

Uptake of water from a Kandosol subsoil: I. Determination of soil water diffusivity

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Abstract

Aims To determine soil water diffusivity, $D(\theta)$, on undisturbed field soil at medium to low water content (suction range from 10 to 150 m of water), for the purpose of modeling the uptake of water by plant roots.

Methods The method is based on the analysis of one-step outflow induced by a turbulent stream of dry air over the exposed end of a soil core, with the other end of the core enclosed. The outflow is measured through time as the change in the weight of the core as it sits on a recording balance. $D(\theta)$ is calculated by deconvoluting the measured outflow function.

Results Over the suction range of 10 to 150 m of water, $D(\theta)$ calculated on the undisturbed soil ranged from 20×10^{-9} to 10×10^{-9} [$\text{m}^2 \text{s}^{-1}$], substantially higher than other published estimates over this range in suction.

Conclusions These unusually large values cast doubt on the view that flow of water to roots limits uptake of water from the targeted subsoil.

Keywords Root water uptake · Plant water uptake · Undisturbed soil · Outflow · Evaporation · Numerical analysis · One-dimensional flow equation

Introduction

Uptake of water from the subsoil markedly increases the yield of crops that are relying on such water during grain filling (Kirkegaard et al. 2007; Angus and van Herwaarden 2001). Yet, crops typically fail to extract substantial amounts of seemingly available water from the bottom third of their rooting zones by the time they have matured (Schultz 1972, 1971; Hurd 1974; Walter and Barley 1974; Jordan and Miller 1980; Kirkegaard et al. 2007; Robertson et al. 1993a, b; Thomas et al. 1995; Christopher et al. 2008). Mechanistic understanding of what limits the uptake of this residual water remains poor (Passioura and Angus 2010). Popular simulation models rely on empirical time constants for describing the rate of uptake from a given layer of soil (APSIM (Keating et al. 2003), CERES (Ritchie 1985)) but these time constants typically have to be determined anew for new circumstances.

Intriguingly coherent patterns of rates of water uptake across the whole root zone suggest that the disposition of water uptake may be primarily under the control of the plants (Dardanelli et al. 2004). However, the usefulness of empirical time constants, which

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implies that the rate of uptake from a given soil layer is proportional to the amount of available water remaining, suggests that the rate of movement of water through the soil may be limiting. If that is so, then the values of soil water diffusivity, $D(\theta)$, would be important. Paradoxically, theoretical estimates of what the time constants might be, given typical published values of $D(\theta)$ in soil at medium to low water content (Rose 1968) and measured root length density (length of root per unit volume of soil), are of the order of a few days, which would give ample time for all but very sparse roots to extract almost all of the available water (Passioura 1983).

However, published information on $D(\theta)$ on undisturbed soil is scant, especially on subsoil, and the values could be substantially lower than those in repacked soil. Further, given the strong clumping of roots in Kandosol subsoil (White and Kirkegaard 2010), the characteristic distance for the flow of water to absorptive roots, and hence the characteristic time for uptake, may be much larger than a simple analysis based on randomly distributed roots (Passioura 1991). Such clumping increases the likelihood that flow through the soil, and hence the values of $D(\theta)$, may be limiting uptake.

Accordingly, we set out to determine $D(\theta)$ in an undisturbed Kandosol subsoil on which much agronomic information, including rate of uptake from the subsoil, was available (Kirkegaard et al. 2007). This paper on $D(\theta)$ in the subsoil is the first part of a series of two. The second part explores factors controlling the uptake of water by plant roots from large cores of the same undisturbed subsoil in controlled conditions.

Soil water diffusivity, $D(\theta)$

Soil water diffusivity, $D(\theta)$ [$\text{m}^2 \text{s}^{-1}$], is the product of the hydraulic conductivity, K [ms^{-1}], and the slope of the soil water retention curve, $dh/d\theta$ [m], at a particular soil volumetric water content, θ , where h [m] is the soil matric suction:

$$D(\theta) = K(\theta) \times dh/d\theta \quad (1)$$

Neglecting gravity, the relationship between the flux of water, q , K and $D(\theta)$ is:

$$q = -D(\theta) \frac{d\theta}{dx} = K(h) \frac{dh}{dx} \quad (2)$$

where x [m] is distance. For modeling uptake of water by roots from the soil, the range of suction over which the soil is most likely to be limiting this uptake is from about 10 m to 150 m, for $D(\theta)$ is close to minimal over this range in a variety of repacked soils (Rose 1968).

The method of Rose (1968), essentially one-step outflow, gives the most reliable measurements. It uses evaporation from one end of an otherwise enclosed cylinder of soil under a turbulent condition, and destructively samples the soil core to determine the water content profile. $D(\theta)$ is then determined using the analytical solution of Matano (1933) and employs the Boltzmann transform (Boltzmann 1894), whereby the absolute integrity of the data can be verified and one can be sure that the calculated $D(\theta)$ is a function of water content alone. However, on undisturbed soil, this technique is experimentally difficult as the soil becomes very hard when air dry and difficult to section. Also, the effects of heterogeneity on water retention, even at small scales, limit the reliability of the analysis.

Many attempts have been made to determine $D(\theta)$ using one-step outflow without sectioning the soil (Crescimanno and Iovino 1995; Doering 1965; Gardner 1956; Gupta et al. 1974; Hopmans et al. 1992; Londra and Valiantzas 2011; Muazu et al. 1990; Passioura 1977; Valiantzas et al. 2007; van Dam et al. 1992; Zia-ul-Haque 1990), but most have dealt only with low to medium water suctions and many are unsuitable for undisturbed soil. The analysis of Passioura (1977) has been used to determine $D(\theta)$ at h from 10 to 70 m of water on repacked soil, and works well if the $D(\theta)$ function is monotonic, approximately exponential, and does not increase with decreasing θ , as sometimes happens when h exceeds about 100 m (Philip 1955; Rose 1968).

The method described here is based on deconvolution of the measured outflow during evaporation into turbulent dry air by numerically solving the one-dimensional flow equation (explained in detail below). Because of the initially rapid evaporation, the method necessarily generates large gradients in temperature near the soil surface but these soon become negligibly small as discussed below.

Materials and method

Theory

Water evaporates from the surface of wet soil in three stages (Idso et al. 1974). In stage one, the rate of evaporation depends on energy exchange at the surface, and is approximately linear with time, approximately, because of the limited flow of sensible heat to the soil surface during the early part of this stage. In stage two, the evaporation boundary condition is replaced by a constant soil water content at the surface, the soil core can be treated as semi-infinite, and cumulative evaporation proceeds as \sqrt{t} (neglecting gravity and assuming homogeneous conditions). In stage three, the finite length of the core becomes evident, and a zero flux boundary condition at $x = L$, the bottom of the core, results in θ falling increasingly below its initial value.

Evaporation takes place at the top end of a vertical core, $x = 0$, where, for the analysis described herein, it is assumed that the water content is reduced to θ_f at the onset of evaporation. Neglecting gravity for the short columns used in this study, the diffusion equation for one-dimensional flow of water in a stable soil of finite length is Eq. 3 subject to the conditions in Eq. 4. The influence of gravity was tested using the HYDRUS-1D (one-dimensional) numerical soil water flow model (Simunek et al. 2008) (which accounts for gravity), where the experiment was simulated twice: Firstly with the evaporation boundary condition at the top and secondly with the evaporation boundary condition at the bottom. The flux was the same for both simulations (data not shown).

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial x} \left(D(\theta) \frac{\partial \theta}{\partial x} \right) \quad (3)$$

$$\begin{aligned} \theta &= \theta_i, & 0 \leq x \leq L, & t = 0 \\ \theta &= \theta_f, & x = 0, & t > 0 \\ \frac{\partial \theta}{\partial x} &= 0, & x = L, & t > 0 \end{aligned} \quad (4)$$

In practice, θ_f is not attained at $x=0$ instantly, because evaporation is at first only limited by the ability of the atmosphere to remove water from soil.

Initially, therefore, the rate of evaporation, dE/dt , is proportional to the difference in humidity between the soil surface, w_s , and the adjacent atmosphere, w_0 :

$$\frac{dE}{dt} = \kappa(w_0 - w_s) \quad x = 0 \quad (5)$$

Where κ is a proportionality constant that incorporates the boundary layer resistance between the evaporating soil surface and the air stream. Equation 5 defines stage one evaporation, and in the experimental system described herein, typically lasts less than 5 min. Thereafter, the evaporation rate is determined by the soil hydraulic properties.

Experimental overview

Undisturbed field soil

Undisturbed soil samples were collected from a field (30 cm depth) located in south-eastern Australia (34° 43' S, 147° 48' E), the soil is a red Kandosol (Isbell 2002) of light clay texture.

Three replicate undisturbed soil cores (length = 6.0 cm, inside diameter = 3.0 cm) were used for the evaporation experiment described below. In order to test the repeatability of the evaporation method, evaporation was measured twice from each undisturbed soil core at two different initial suctions: Firstly the cores were equilibrated at a suction of 0.5 m of water and the evaporation was measured, then the cores were equilibrated at a suction of 1.0 m of water and the evaporation was measured again.

Soil water retention

The soil water retention was measured using two methods: (1) for suctions at 0.5 and 1.0 m of water, a porous ceramic tension table was used and (2) for suctions at 10, 50, 100 and 150 m of water, pressure plate apparatus was used.

Evaporative procedure

The samples were allowed to saturate from the base up and then drained to a suction of either 0.5 or 1.0 m of water and weighed, giving the initial water content, θ_i . The base of the core, $x = L$, was then sealed, and the top, $x=0$, subjected to rapid evaporation. An air outlet

was devised to supply a controlled, continuous flow of air (nominally 50 L min^{-1}) onto the top of the soil sample. The outlet of the air stream was positioned 20 cm directly above the soil surface. The velocity of the air stream was sufficiently fast to create a highly turbulent atmosphere just above the soil surface, thereby reducing the boundary layer between the air stream and the evaporating soil surface.

To ensure that the viscosity of the soil water remained constant, at least once the rapid evaporation during the first stage was over, the experiment was housed in a temperature controlled cabinet, maintained at $29 \text{ }^\circ\text{C} \pm 0.5$, a few degrees higher than that of the laboratory. This was checked by logging the temperature using copper constantan thermocouples positioned in two locations: inside the temperature controlled cabinet and at the air outlet inside the air stream. The diurnal fluctuation in ambient laboratory temperature was between 2 and 3 $^\circ\text{C}$ and the temperature of the air stream was typically within 0.5 $^\circ\text{C}$ of the ambient temperature inside the cabinet. To test for cooling on expansion, the thermocouple located at the air outlet was placed 3 cm below the air outlet, in the air-stream: the cooling on expansion was typically 1.0 to 1.5 $^\circ\text{C}$. The airstream was provided by a compressor and its dewpoint did not exceed 1 $^\circ\text{C}$.

The sample was positioned on a recording balance and the air stream was automatically turned off with a solenoid and timer for 10 s periodically. During this time the balance stabilized and the weight was measured automatically to generate a time series of weight. For the first 15 min of evaporation, when the rate of evaporation was changing rapidly, the weight was measured approximately every 150 s. Thereafter, the sampling interval was manually increased to 5 min, then 10 min and 20 min as the rate of evaporation diminished. The measurements ended when the rate of water loss became undetectable by the balance (10 μg resolution), at which point θ was assumed to be constant throughout the core and the final water content, θ_f , was then known.

Estimation of $D(\theta)$ by deconvolution of cumulative water loss through time

The data of cumulative water loss through time was deconvoluted to estimate $D(\theta)$ by numerically solving the one-dimensional flow equation, Eq. 3, subject to

the conditions in Eq. 4, where a constant boundary condition was set at the evaporating surface by fixing θ at $x=0$ equal to the θ_f measured in the experiment, and a zero flux boundary condition was set at $x=L$. Two simple functions were chosen to represent $D(\theta)$, each with three tunable parameters, a quadratic, Eq. 6, and an exponential, Eq. 7.

$$D(\theta) = a_0 + a_1\theta + a_2\theta^2 \quad (6)$$

$$D(\theta) = b_0 + b_1 \exp(b_2\theta) \quad (7)$$

These functions were chosen because their shapes approximate the $D(\theta)$ calculations made by Philip (1955) and the measurements by Rose (1968).

A program to solve Eq. 3, subject to the initial and boundary conditions in Eq. 4, was written in MATLAB®, modified from Campbell (1985). Equation 3 was expressed in finite difference form and the derivative at the three space coordinates ($i-1$, i , $i+1$) used to form a Jacobian matrix. The system of linear equations was then solved using the Thomas algorithm (Conte and De Boor 1972).

Each evaporation experiment was simulated using the experimental values of θ_i , θ_f , the length of the sample and an initial estimate of the parameters in either Eqs. 6 or 7 chosen to approximate the form of $D(\theta)$. An objective function was thereby created for the error between the cumulative evaporation from the experiment and simulation at each time point. These errors were minimized, using the least squares criterion, by optimizing the three $D(\theta)$ parameters in either Eqs. 6 or 7, using the downhill simplex optimization routine (Nelder and Mead 1965). The code we used was based on the “amoeba” of Press et al. (1986), converted from Fortran to MATLAB® by Keffer (1999). The iterative procedure was continued until the minimum error was reached or the maximum number of iterations was exceeded, both user defined.

We tested the ability of the downhill simplex to optimize to a unique solution by numerically generating evaporation data, using both eqs. 6 and 7, and starting the downhill simplex optimization routine with $D(\theta)$ parameters 75 % above and below the original parameters. In all cases the optimized $D(\theta)$ parameters were the same as those used in the original simulation.

The model was tested by comparing, at each time step, two different calculations of the quantity of

water, E [m], lost by evaporation: (1) by subtracting the integral of θ with space at a particular time, $t = i$, from the initial quantity of water in the soil, W_0 , (Eq. 8), and (2) the integral of the flux density with time at the evaporating surface using Eq. 9.

$$E = W_0 - \left[\int_{x=0}^{x=L} \theta(x, t) dx \right]_{t=i} \quad (8)$$

$$E = \left[\int_{t=0}^{t=i} D(\theta) \frac{\delta \theta}{\delta x} dt \right]_{x=0} \quad (9)$$

The accuracy of the program was tested by calculating the absolute difference between Eqs. 8 and 9 and expressing it as a percentage of the quantity of water lost as calculated from the integral of water content with space (Eq. 8). This error decreased with the number of space steps used and also with increasing time, as the major perturbations in θ in the first few distance steps at the start of the analysis became progressively damped. After 1000 s the error was less than 1 % with 100 distance steps, and less than 0.01 % with 1000 steps. We used 100 steps as the default in the analysis.

Summary of the procedure for obtaining $D(\theta)$ is as follows

Experiment

1. Equilibrate soil core at a given soil water suction and calculate θ_i from the soil water retention curve.
2. Seal the base of the core and place core on a recording balance.
3. Expose the top of the core to a turbulent atmosphere of constant vapour pressure and record the cumulative evaporation with time, $E(t)$, until dE/dt becomes negligibly close to zero and determine θ_f .

Analysis

1. Set up the objective function as the error between the cumulative evaporation from the experiment and simulation at each time point.
2. Set up the simulation by numerically solving Eq. 3 subject to the conditions in Eq. 4, using θ_i and θ_f determined above from the evaporation experiment and an initial guess at the $D(\theta)$

parameters a_0 , a_1 and a_2 in Eq. 6 or b_0 , b_1 and b_2 in Eq. 7.

3. Minimize the objective function using the least squares criterion by optimizing the $D(\theta)$ parameters a_0 , a_1 and a_2 in Eq. 6 or b_0 , b_1 and b_2 in Eq. 7, using the downhill simplex optimization routine (Nelder and Mead 1965).

Validation against the analyses of Doering (1965) and Passioura (1977)

The analysis described above was compared against the analyses of Doering (1965) and Passioura (1977). Neither of these is restricted to a specific function (such as quadratic or exponential) and both have been shown to accord reasonably with the analysis of Rose (1968). Doering's method works well when $D(\theta)$ is fairly flat, and Passioura's works well when $D(\theta)$ is strongly exponential, but overestimates $D(\theta)$ by about 25 % when $D(\theta)$ is flat, as happens especially when mean θ approaches its final value (Passioura 1977). Both of these methods estimate D at successive mean water contents during the outflow. By contrast, the deconvolution method estimates the parameters over the designated functions, quadratic or exponential, over the whole range of water contents, from initial to final, simultaneously.

Doering (1965) estimated $D(\theta)$ from one-step outflow by assuming that D was constant with distance in the core at a given time, but varied with time as the core dried. His approximate equation, derived from analysis of the one-dimensional diffusion equation is:

$$D(\theta) = - \frac{4L^2}{\pi(\theta - \theta_f)} \times \frac{\delta \theta}{\delta t} \quad (10)$$

Passioura (1977) estimated $D(\theta)$ where it is expected to be rising strongly exponentially, by noting that θ varies little with x at any given time, except where x is small, and that therefore, during the third stage of evaporation or liquid outflow, $d\theta/dt$ will be approximately constant where x is large enough—in practice, larger than about $0.2L$. This led to the following procedure:

1. Cumulative outflow is plotted with $t^{1/2}$ and the third stage identified.

2. From the third stage outflow data, $D(\theta)$ is calculated using Eq. 11.

$$D(\theta) = \delta F / \delta W_R \times L^2 / 2 \tag{11}$$

Where F is the rate of outflow and W_R is the water remaining in the soil.

3. The natural log of $D(\theta)$ is plotted against mean θ , $\bar{\theta}$, and the slope, B , of this curve calculated at:

$$\bar{\theta} = (\theta_i + \theta_f) / 2 \tag{12}$$

4. Approximations of small and large $\bar{\theta}$ are made using Eq. 13 for small $\bar{\theta}$ and Eq. 14 for large $\bar{\theta}$, where $\delta \approx 0.61/B$.

$$\theta = \theta_f + \pi/2(\bar{\theta} - \theta_f) \tag{13}$$

$$\theta = \bar{\theta} + \delta \tag{14}$$

5. The actual θ for D is determined by plotting the small and large $\bar{\theta}$ s against $\bar{\theta}$ and the region where the two lines meet is then smoothed by drawing a third line between the midpoints of the first two.

Boundary condition analysis

Evaporation was measured from the top of the core, $x = 0$, where, for the analysis, it was assumed that the water content was reduced to θ_f at the onset of evaporation. The acceptability of this assumption was tested by measuring the temperature at the soil surface (Fig. 1): there was an initial temperature depression of about 9 °C, that lasted for approximately 5 min, before the temperature started to increase back toward the ambient temperature.

The large initial temperature depression at the soil surface was due to latent heat required to change liquid water to vapour. The maximum temperature depression was steady for approximately 5 min and during this time it is reasonable to assume that liquid water was evaporating

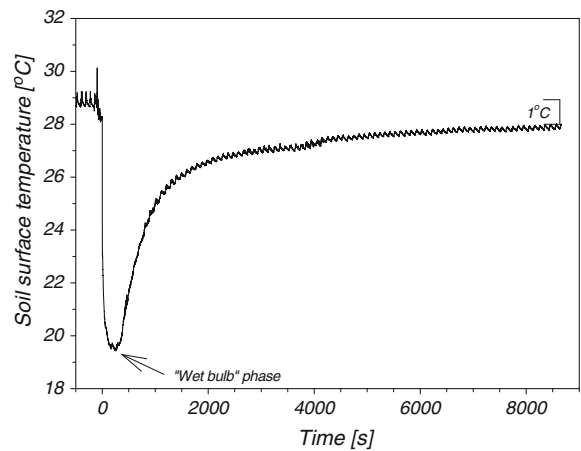


Fig. 1 Soil surface temperature, undisturbed field soil, measured by thermocouple as a function of time. The airstream is started at time = 0

fairly steadily from the soil surface and the system was behaving like a “wet bulb” thermometer. Thereafter, the temperature at the soil surface increased sharply and did so at the same time as the rate of evaporation was falling rapidly, as stage one ended and stage two began (Fig. 2).

The temperature of the air stream was between 28 and 29 °C and the dewpoint was between 0 and 1 °C, which corresponds to a vapour pressure of about 0.7 kPa. Assuming initially that the relative humidity

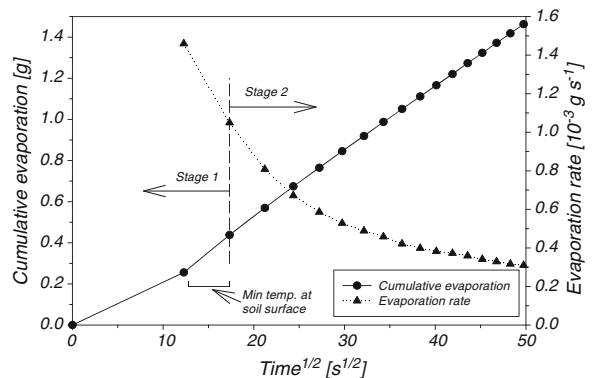


Fig. 2 Typical plot of cumulative evaporation and rate of evaporation as a function of time^{1/2} for the first 2500 s. The minimum temperature depression at the soil surface was attained around 250 s (~15.8 s^{1/2}) and the transition from stage 1 to stage 2 drying was evident at 300 s (~17.3 s^{1/2}). The rate of evaporation decreases approximately 25 % from when it is first measured at 150 s (~12.3 s^{1/2}) to the second measurement at 300 s. From the first measurement at 150 s to the fourth measurement at 600 s (~24.5 s^{1/2}) the rate of evaporation decreases approximately 50 %

of the soil surface was very close to 100 % (consistent with h of 1 m of water), at 28 °C the vapour pressure at the soil surface would be 3.8 kPa. When the initial rapid evaporation lowered the surface temperature to about 18 °C, it thereby reduced the saturated vapour pressure at the soil surface from 3.8 kPa (at 28 °C) to 2.1 kPa (at 18 °C). This effectively decreased the difference in vapour pressure across the boundary layer by about 50 %, which was maintained during the “wet bulb” phase (Fig. 1). The subsequent rise in temperature implies that the relative humidity at the soil surface was falling, consistent with the transition from the first to the second stage of drying, where the surface water content is constant: a 5 % fall in the relative humidity at the soil surface, from 100 to 95 %, corresponds to a suction of 700 m of water, at which the soil water content is typically within 5 % of its final value.

Figure 1 shows that eventually the soil surface temperature comes to within 1 °C of the ambient cabinet temperature (29 °C) after 10^4 s, about 1 % of the total time taken for the determination of $D(\theta)$. The difference of 1 °C between the soil surface temperature and the ambient temperature of the cabinet, was due to the cooling on expansion of the air stream, which was typically 1.0 to 1.5 °C (data not shown).

Results

$D(\theta)$ of undisturbed field soil

Figure 3 shows a typical plot of: (1) evaporation measured from an undisturbed field soil and (2) the absolute model error expressed as a fraction of the experimental data (error = $|\text{exp.} - \text{modell}|/\text{exp.}$) when using a quadratic (Eq. 6) and exponential (Eq. 7) function for $D(\theta)$. In most cases the error of the exponential $D(\theta)$ and quadratic $D(\theta)$ models is large and variable at small times, consistent with the assumption that the second stage of evaporation starts at time zero, but then falls to less than 1 % after 1×10^5 s ($\sim 300 \text{ s}^2$) (Fig. 3).

Figure 4 shows: (1) the means for the optimized quadratic and exponential $D(\theta)$ functions used to simulate the evaporation data as well as those for the Doering (1965) and Passioura (1977) analyses ($n=6$, three replicate soil cores ran twice each), and (2) the

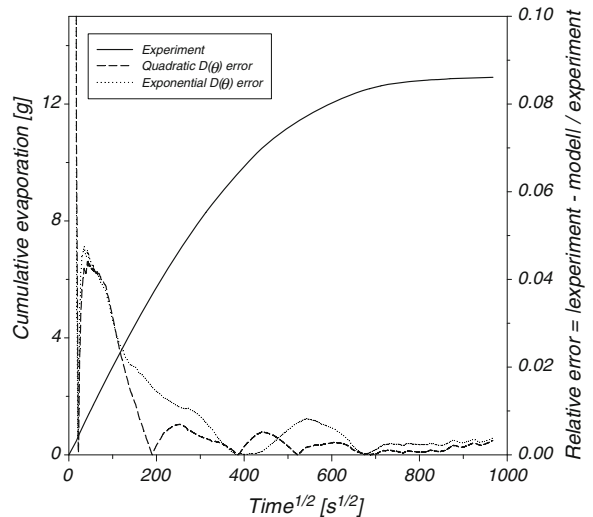


Fig. 3 Typical undisturbed soil replicate: measured cumulative evaporation (left y-axis) and absolute value of the relative modeling error (right y-axis) as a function of time^{1/2} when using quadratic (dashed line) and exponential (dotted line) $D(\theta)$. The sign of the error changes wherever the plot touches the x-axis

soil water retention data from 10 to 150 m of water suction, the range of interest for modeling the flow of water to the plant roots (the drained upper limit of plant available water for this soil is $0.25 \text{ [m}^3 \text{ m}^{-3}]$ and

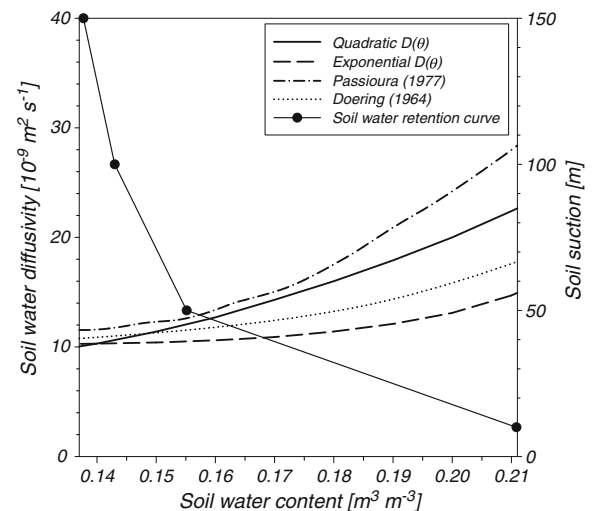


Fig. 4 Mean values of $D(\theta)$ over all 6 replicates for; (1) optimized quadratic (Eq. 6 where $a_0=1.682 \times 10^{-8}$, $a_1=-1.917 \times 10^{-7}$ and $a_2=1.038 \times 10^{-6}$) and exponential (Eq. 7 where $b_0=1.035 \times 10^{-8}$, $b_1=8.238 \times 10^{-13}$ and $b_2=4.096 \times 10$) $D(\theta)$ functions and analyses of Passioura (1977) and Doering (1965) (left y-axis) and (2) soil water retention curve (right y-axis)

is reported in Fig. 1 of Kirkegaard et al. 2007). The quadratic and exponential $D(\theta)$ functions shown in Fig. 4 are:

quadratic (Eq. 6) $a_0=1.682 \times 10^{-8}$, $a_1=-1.917 \times 10^{-7}$ and $a_2=1.038 \times 10^{-6}$

and exponential (Eq. 7) $b_0=1.035 \times 10^{-8}$, $b_1=8.238 \times 10^{-13}$ and $b_2=4.096 \times 10$

In the suction range from 10 to 150 m of water, the mean quadratic $D(\theta)$ ranged from 22×10^{-9} to 10×10^{-9} [$\text{m}^2 \text{s}^{-1}$] and the mean exponential $D(\theta)$ ranged from 14×10^{-9} to 10×10^{-9} [$\text{m}^2 \text{s}^{-1}$].

Discussion

The rationale for this work was to measure soil water diffusivity, $D(\theta)$, on undisturbed field soil, which is a necessary function for understanding what may limit the uptake of water by crops from the subsoil. Crops often leave substantial amounts of seemingly available water in the subsoil at harvest (e.g. most recently Christopher et al. (2008) and Kirkegaard et al. (2007)), and the reasons why are unclear. It is often assumed that flow of water through the soil may be limiting uptake when the available water is starting to run out, at suctions above about, say, 50 m, but common estimates of D for this stage are in the order $10^{-9} \text{m}^2 \text{s}^{-1}$ (e.g. Rose 1968; Passioura 1977, 1980 and Stirzaker and Passioura 1996), which is large enough to provide almost complete uptake by even sparse roots during the few weeks of grain filling (Passioura 1983, 1991).

This can be illustrated using the framework provided by Passioura (1991), where the time constant for the uptake of water by a root in a cylinder of soil of radius b (i.e. average distance to the water shed between adjacent roots) is $2b^2/D$. The time constant is the time taken for the average water content between adjacent roots to fall to $1/e$ (i.e. ~ 0.37) of a given starting value. Assuming the root length density to be approximately 0.1 [cm cm^{-3}] (resulting in b of about 2 cm), as was measured in the same field from which the soil samples used in this study were taken (White and Kirkegaard 2010; Kirkegaard et al. 2007) and, given that we calculate D to reach a constant minimum of approximately 10×10^{-9} [$\text{m}^2 \text{s}^{-1}$] from 50 to 150 m of suction (Fig. 4) or about 10 [$\text{cm}^2 \text{d}^{-1}$], the time constant would be about 1 day. That is, the amount of water remaining in the water shed

between adjacent roots, separated by distance b , would be reduced by a factor of about 2.7 ($1/0.37$) every day. Thus, if the roots are maintaining a large suction (say, 150 m) and therefore a low water content at their surfaces, then only about 5 % of the initially available soil water would be left after only 3 days. If the root length density was only 0.01 [cm cm^{-3}], then by the same argument it would take the roots only about a fortnight to extract almost all of the available soil water. Yet paradoxically, roots often fail to extract much of the available soil water in the subsoil by the time of harvest (Christopher et al. 2008; Kirkegaard et al. 2007).

We hypothesized that D might be much smaller in undisturbed soil than in the repacked soils that almost all estimations of $D(\theta)$ have been made on, and that this could account for the slow uptake. Our calculations showed instead that D was an order of magnitude larger than had previously been reported at suctions prevailing during the uptake of the last half of the available water supply (Fig. 4)—cf. Rose (1968), who showed that $D(\theta)$ obtained a minimum value of approximately 10^{-9} [$\text{m}^2 \text{s}^{-1}$] at a suction of approximately 150 m, for several soils. Further, this was not because the samples were undisturbed, because the same samples broken up and repacked to the same bulk density gave similar $D(\theta)$ (data not shown).

We explored the possibility that the large values of D might be an artifact arising from the large depressions of temperature at the surfaces of the cores of soil during the rapid evaporation into dry turbulent air that occurred at the start of each experiment. However, the temperatures returned to close to ambient within a sufficiently short time (Figs. 1 and 2), thereby avoiding temperature induced water flow and the associated errors discussed in detail by van Grinsven et al. (1985).

We tested the technique, introduced in this paper, of deconvoluting the evaporation data to arrive at values of the parameters in likely approximate functions for $D(\theta)$ (quadratic and exponential) by comparing it with the techniques of Doering (1965) and Passioura (1977), which had previously been shown to agree tolerably well with the technique of Rose (1968), which still remains the standard for accurate measurement of $D(\theta)$, but is restricted to repacked soil.

The deconvolution technique estimates $D(\theta)$ as a function covering the complete range of θ , from its initial value to its final, in a way that gives equal value to the data at every stage of the drying, whereas the

techniques of Doering (1965) and Passioura (1977) estimate $D(\theta)$ independently at any given mean water content. It is therefore possible that they may not converge over the range of suctions of most interest (50 to 150 m). Nevertheless, they did converge within a range of about $\pm 30\%$ at these large suctions.

As discussed above, these unusually large values of $D(\theta)$ we calculated in the Kandosol subsoil, cf. Rose (1968), cast doubt on the possibility that flow of water through the soil on the scale of the rhizosphere (mm) is in itself limiting the rate of uptake of water by the roots. Nevertheless, strong clumping of the roots into pre-existing pores (Passioura 1991; White and Kirkegaard 2010), which may be tens of mm apart, could still generate limiting flow rates in the soil. This and other possibilities are explored in part II of this series.

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References

- Angus JF, van Herwaarden AF (2001) Increasing water use and water use efficiency in dryland wheat. *Agron J* 93(2):290–298
- Boltzmann L (1894) Zur integration des diffusionsgleichung bei variabeln diffusions coefficienten. *Ann Phys* 53:959–964
- Campbell GS (1985) Soil physics with BASIC: transport models for soil-plant systems. *Developments in soil science*, vol 14. Elsevier, Amsterdam
- Christopher JT, Manschadi AM, Hammer GL, Borrell AK (2008) Developmental and physiological traits associated with high yield and stay-green phenotype in wheat. *Aust J Agric Res* 59(4):354–364
- Conte SD, De Boor C (1972) Elementary numerical analysis: an algorithmic approach. *International series in pure and applied mathematics*, 2nd edn. McGraw-Hill, New York
- Crescimanno G, Iovino M (1995) Parameter-estimation by inverse method based on one-step and multistep outflow experiments. *Geoderma* 68(4):257–277
- Dardanelli JL, Ritchie JT, Calmon M, Andriani JM, Collino DJ (2004) An empirical model for root water uptake. *Field Crop Res* 87(1):59–71
- Doering EJ (1965) Soil-water diffusivity by the one-step method. *Soil Sci* 99(5):322–326
- Gardner WR (1956) Calculation of capillary conductivity from pressure plate outflow data. *Soil Sci Soc Am Proc* 20:317–320
- Gupta SC, Farrell DA, Larson WE (1974) Determining effective soil-water diffusivities from one-step outflow experiments. *Soil Sci Soc Am J* 38(5):710–716
- Hopmans JW, Vogel T, Koblik PD (1992) X-Ray tomography of soil-water distribution in one-step outflow experiments. *Soil Sci Soc Am J* 56(2):355–362
- Hurd EA (1974) Phenotype and drought tolerance in wheat. *Agric Meteorol* 14(1–2):39–55
- Idso S, Reginato R, Jackson R, Kimballa B, Nakayama F (1974) The three stages of drying of a field soil. *Soil Sci Soc Am J* 38(5):831–837
- Isbell RF (2002) The Australian soil classification, vol 4. Australian soil and land survey handbook series. CSIRO Publishing, Melbourne
- Jordan WR, Miller FR (1980) Genetic Variability in Sorghum Root Systems: Implication for Drought Tolerance. In: Turner NC, Kramer PJ (eds) *Adaptation of Plants to Water and High Temperature Stress*. Wiley Interscience, New York, pp 383–399
- Keating BA, Carberry PS, Hammer GL, Probert ME, Robertson MJ, Holzworth D, Huth NI, Hargreaves JNG, Meinke H, Hochman Z, Mclean G, Verburg K, Snow V, Dimes JP, Silburn M, Wang E, Brown S, Bristow KL, Asseng S, Chapman S, Mccown RL, Freebairn DM, Smith CJ (2003) An overview of Apsim, a model designed for farming systems simulation. *Eur J Agron* 18(3–4):267–288
- Keffer D (1999) ChE 505 Library of MATLAB® Subroutines. <http://clausius.engr.utk.edu/che505/text/codes.html>. Accessed 20 October 2006
- Kirkegaard JA, Lilley JM, Howe GN, Graham JM (2007) Impact of subsoil water use on wheat yield. *Aust J Agric Res* 58(4):303–315
- Londra PA, Valiantzas JD (2011) Soil water diffusivity determination using a new two-point outflow method. *Soil Sci Soc Am J* 75(4):1343–1346. doi:10.2136/sssaj2010.0448
- Matano C (1933) On the relation between the diffusion-coefficients and concentrations of solid metals (The Nickel-Copper System). *Jpn J Phy* 8:109–113
- Muazu S, Skopp J, Swartzendruber D (1990) Soil-water diffusivity determination by a modified one-step outflow method. *Soil Sci Soc Am J* 54(4):1184–1186
- Nelder JA, Mead R (1965) A simplex method for function minimization. *Comput J* 7:308–313
- Passioura JB (1977) Determining soil water diffusivities from one-step outflow experiments. *Aust J Soil Res* 15(1):1–8
- Passioura JB (1980) The transport of water from soil to shoot in wheat seedlings. *J Exp Bot* 31(120):333–345
- Passioura JB (1983) Roots and drought resistance. *Agric Water Manag* 7(1/3):265–280
- Passioura JB (1991) Soil structure and plant-growth. *Aust J Soil Res* 29(6):717–728
- Passioura JB, Angus JF (2010) Improving Productivity of Crops in Water-Limited Environments. In: Sparks DL (ed) *Advances in Agronomy*, Vol 106, vol 106. *Advances in Agronomy*, pp 37–75
- Philip JR (1955) The concept of diffusion applied to soil water. *Proc Nat Acad Sci Ind A* 24:93–104
- Press WH, Flannery BP, Teukolsky SA, Vetterling WT (1986) *Numerical recipes: The art of scientific computing*. Cambridge University Press, Cambridge

- Ritchie JT (1985) A user-oriented model of the soil water balance in wheat. In: Wheat growth and modelling/edited by W. Day and R. K. Atkin. NATO ASI series: series A. Life sciences, vol v.86. Plenum in cooperation with NATO Scientific Affairs Division, New York, pp 293–305
- Robertson MJ, Fukai S, Ludlow MM, Hammer GL (1993a) Water Extraction by Grain-Sorghum in a Subhumid Environment. 1. Analysis of the Water Extraction Pattern. *Field Crop Res* 33(1–2):81–97
- Robertson MJ, Fukai S, Ludlow MM, Hammer GL (1993b) Water Extraction by Grain-Sorghum in a Subhumid Environment. 2. Extraction in Relation to Root-Growth. *Field Crop Res* 33(1–2):99–112
- Rose DA (1968) Water movement in porous materials III. Evaporation of water from soil. *Br J Appl Phys* 1(2):1779–1791
- Schultz JE (1971) Soil water changes under fallow-crop treatments in relation to soil type, rainfall and yield of wheat. *Aust J Exp Agric Anim Husb* 11:236–242
- Schultz JE (1972) The effect of surface treatments on soil water storage and yield of wheat. *Aust J Exp Agric Anim Husb* 12(56)
- Simunek J, van Genuchten MT, Sejna M (2008) Development and applications of the HYDRUS and STANMOD software packages and related codes. *Vadose Zone J* 7(2):587–600
- Stirzaker RJ, Passioura JB (1996) The water relations of the root-soil interface. *Plant Cell Environ* 19(2):201–208
- Thomas FS, Hammer GL (1995) Growth and yield response of barley and chickpea to water stress under three environments in southeast Queensland. II. Root growth and soil water extraction pattern. *Aust J Agric Res* 46(1):35–48
- Valiantzas JD, Londra P, Salsalou A (2007) Explicit formulae for soil water diffusivity using the one-step outflow technique. *Soil Sci Soc Am J* 71(6):1685–1693
- van Dam JC, Stricker JNM, Droogers P (1992) Inverse method for determining soil hydraulic functions from one-step outflow experiments. *Soil Sci Soc Am J* 56(4):1042–1050
- van Grinsven JJM, Dirksen C, Bouten W (1985) Evaluation of the hot air method for measuring soil water diffusivity. *Soil Sci Soc Am J* 49(5):1093–1099
- Walter CJ, Barley KP (1974) The Depletion of Soil Water by Wheat at Low, Intermediate, and High Rates of Seeding. *Transactions, 10th International Congress of Soil Science*, I:150–158
- White RG, Kirkegaard JA (2010) The distribution and abundance of wheat roots in a dense, structured subsoil—implications for water uptake. *Plant Cell Environ* 33(2):133–148
- Zia-ul-Haque (1990) A Computerized One-Step Outflow Method for Measurement of Soil Water Diffusivity. *Soil physics: application under stress environments Proceedings of the International Symposium on Applied Soil Physics in Stress Environments, Islamabad, Pakistan, 22–26 January 1989:70–77*