by Smith et al. (1970), is the role of the fractures in transmitting flow through the chalk unsaturated zone (perhaps the key contributions to this debate come from Smith et al., 1970; Foster, 1975; Wellings, 1984; Cooper et al., 1990; Hodnett and Bell, 1990; Price et al., 2000; Mahamood-ul-Hassan and Gregory, 2002; Haria et al., 2003). Most workers since Wellings (1984) have concluded that matrix flow is dominant, but instances when conditions likely to initiate fracture flow (based on observations of ψ exceeding the threshold associated with fracture activation) exist near the top of the profile have been reported. Within the CUZ model, it is possible to explicitly differentiate between matrix and fracture flow, since the hydraulic conductivity in both domains is a unique function of ψ, and the head gradient can be extracted from the simulated ψ distribution. Figure 13 shows simulated flow in the matrix and the fractures throughout the profile at WF. Fracture flow occurred down to a depth of 1 m, but below this flow was solely transmitted through the matrix. Fracture flow generally occurred in the winter, but also occurred in the top 0.5 m of the profile following the large rainfall event in the summer of 2004. At WI the patterns were very similar, although flow was slightly more attenuated than at WF.

At WF, for 2004/5, the water table fluctuated between around 32 and 44 m below ground level. In the model, it was necessary to fix the water table at 40 m. The simulated flux at 35 m, shown in Figure 13, can be assumed to be at least indicative of the actual recharge flux. It can be seen that the recharge flux is attentuated such that it is almost constant over time. At WI, where the water table is about 70 m deep, a similar result is found, with the recharge signal even more strongly attentuated. If the results of these simulations are to be believed, variations in the water table elevation could not have been caused by changes in the recharge flux over time, and hence must have been caused by changes in the lateral head gradient differential in the saturated zone. We speculate that changes in the elevation of the water table at the interfluve may therefore be largely caused by the propagation of a pressure wave laterally through the saturated zone, initiated by recharge occurring where the unsaturated zone thickness is much less.

A serious limitation of the modelling study thus far is that it only considered data from two years, 2004 and 2005. Comparing the rainfall and potential evaporation data with the long term (30 years) record from the area, Figure 14, shows that apart from two wet months (August and October 2004) the period generally received less than average rainfall. In fact, the period of 2004-6 has been described by the Department for Environment, Food and Rural affairs, DEFRA, as the worst drought in southeast England in the last 100 years (DEFRA, 2007). Therefore it can be expected that more fracture flow occurs in more typical years. As no data were available to test the model during wetter conditions, a simple sensitivity analysis was carried out. The rainfall intensity was increased progressively from 1% up to 20% (that is, every single rainfall event in the 2 year period was increased by these scale factors). The corresponding change in the occurrence of fracture flow throughout the profile at WI is presented in Figure 15 where it can be seen that the occurrence of fracture flow highly sensitive to the rainfall intensity. Increasing the rainfall by 4% resulted in fracture flow at depths of up to 10 m. An increase of 10% leads to fracture flow throughout the entire profile. Figure 16 shows the recharge fluxes (approximated by the simulated flux at 65 m depth) split into matrix flow, fracture flow and total flow, for three rainfall scenarios (normal, 10% and 20% increase in rainfall). For a 10% increase in rainfall 10% of the recharge is transmitted through the fractures. Furthermore, fracture flow is no longer associated with any particular rainfall events, rather it is steady. For a 20% increase in rainfall, flow through the fractures is more variable, and at certain times dominates the recharge signal. In other words, at some point between 10 and 20%, the behaviour of the recharge switched between a completely attenuated, steady response, and a seasonally dynamic response, comprising temporally discrete rapid recharge events.

The same analysis was performed for WF assuming this time that the recharge flux can be approximated by the simulated flux at 30 m depth (see Figure 17). Here, because of the reduced unsaturated zone thickness, there is less attenuation of the recharge flux, and seasonal variations in recharge associated with fracture flow are present for an increase in rainfall of just 10%, although matrix flow still generally dominates the recharge pattern. It is notable that the fracture event for the 10% rainfall scenario is delayed as compared with with 20% rainfall scenario. Hence, the fractures in the CUZ model are not behaving as simple bypass pathways which are either on or off. Rather they allow significant attenuation to occur, depending on the intensity of rainfall. The inference from this work, therefore, is that recharge models that use a simple bypass mechanism to represent fracture flow (Rushton et al., 1989; Ragab et al., 1997; Andrews et al., 1997; Bradford et al., 2002) are of questionable value.

5 Conclusions

In this paper we have presented a methodology for modelling flow in the chalk unsaturated zone, accounting for vertical heterogeneity in the soil and weathered chalk layers, using a parsimonious, Richards' equation based approach, which is able to simulate flow in both the matrix and the fractures. A rational approach was taken to identify appropriate model parameters. Those parameters which are liable to be site specific and are not amenable to laboratory investigation were identified using a Monte Carlo methodology. This was carried out in two stages. Firstly, parameters associated with the soil moisture characteristic relationships at various depths in the profile are identified using parametric relationships, which derive from the Kosugi (1996) model. Secondly, parameters associated with hydraulic conductivity are identified by inverse modelling, using a Richards equation based, equivalent composite medium model. For the period studied the model was seen to perform well in reproducing the observed soil moisture status (i.e. water content and matric potential) at the two field sites. However, there were two limitations. Firstly, observed data were only available in the near surface, whereas interpretations were made from the entire profile, down to the water table. Secondly, the period studied was unusually dry, hence the model was not tested for the entire realistic range of field conditions.

The model has enabled a number of useful insights to be made. During the period studied zero flux planes developed in the top 7 m of of the profile. Above this, a large amount of storage was potentially available to satisfy evaporative demand. Beneath the ZFP the model suggests that the unsaturated zone drains continuously into the water table. As a result, recharge is continuous throughout the year, albeit with potentially differing rates, which has important implications for the representation of recharge in groundwater models, which have perhaps been largely overlooked in the past. Failure to recognise this is also likely to lead to errors in the estimation of parameters for unconfined chalk aquifers.

As the period studied was during a drought, a sensitivity study was carried out to explore the effect of increased rainfall intensity. It was found that the frequency, duration and depth of flow in the fractures, and consequently the recharge rates and patterns were highly sensitive to rainfall intensity. A relatively moderate increase in rainfall intensity (say of the order of 10%) may result in fracture flow being initiated down to greater depths, even right down to the water table, and a seasonal, or event based, recharge pattern may become evident. This non-linear behaviour, is likely to be important when it comes to understanding groundwater flooding in Chalk catchments (see also Pinault et al., 2005). However, the model developed in this study has not yet been verified against field data under wet, or high rainfall, conditions.

Acknowledgements

This study was possible because of the work of Ned Hewitt, Roger Wyatt, Amanda Lloyd, Andy Dixon and Paul Rosier from CEH Wallingford, who installed and maintained the instrumentation and collected the field data. David Cooper also provide invaluable advice and guidance.

This work was carried out as part of a CASE studentship funded by the Natural Environmental Research Council and the Centre for Ecology and Hydrology, Wallingford.

References

Allen, D. J., Brewerton, L. J., Coleby, L., Gibbs, B. R., Lewis, M. A., MacDonald, A. M., wagstaff, S. J., Williams, A. T., 1997. The physical properties of major aquifers in England and Wales. Technical report wd/97/34, British Geological Survey.

Allshorn, S. J. L., Bottrell, S. H., West, L. J., Odling, N. E., 2007. Rapid karstic bypass flow in the unsaturated zone of the Yorkshire chalk aquifer and implications for contaminant transport. Geological Society London Special Publications 279 (1), 111–122.

Andrews, R. J., Lloyd, J. W., Lerner, D. N., 1997. Modelling of nitrate leaching from arable land into unsaturated soil and chalk 1. Development of a management model for applications of sewage sludge and fertilizer. Journal of Hydrology 200, 179–197.

Barker, J. A., Foster, S. S. D., 1981. A diffusion exchange model for solute movement in fissured porous rock. Quart. J. Eng. Geol. 14, 17–24.

Barraclough, D., Gardner, C. M. K., Wellings, S. R., Cooper, J. D., 1994. A tracer investigation into the importance of fissure flow in the unsaturated zone of the British Upper Chalk. Journal of Hydrology 156, 459–469.

Bradford, R., Ragab, R., Crooks, S., Bouraouri, F., Peters, E., 2002. Simplicity versus complexity in modelling groundwater recharge in Chalk catchments. Hydrol. Earth Syst. Sci. 6, 927–937.

Brouyère, S., 2006. Modelling the migration of contaminants through variably saturated dual-porosity, dual-permeability Chalk. Journal of Contaminant Hydrology 82, 195–219.

Brouyère, S., Dassargues, A., Hallet, V., 2004. Migration of contaminants through the unsaturated zone overlying the Hesbaye chalky aquifer in Belgium: a field investigation. Journal of Contaminant Hydrology 72, 135–164.

Brutsaert, W., 1967. Some methods of calculating unsaturated permeability. Trans. ASAE 10, 400–404.

Burdine, N. T., 1953. Relative permeability calculation from size distribution data. Trans. AIME 198, 71–78.

Cassiani, G., Binley, A., 2005. Modeling unsaturated flow in a layered formation under quasi-steady state conditions using geophysical data constraints. Advances in water resources 28, 467–477.

Cooper, J. D., Gardner, C. M. K., MacKensie, N., 1990. Soil water controls on recharge to aquifers. European Journal of Soil Science 41, 613–630.

Dahan, O., Nativ, R., Adar, E., Berkowitz, B., 1998. A measurement system to determine water flux and solute transport through fractures in the unsaturated zone. Groundwater 36 (3), 444–449.

Dahan, O., Nativ, R., Adar, E., Berkowitz, B., Ronen, Z., 1999. Field observation of flow in a fracture intersecting unsaturated chalk. Water Resources Research 35 (11), 3315–3326.

DEFRA, 2007. http://www.defra.gov.uk/Environment/water/resources/drought/index.htm. Department for Environment, Food and Rural affairs, UK.

Doughty, C., 1999. Investigation of conceptual and numerical approaches for evaluating moisture, gas, chemical and heat transport in fractured unsaturated rock. Journal of Contaminant Hydrology 38, 69–106.

Downing, R. A., 1998. Groundwater: our hidden asset. Tech. rep., British Geological Survey, Keyworth, Nottingham.

Downing, R. A., Price, M., Jones, G. P., 1993. The Hydrogeology of the Chalk of North-west Europe. Oxford University Press.

Feddes, R. A., Kowalik, P., Kolinska-Malinka, K., Zaradny, H., 1976. Simulation of field water uptake by plants using a soil water dependent root extraction function. Journal of Hydrology 31.

Foster, S. S. D., 1975. The Chalk groundwater tritium anomaly - a possible explanation. Journal of Hydrology 25, 159–65.

Gerke, H. H., van Genuchten, M. T., 1993. A dual-porosity model for simulating the preferential movement of water and solutes in structured porous media. Water Resources Research 29 (2), 305–319.

Gerke, H. H., van Genuchten, M. T., 1996. Macroscopic representation of structural geometry for simulating water and solute movement in dual-porosity media. Advances in Water Resources 19 (6), 343–357.

Gooddy, D. C., Mathias, S. A., Harrison, I., Lapworth, D. J., Kim, A. W., 2007. The significance of colloids in the transport of pesticides through Chalk. Science of the Total Environment 385 (1-3), 262–271.

Grindley, J., 1969. The Calculation of Actual Evaporation and Soil Moisture Deficit over Specified Catchment Areas, Hydrological Memorandum 38. Tech. rep., Meteorological Office.

Haria, A. H., Hodnett, M. G., Johnson, A. C., 2003. Mechanism of groundwater recharge and pesticide penetration to a chalk aquifer in southern England. Journal of Hydrology 275, 122–137.

Hodnett, M. G., Bell, J. P., 1990. Processes of Water Movement Through a Chalk Coombe Deposit in Southeast England. Hydrological Process. 4, 361–372.

Hoffmann-Reim, H., van Genuchten, M. T., Fluhler, H., 1999. General model for the hydraulic conductivity of unsaturated soils. In: van Genuchten, M. T., Leij, F. J., Wu, L. (Eds.), Chracterization and Measurement of the Hydraulic Properties of Unsaturated Porous Media: Proceedings of the International Workshop. Riverside, California, pp. 31–42.

Ireson, A. M., Wheater, H. S., Butler, A. P., Finch, J., Cooper, J. D., Wyatt, R. G., Hewitt, E. J., 2005. Field monitoring of matric potential and soil water content in the Chalk unsaturated zone. In: Advanced experimental unsaturated soil mechanics. Experus 2005. A. A. Balkema, London.

Ireson, A. M., Wheater, H. S., Butler, A. P., Mathias, S. A., Finch, J., Cooper, J. D., 2006. Hydrological processes in the Chalk unsaturated zone - insights from an intensive field monitoring programme. Journal of Hydrology 330, 29–43.

Jackson, B. M., Wheater, H. S., Mathias, S. A., McIntyre, N., Butler, A. P., 2006. A simple model of variable residence time flow and nutrient transport in the chalk. Journal of Hydrology 330, 221–234.

Jackson, B. M., Wheater, H. S., Wade, A. J., Butterfield, D., Mathias, S. A., Ireson, A. M., Butler, A. P., McIntyre, N. R., Whitehead, P. G., 2007. Analysis of water-level response to rainfall and implications for recharge pathways in the Chalk aquifer, SE England. Ecological Modelling 209, 604–620.

Jacobs, 2006. Making Space for Water. Groundwater flooding records collation, monitoring and risk assessment. Extended Report (Chalk Aquifers). Tech. Rep. HA5, Environment Agency.

Kloppmann, W., Dever, L., Edmunds, W. M., 1998. Residence time of Chalk groundwaters in the Paris Basin and the North German Basin: a geochemical approach. Applied Geochemistry 13 (5), 593–606.

Kosugi, K., 1994. Three-parameter lognormal distribution model for soil water retention. Water Resources Research 30 (4), 891–901.

Kosugi, K., 1996. Lognormal distribution model for unsaturated soil hydraulic properties. Water Resources Research 32 (9), 2697–2703.

Kosugi, K., 1999. General model for unsaturated hydraulic conductivity for soils with lognormal pore-size distribution. Soil Science Society of America Journal 63, 270–277.

Kwicklis, E. M., Healy, R. W., 1993. Numerical investigation of steady liquid water-flow in a variably saturated fracture network. Water Resources Research 29, 4091–4102.

Larsbo, M., Roulier, S., Stenemo, F., Kasteel, R., Jarvis, N., 2005. An improved dual-permeability model of water flow and solute transport in the vadose zone.

Vadose Zone Journal 4, 398–406.

Lee, L. J. E., Lawrence, D. S. L., Price, M., 2006. Analysis of water-level response to rainfall and implications for recharge pathways in the Chalk aquifer, SE England. Journal of Hydrology 330, 604–620.

Lewis, M. A., Jones, H. K., Macdonald, D. M. J., Price, M., Barker, J. A., Shearer, J. A., Wesselink, T. R., Evans, D. J., 1993a. Groundwater storage in British aquifers: Chalk. R&D Note 169, National Rivers Authority, Bristol.

Lewis, M. A., Jones, H. K., Macdonald, D. M. J., Price, M., Barker, J. A., Shearer, J. A., Wesselink, T. R., Evans, D. J., 1993b. Groundwater storage in British aquifers: Chalk. Project Record 128/8/A, British Geological Survey, Hydrogeology Group.

Liu, H. H., Doughty, C., Bodvarsson, G. S., 1998. An active fracture model for unsaturated flow and transport in fractured rocks. Water Resources Research 34, 2633–2646.

Liu, H. H., Haukwa, C. B., Ahlers, C. F., Bodvarsson, G. S., Flint, A. L., Guertal, W. B., 2003. Modeling flow and transport in unsaturated fractured rock: an evaluation of the continuum approach. Journal of contaminant hydrology 62, 173–188.

Mahamood-ul-Hassan, M., Gregory, P. J., 2002. Dynamics of water movement on Chalkland. Journal of Hydrology 257, 27–41.

Mathias, S. A., 2005. Transient simulations of flow and transport in the Chalk unsaturated zone. Ph.D. thesis, Imperial College London.

Mathias, S. A., Butler, A. P., Ireson, A. M., Jackson, B. M., McIntyre, N., Wheater, H. S., 2007. Recent advances in modelling nitrate transport in the Chalk unsaturated zone. Quarterly Journal of Engineering Geology 40, 353–359.

Mathias, S. A., Butler, A. P., Jackson, B. M., Wheater, H. S., 2006. Transient simulations of flow and transport in the Chalk unsaturated zone. Journal of Hydrology 330, 10–28.

Mathias, S. A., Butler, A. P., McIntyre, N., Wheater, H. S., 2005. The significance of flow in the matrix of the Chalk unsaturated zone. Journal of Hydrology 310, 62–77.

Mualem, Y., 1976. A new model of predicting hydraulic conductivity of unsaturated porous media. Water Resources Research 12, 513–522.

Nativ, R., Adar, E., Dahan, O., Geyh, M., 1995. Water recharge and solute transport through the vadose zone fo fractured Chalk under desert conditions. Water Resources Research 31, 253–261.

Nativ, R., Nissim, I., 1992. Characterization of a desert aquitard- hydrologic and hydrochemical considerations. Groundwater 30 (4), 598–606.

Oakes, D. B., 1977. The movement of water and solutes through the unsaturated zone of the Chalk of the United Kingdom. In: Proc. 3rd Int. Hydrol. Symp. Colorado State Univ. Fort Collins, USA.

Oakes, D. B., Young, C. P., Foster, S. S. D., 1981. The effects of farming practices on groundwater quality in the United Kingdom. The Science of the Total Environment 21, 17–30.

Peters, R. R., Klavetter, E. A., 1988. A Continuum Model for Water Movement in an Unsaturated Fractured Rock Mass. Water Resources Research 24 (3), 416–430.

Pinault, J. L., Amraoui, N., Golaz, C., 2005. Groundwater-induced flooding in macropore-dominated hydrological system in the context of climate changes. Water Resources Research 41.

Price, M., Downing, R. A., Edmunds, W. M., 1993. The Chalk as an aquifer. In: Downing, R. A., Price, M., Jones, G. P. (Eds.), The Hydrogeology of the Chalk of North-West Europe. Clarendon Press, Oxford.

Price, M., Low, R. G., McCann, C., 2000. Mechanisms of water storage and flow in the unsaturated zone of the Chalk aquifer. Journal of Hydrology 233, 54–71.

Ragab, R., Finch, J., Harding, R., 1997. Estimation of groundwater recharge to Chalk and sandstone aquifers using simple soil models. Journal of Hydrology 190, 19–41.

Richards, L. A., 1931. Capillary conduction of liquids through porous mediums. Physics 1, 318–333.

Roberts, J., Rosier, P., Smith, D. M., 2005. The impact of broadleaved woodland on water resources in lowland UK: II. Evaporation estimates from sensible heat flux measurements over beech woodland and grass on chalk sites in Hampshire. Hydrology and Earth System Sciences 9 (6), 607–613.

Rushton, K. R., Connorton, B. J., Tomlinson, L. M., 1989. Estimation of the groundwater resources of the Berkshire Downs supported by mathematical modelling. Quart. J. Eng. Geol. 22, 329–341.

Schaap, M. G., Leij, F. J., 2000. Improved Prediction of Unsaturated Hydraulic Conductivity with the Mualem-van Genuchten Model. Soil Science Society of America Journal 64.

Smith, D. B., Wearn, P. L., Richards, H. J., Rowe, P. C., 1970. Water movement in the unsaturated zone of high and low permeability strata using natural tritium. In: Isotope Hydrology. Atomic Energy Agency, Vienna.

Thompson, N., Barry, I. A., Ayles, M., 1981. The Meteorological Office rainfall and evaporation calculation system: MORECS. Tech. rep., Meteorological Office, Bracknell, UK.

Tocci, M. D., Kelley, C. T., Miller, C. T., 1997. Accurate and economical solution of the pressure-head form of Richards' equation by the method of lines. Advances in Water Resources 20 (1), 1–14.

Van den Daele, G. F. A., Barker, J. A., Connell, L. D., Atkinson, T. C., Darling, W. G., Cooper, J. D., 2007. Unsaturated flow and solute transport through the Chalk: Tracer test and dual permeability modelling. Journal of Hydrology 342, 157–172.

van Genuchten, M. T., 1980. A Closed-form Equation for Predicting the Hydraulic Conductivity in Unsaturated Soils. Soil Science Society of America Journal 44, 892–898.

Wang, J. S. Y., Narasimhan, T. N., 1985. Hydrologic mechanisms governing fluid-flow in a partially saturated, fractured, porous-medium. Water Resources Research 21, 1861–1874.

Wellings, S. R., 1984. Recharge of the Upper Chalk aquifer at a site in Hampshire, England, 1. Water balance and unsaturated flow. Journal of Hydrology 69, 259–273.

Wellings, S. R., Bell, J. P., 1980. Movement of water and nitrate in the unsaturated zone of the Upper Chalk near Winchester, Hants., England. Journal of Hydrology 48, 119–136.

Wheater, H. S., Neal, C., Peach, D., 2006. Hydro-ecological functioning of the Pang and Lambourn catchments, UK: An introduction to the special issue. Journal of Hydrology 330, 1–9.

Young, C. P., Oakes, D. B., Wilkinson, W. B., 1976. Prediction of Future Nitrate Concentrations in Ground Water. Groundwater 14 (6), 426–438.

Appendix A: Alternative models for the relative hydraulic conductivity

For variably saturated porous media, the hydraulic conductivity, $K(\psi)$ is given by the product of the saturated hydraulic conductivity, K_s and the relative permeability, $K_r(\psi)$. Various different forms have been proposed for the $K_r(\psi)$ relationship. Kosugi (1996) considers both the Mualem (1976) and the Burdine (1953) relationships, which are both special cases of the general relationship proposed by Hoffmann-Reim et al. (1999) (cited by Schaap and Leij, 2000)

$$K(\psi) = K_s S_e^L \left(\frac{\int_0^{S_e} \psi^{-\alpha} dS_e}{\int_0^1 \psi^{-\alpha} dS_e} \right)^{\beta} \tag{8}$$

where L is a parameter typically related to the tortuosity and pore connectivity (Mualem, 1976), and α and β are parameters which determine the form of the relationship. For the Mualem relationship, $\alpha = 1$ and $\beta = 2$, and for the Burdine relationship $\alpha = 2$ and $\beta = 1$. Furthermore, the Kozeny relationship (Brutsaert, 1967), is given by setting $\beta = 0$. The solution to Equation 8 will depend on the form of the $S_e(\psi)$ relationship used. Kosugi (1999) showed that unlike with the van Genuchten (1980) model, using the KS model for $S_e(\psi)$ Equation 8 can be solved for non-integer parameter combinations of α and β, to yield the equation

$$K(\psi) = K_s.S_e^L \left(\frac{1}{2} \mathrm{erfc} \left[\mathrm{erfc}^{-1}(2S_e) + \frac{\alpha\sigma}{\sqrt{2}} \right] \right)^{\beta} \tag{9}$$

where σ is a KS model parameter. By treating L and α as fitting parameters, and setting $\beta = 1$, Kosugi was able to obtain an improved description of the observed $K(\psi)$ relationships for a large number of soils, as compared with the results using the Burdine (1953) and Mualem (1976) models. In this study, since we do not have observed $K(\psi)$ data for the Chalk, we examined the performance of the model for a number of integer combinations of these parameters, including each of the established relationships, as well as for the case when $\alpha = 1$ and $\beta = 1$, which we refer to as the 'modified Mualem' model. For each model, a 1000 realisation Monte Carlo simulation was performed to identify the parameters K_s^f, K_s^m and L^f (as in the second calibration stage described earlier). Additional model parameters were taken from the first calibration stage for WF, and observed matric potential data from 2004 was used to gauge the model performance. Figure 18 shows the performance for the optimum parameter set for each of the four model configurations considered at 0.2, 1.0 and 3.0 m depth. Additionally, the RMSE between each model result and the observed data was calculated. It was found that the modified Mualem model performed significantly better than the alternatives, with an RMSE of 4.4 (the Mualem, Kozeny and Burdine models had RMSE values of 5.15, 5.4 and 5.5 respectively), and was consequently adopted for the CUZ model developed in this study. The integrated form of Equation 8 with the Kosugi relationship for $S_e(\psi)$ and $\alpha = \beta = 1$, is given by item 8 in Table 1.

Inputs: ψ, z and 17 parameters:

$\theta_r^m, \theta_s^m, \theta_r^f, \theta_s^f, w_{f,0}, w_{f,\infty}, \psi_1^m, \psi_2^m, \psi_{1,0}^f, \psi_{1,\infty}^f, \psi_2^f, K_s^m, K_s^f, L^m, L^f, Z_\alpha, Z_\beta$

Initialise constants:

$x_1 = -\sqrt{2}(\mathrm{erf}^{-1}[2S_{e,1}-1]); \quad S_{e,1} = 0.05$ $x_2 = -\sqrt{2}(\mathrm{erf}^{-1}[2S_{e,2}-1]); \quad S_{e,2} = 0.95$	These constants determine the value of S_e at ψ_1 and ψ_2 to characterise the pore size distribution. See section 3.2

		Description
1.	$\psi_1^f = \psi_{1,\infty}^f + \frac{\psi_{1,0}^f - \psi_{1,\infty}^f}{1+\exp\left(-Z_\alpha(z-Z_\beta)\right)}$	Depth dependent Fracture pore size dist.(1) and domain size (2)
2.	$w_f = w_{f,\infty} + \frac{w_{f,0} - w_{f,\infty}}{1+\exp\left(Z_\alpha(z-Z_\beta)\right)}$	

Repeat steps 3–8 for matrix and fracture domains

3.	$\sigma = \frac{ln\left(\frac{\psi_2}{\psi_1}\right)}{x_2 - x_1}$	Transform to get KS model parameters (3&4)
4.	$\psi_0 = \frac{\psi_1}{e^{(x_1+\sigma)\sigma}}$	
5.	$S_e = 0.5 + 0.5\mathrm{erf}\left(-\frac{[\ln(\psi/\psi_0)/\sigma - \sigma]}{\sqrt{2}}\right)$	Effective saturation (S_e^m/S_e^f)
6.	$\theta = \theta_r + S_e(\theta_s - \theta_r)$	Water content (θ^m/θ^f)
7.	$C = \frac{\theta_s - \theta_r}{(2\pi)^{1/2}\sigma(-\psi)} \exp\left(-\frac{[\ln(\psi/\psi_0) - \sigma^2]^2}{2\sigma^2}\right)$	Specific capacity (C^m/C^f)
8.	$K = K_s S_e^L \left[0.5 + 0.5\mathrm{erf}\left(\mathrm{erf}^{-1}[2S_e - 1] - \frac{\sigma}{\sqrt{2}}\right)\right]$	Hydraulic conductivity (K^m/K^f)

9.	$\theta(\psi) = w_f\theta^f(\psi) + (1-w_f)\theta^m(\psi)$	Bulk water content
10.	$C(\psi) = w_f C^f(\psi) + (1-w_f)C^m(\psi)$	Bulk specific capacity
11.	$K(\psi) = w_f K^f(\psi) + (1-w_f)K^m(\psi)$	Bulk hydraulic conductivity

Outputs: θ, C and K

For a description of all the parameters and variables, see the list of notation

Table 1

Summary of the equations used to obtain the hydraulic properties as a function of matric potential and depth

Parameter[♭]	Identification method	Parameter value	
		Warren Farm	West Ilsley
θ_r^m	Price et al. (2000); Mathias et al. (2006)	0	0
θ_s^m	Price et al. (2000); Mathias et al. (2006)	0.35	0.35
θ_r^f	Mathias et al. (2006)	0	0
θ_s^f	Mathias et al. (2006)	1	1
$w_{f,0}$	Optimisation[†]	0.12	0.14
$w_{f,\infty}$	Price et al. (1993); Mathias et al. (2006)	0.01	0.01
ψ_1^m	Price et al. (2000); Mathias et al. (2006)[**]	-95.2 m	-95.2 m
ψ_2^m	Price et al. (2000); Mathias et al. (2006)[**]	-14.1 m	-14.1 m
$\psi_{1,0}^f$	Optimisation[†]	-40.1 m	-48.3 m
$\psi_{1,\infty}^f$	Optimisation[†]	-1.29 m	2.99 m
ψ_2^f	Fixed[†‡]	-0.1 m	-0.1 m
K_s^m	Optimisation[§]	0.53 mm/day	1.01 mm/day
K_s^f	Optimisation[§]	2.83 m/day	1.73 m/day
L^m	Mualem (1976)[***]	0.5	0.5
L^f	Optimisation[§]	4.08	3.68
Z_α	Optimisation[†]	-1.4 m^{-1}	-9.5 m^{-1}
Z_β	Optimisation[†]	0.89 m	0.49 m

♭ See nomenclature for parameter descriptions.

* Note the distinction between the fracture domain saturated water content, θ_s^f which is 100%, and the fracture domain fraction, $w_{f,0}$ and $w_{f,\infty}$, which are equivalent to bulk fracture porosity.

** These parameters were derived from existing (Brooks and Corey, 1966) model parameterisations for the English chalk matrix (Mathias, 2005; Mathias et al., 2006), which are based on the experimental data obtained by Price et al. (2000).

*** The matrix conductivity exponent parameter is insensitive.

† These parameters are classified as 'soil moisture' parameters, as they can be identified from the $\theta(\psi, z)$ data alone.

‡ Arbitrarily fixing the value of this parameter did not affect the model performance, and doing so enabled the remaining parameter space to be explored more thoroughly.

§ These parameters are classified as 'hydraulic conductivity' parameters, as they are associated with the hydraulic conductivity, and can be identified by inverse modelling.

Table 2
Summary of all model parameters

Fig. 1. Photographs of the Chalk profile over various depth horizons at West Ilsley

Fig. 2. The Chalk profile at West Ilsley, and statistical properties of the water content data recorded between January and July of 2003

Fig. 3. Parameter distributions with depth, to account for vertical heterogeneity in the near surface

Fig. 4. The effect of changing the fracture pore size distribution scaling parameters on the fracture effective saturation curve

Fig. 5. Stage one calibration results for Warren Farm soil moisture parameters

Fig. 6. Stage one calibration results for West Ilsley soil moisture parameters

Fig. 7. Dotty plots of the model performance (objective function to be minimised) against parameter values for Warren Farm. Note the different units of K_s^m and K_s^f.

Fig. 8. Model performance (optimum simulation) plotted against observed data for Warren Farm

Fig. 9. Dotty plots of the model performance (objective function to be minimised) against parameter values for West Ilsley. Note the different units of K_s^m and K_s^f.

Fig. 10. Model performance (optimum simulation) plotted against observed data for West Ilsley

Fig. 11. Simulated water content in the near surface, demonstrating attenuation by the soil and weathered Chalk layers

Fig. 12. Simulated zero flux planes and observed water table response for Warren Farm

Fig. 13. Simulated matrix and fracture flow throughout the profile at Warren Farm

Fig. 14. Monthly rainfall and potential evaporation recorded at the automatic weather station at Wallingford (SU461189)

Fig. 15. Fracture flow occurrence in the West Ilsley profile as rainfall is increased

Fig. 16. Recharge flux (approximated by the flux at 65 m depth) at West Ilsley as total rainfall is increased

Fig. 17. Recharge flux (approximated by the flux at 30 m depth) at Warren Farm as total rainfall is increased

Fig. 18. Optimum performance of the alternative models for hydraulic conductivity