



## Comparison of the root water uptake term of four simulation models

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## Abstract

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Water uptake by plant roots is an important component of the soil water balance. In this report we studied four water uptake models, of different complexity, that were all embedded in a greater model dealing with transport of water in (an unsaturated) soil. Though also some attention was paid to performance of the routines by themselves, the focus was directed to their functioning as a part of the greater models. We examined the results of two scenarios of potential transpiration and precipitation, comprising a period of 16 days. As could be expected the models yielded different results, but the differences in actual transpiration are modest due to feedback mechanisms.

Keywords: model comparison, root length density, root water uptake, root zone, simulation model, soil, transpiration

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# Preface

On 10-12 September 2008 a WIMEK-NUPUS-PE&RC Workshop entitled *Roots, An Interdisciplinary Link* was held in Wageningen. During and after some discussions, the authors of this report decided to perform a comparison of the water uptake routines of models they presented at that workshop. This report is the result of that comparison.



# Summary

Most models dealing with the water cycle in the vadose zone of the soil treat the calculation of macroscopic transport of water in the soil profile in essentially the same way, by numerically solving Richards equation. The treatment of boundary conditions, e.g. soil evaporation and drainage, however, shows much more differences. This applies a fortiori to the description of water uptake by a root system as here not only physical but also biological phenomena play a role.

The goal of this report is to compare four water uptake (WU) routines of diverging complexity, both as they operate as stand-alone, and as they function in the greater models they are part of. The soil models used were SWAP (1D) (Kroes et al., 2008), FUSSIM2 (2D) (Heinen and De Willigen 1998; Heinen, 2001) and RSWMS (3D) (Javaux et al., 2008). Within SWAP two root WU functions are presented: the macroscopic Feddes function (Feddes et al., 1978) (SWAP-macro), and the recently developed microscopic root water uptake model of De Jong van Lier et al. (2008) (SWAP-micro). In FUSSIM2 the root WU model of De Willigen and Van Noordwijk (1987) is used, and the WU model in RSWMS is obtained by coupling the Richards equation to the Doussan equation (Doussan et al., 1998), which explicitly solves the water flow in a root system given its 3D architecture. Besides the differences in dimensionality of the models, the complexity of the processes considered in root water uptake increases from SWAP-macro, SWAP-micro, FUSSIM2 to RSWMS. The RSWMS model is the most complex model that takes into account the following aspects: pressure head in soil, pressure head at soil root interface, root water potential, radial root resistance, and axial root resistance. Except for the axial root resistance in FUSSIM2 these aspects are also considered. In both SWAP models the root parameters are not considered. In SWAP-micro both the pressure head in the soil and at the soil-root interface is considered, while SWAP-macro only considers pressure head in the soil.

Before comparing the WU models, we first established that the numerical solution of the Richards equation in the three full models were identical by mutual comparison for an infiltration scenario.

Next water uptake from a 1D soil column was simulated for a fixed root length density distribution and a constant daily required amount of transpiration. Computations were done for three soil types: a sand, a clay and a loam. The following findings were obtained.

- In case a snapshot of WU is taken when all models were subject to the same pressure head distribution in the soil, the WU uptake distribution with depth differed between the four models. This reveals that the mathematical description of the models is truly different.
- For a 30 d period of transpiration with one rainfall event at d 15, large differences exist in the time of onset of transpiration reduction and pressure head distribution in the (bulk) soil with depth, but differences in cumulative transpiration over the period of 30 days were (relatively) small. So, apparently, in the full models (Richards equation plus root water uptake function) the pattern of water uptake differs not so much. This is caused by feedback mechanisms: the tendency of the soil to aim at equilibrium of total head and consequently at evening out of differences in total head, and secondly by the fact that in all water uptake routines the uptake in a certain layer depends directly or indirectly on the pressure head in that layer, where lower values of pressure head lead generally to lower uptake. In case of SWAP-macro uptake is completely determined by the local pressure head, for the other three models the uptake in a certain layer is also determined by the uptake possibilities in other layers. This can lead to total compensation, where uptake in some layers can make up for uptake deficit in others.
- At wet conditions, water uptake is proportional to the root length density distribution in the soil. At dry situations, the SWAP-micro, FUSSIM2 and RSWMS models predict a shift in water uptake to wetter layers in order to fulfill the demand. The compensation in all three models occurs as a 'natural' consequence of the mathematical description of uptake. However, each model differs in the exact compensation effect.

- In case the daily transpiration demand was sinusoidally distributed over the day the total actual uptake by the SWAP-micro, FUSSIM2 and RSWMS models was less than when it was taken constant over the day. Opposite to the SWAP-macro model, these models are sensitive to the instantaneous transpiration flux. It seems that RSWMS is more sensitive to the instantaneous flux than the other models. It is probably due to the three dimensional character of RSWMS. Indeed, as soon as the potential demand is high, the local fluxes increase as well, which create a sudden drop of water content and conductivity in the voxels close to the root nodes. As the lateral redistribution is not instantaneous (as it is in 2D or 1D models, when the depth-averaged water potential is felt by the root), high flux may create more rapidly local low potentials, which generate stress during the middle of the day.

A model, by definition, is a simplification of part of the real world. In making a model one tries to leave out as much as possible, with the intent to include only the processes which really do matter for the phenomena one wants to study. It is therefore difficult to give a general recommendation as to which of the models discussed here can best be used, this depends on the purpose of the user and the data available. For instance, if one is interested in simulation of the transpiration in the growing season and data on distribution of root length density are not available SWAP-macro seems a suitable choice. At the other end of the spectrum one finds the model RSWMS that is more flexible and by which subtleties of differences in radial and axial conductance can be investigated at the scale of a single plant. Another example is the actual flow pattern in the root zone. If this flow pattern is predominantly vertical, as in close, uniform covered cultivated soils, a one-dimensional approach as used by SWAP-macro and SWAP-micro may suffice. However, at two-dimensional or radial symmetric flow patterns for instance in case of drip irrigation, FUSSIM2 might be more suitable. In case of three-dimensional patterns analysis by RWSMS may be justified.

# 1 Introduction

The proper estimation of water extraction by plant roots is of interest for a range of different environmental and agricultural applications. The first root water uptake models developed in the field of soil sciences appeared in the 60's of the previous century. Since then, numerous models have appeared with different theoretical bases, assumptions, processes and dimensionality.

In this report, we compare four models (denoted by SWAP-macro, SWAP-micro, FUSSIM2 and RSWMS), relying on very different uptake concepts, at water scarce conditions. The models have some characteristics in common: they solve Richards equation by the same numerical methods, and they apply to the same time scale (a growing season, a year) and spatial scale (an area of some square meters up to one hectare, a depth of the rootable part of the vadose zone in case of arable crops which amounts to 1 - 1.5 m). SWAP-macro and FUSSIM2 have also been applied to periods of decades of years and regional spatial scale. Where the models do differ is in the treatment of water uptake by plant roots and bare soil evaporation. For the sake of comparison we do not consider soil evaporation here.

Extensive reviews of concepts for soil water extraction by roots have been given by Feddes and Raats (2004) and Hopmans and Bristow (2002). These reviews distinguish between microscopic models, which consider the radial flow towards single roots, and macroscopic models which view the root zone as a soil-root continuum with vertical gradients in water content and root density. Today, in addition to these two types of models a series of *hybrid* models have been developed, which work at the plant scale but explicitly consider the water movement to each root or solve local equations to predict 2D or 3D water flow. An example of a hybrid model is given by Pronk et al. (2007) who coupled FUSSIM2 to a plant growth model.

The availability of such a wide range of root water uptake concepts makes the choice less easy for specific applications. Comparison between models is, therefore, needed in order to assess how the underlying assumptions or concepts may affect root water uptake predictions.

A well-known macroscopic model is the Feddes model (Feddes et al., 1978; Belmans et al., 1983). Although this model has been very useful, it has also some severe shortcomings for specific applications. For instance, the model does not consider compensation of root water uptake when drought or oxygen stress occurs in part of the root zone. Also, the empirical reduction function for root water extraction only implicitly accounts for the effect of soil hydraulic functions, radial and longitudinal root resistances and root water potentials. Therefore the coefficients of this empirical reduction function require calibration to specific vegetation - soil - climate combinations. The Feddes concept has been implemented in the SWAP model (Kroes et al., 2008).

In their thesis, de Willigen and van Noordwijk (1987) focused on a more physical, microscopic approach to model both water and nutrient uptake. Different from the common approach followed by soil physicists, they did not stop at the soil-root interface, but included a radial resistance for water flow inside the roots. Their concept has been implemented in the FUSSIM2 model (Heinen and De Willigen, 1998), which focuses on two-dimensional transport processes in the vadose zone. This model has been very useful to clarify the role of various physical factors in root water uptake, such as soil hydraulic functions, root length density, transpiration rate and radial root resistance.

A similar physical approach for root water uptake has been followed by de Jong van Lier et al. (2008), although they did stop at the root - soil interface. They reasoned that in situations with serious soil water deficit, the main hydraulic resistance occurs in the soil. Therefore they focused on the water movement in the soil and considered the root system as a black box which just extracts water. Their concept has been implemented in the SWAP model (Kroes et al., 2008) and includes osmotic stress due to salinity and compensation when stress occurs in certain parts of the root zone.

In recent years the increasing computational capacity and development of microscopic measurement techniques for root water uptake create avenues for an even more detailed physical based modeling approach. A clear example is the RSWMS model (Javaux et al., 2008) which accommodates 3-dimensional rooting patterns with detailed water movement. RSWMS simulates 3-dimensional soil water flow, flow towards the roots, and radial and longitudinal flow inside the root system. This creates new research possibilities on the important feedback mechanisms occurring in the rhizosphere when soil moisture becomes limiting.

In this report, we show the performance of various modeling concepts covering a broad range of assumptions for well-defined drought situations. Four models were involved in the comparison in the comparison, these are given by their acronyms SWAP-macro, SWAP-micro, FUSSIM2, and RSWMS. Table 1 gives references for the description and application of the models.

**Table 1**

*References for description and applications of the models.*

<b>Model</b>	<b>Description</b>	<b>Application</b>
SWAP-macro	Kroes et al., 2008	Droogers et al., 2000; Hupet et al., 2004; Van Dam et al., 2006
SWAP-micro	De Jong van Lier et al. 2008	De Jong van Lier et al., 2009
FUSSIM2	Heinen and De Willigen 1998; Heinen, 2001	Heinen, 1997, 2001; Heinen et al. 2003; Pronk et al. 2007
RSWMS	Javaux et al., 2008	Draye et al., 2010

We particularly investigate how the four models cope with hydraulic lift compensation mechanisms and effect of soil on uptake. With hydraulic lift we mean root water excretion, when the xylem pressure heads exceeds the pressure head at the root-soil interface. So hydraulic lift may also denote downward movement of water by the root system. Each of these models also differ by its intrinsic complexity. The importance of such a complexity against modeling performances is also assessed in this report.

For the comparison three scenarios will be considered. In the first one we check whether the models concerned do give similar results with respect to the basic processes of soil water flow. The other two scenarios specifically aim at comparing the respective water uptake routines.

## 2 Governing equations

### 2.1 Richards equation

The partial differential equation solved numerically by the four models is the so-called Richards equation, here given in its general form with a sink term:

$$\frac{\partial \theta}{\partial t} = \nabla \cdot \{K(h)\nabla h\} + \frac{\partial K(h)}{\partial z} - S \quad (1)$$

where  $\theta$  denotes the volumetric water content in soil ( $\text{cm}^3 \text{ cm}^{-3}$ ),  $\nabla \cdot$  is the divergence operator ( $\text{cm}^{-1}$ ),  $\nabla$  is the gradient operator ( $\text{cm}^{-1}$ ),  $z$  the vertical coordinate (positive upward; cm),  $h$  the pressure head (cm),  $K(h)$  the hydraulic conductivity ( $\text{cm d}^{-1}$ ), and  $S$  is a sink term ( $\text{cm}^3 \text{ cm}^{-3} \text{ d}^{-1}$ ) which will be explained in the next section. Eq. (1) is nonlinear both because of the nonlinear relation between  $h$  and  $\theta$ , and that between  $K$  and  $h$  (or  $\theta$ ). Both relations can be expressed in closed form equations, we used the well-known van Genuchten (1980)  $\theta(h)$  function and the Mualem (1976)  $K(h)$  or  $K(\theta)$  functions. The Richards equation is numerically solved in 1D in SWAP, in 2D in FUSSIM2 and in 3D in RSWMS.

### 2.2 Sink term

The four models have a different way of formulating the root water uptake  $S$ . Transpiration reduction due to water stress is present in all the models but three of them (SWAP-macro, SWAP-micro and FUSSIM2) have an explicit reduction function. For some selected parameters and for low and moderate root length densities the reduction functions of these three models will be graphically presented. In addition, for SWAP-macro and SWAP-micro the pressure head below which transpiration reduction occurs is explicitly known. For FUSSIM2 this has to be approximated as will be shown later (section 4.2.2). In RSWMS, there is a limiting xylem pressure head below which transpiration is no longer sustained. The critical pressure head will be presented as a function of root length density for the first three models.

We will give below a brief description of the root water uptake routines for a one-dimensional profile of total length  $L$  (cm) and subdivided in  $n$  layers of thickness  $\Delta z_i$  with a root length density of  $L_{m,i}$  ( $\text{cm cm}^{-3}$ ). The potential transpiration rate is denoted by  $T_P$  ( $\text{cm}^3 \text{ cm}^{-2} \text{ d}^{-1}$ ).

When discussing the uptake routine we will first consider the reduction of potential transpiration due to soil and plant properties and environmental conditions as experienced by a single root, or rather a single soil layer, and next the up-scaling of the single root to a complete root system.

The order of presentation of the models is that of increasing complexity of the reduction function. The reduction in SWAP-macro is determined by the average pressure head in the soil. In SWAP-micro the influence of matric flux potential (the integral of soil conductivity with respect to pressure head), radial flow and root length density is added. FUSSIM2 adds to these factors the root radial conductance and the root water potential. Finally, as most complex model, RSWMS takes also the axial conductance into account. Table 2 gives an overview.

**Table 2***Variables and parameters considered in the water uptake routine of the different models*

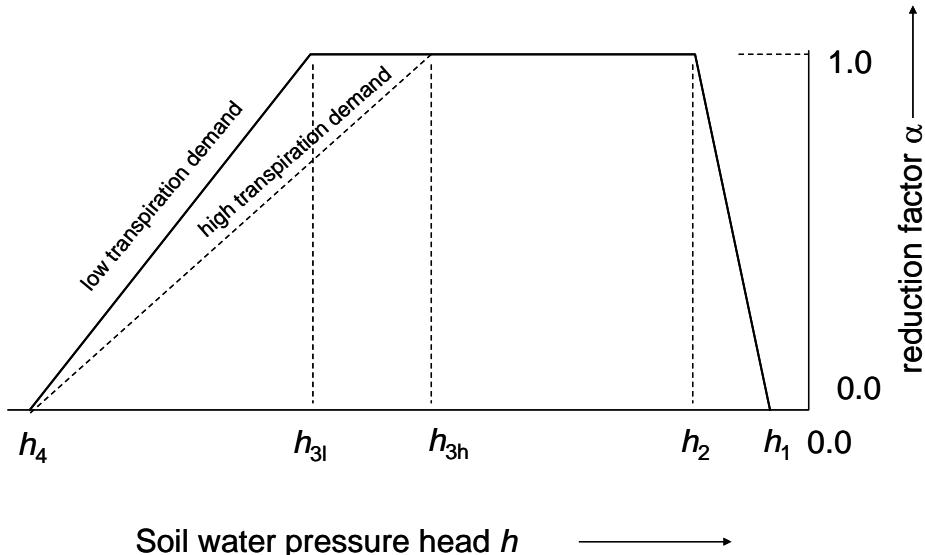
	SWAP		FUSSIM2	RSWMS
	macro	micro		
Pressure head in soil	X	X	X	X
Pressure head at soil root interface		X	X	X
Root water potential			X	X
Radial root resistance			X	X
Axial root resistance				X

### 2.2.1 SWAP-macro

The SWAP model calculates the transport of water in one dimension in an unsaturated soil profile. We start by first considering a single layer. The actual uptake rate ( $S_a$ ) of this layer equals the required uptake rate ( $S_r$ ) multiplied by a coefficient  $\alpha$  that is a function of the soil pressure head in the layer:

$$S_a = \alpha(h) S_r \quad (2)$$

The uptake rate is expressed in  $\text{cm}^3 \text{ cm}^{-3} \text{ d}^{-1}$ . The relation between  $h$  and  $\alpha$  is shown in Figure 1.

**Figure 1***Reduction coefficient ( $\alpha$ ) as a function of pressure head ( $h$ ) as used in SWAP-macro.*

For a monolayer the required uptake rate is the potential transpiration divided by layer thickness:

$$S_r = \frac{T_p}{L} \quad (3)$$

In scaling up from a monolayer to a multilayer system Kroes and van Dam (2003) corrected the required uptake rate of a layer by the relative root length density in that layer

$$S_{r,i} = \frac{\lambda_i T_p}{\Delta z_i} \quad (4)$$

where  $\lambda_i$  is the relative root length density in a layer defined as:

$$\lambda_i = \frac{\Delta z_i L_{rv,i}}{\sum_{i=1}^n \Delta z_i L_{rv,i}} \quad (5)$$

The actual uptake rate of layer  $i$  is thus given as:

$$S_{a,i} = \alpha_i S_{r,i} \quad (6)$$

The total actual uptake rate  $T_a$  of the root system is the sum of the individual uptake rates multiplied by layer thickness:

$$T_a = \sum_{i=1}^n \Delta z_i S_{a,i} = T_p \sum_{i=1}^n \lambda_i \alpha_i \quad (7)$$

Equation (7) implies that in case of small differences in soil pressure head, leading to an almost constant reduction coefficient, the distribution of the water uptake with depth is almost completely determined by the distribution of root length density.

**Summarizing:** for a given pressure head and relative root length distribution the hydraulic properties and absolute root length densities in the soil do not play a role. In a dynamic situation where the moisture content is changing, the soil hydraulic functions play a central role as these determine the decrease in pressure head for a given decrease in moisture content and vertical soil water redistribution. In case of drought stress in certain parts of the root zone, no compensation by extra root water uptake in wetter zones occurs.

## 2.2.2 SWAP-micro

SWAP-micro (De Jong van Lier et al., 2008) takes, contrary to SWAP-macro, the gradients of water content and pressure head from soil to root into account. They start with considering a monolayer: a single root confined within a soil cylinder of radius  $R_1 = 1/\sqrt{\pi L_{rv}}$  (cm). Then they solve the partial differential equation (pde) for radial transport of water in the cylinder to a root with radius  $R_0$  (cm). This pde follows from Eq. (1) without a sink term in radial coordinates and disregarding gravity:

$$\frac{\partial \theta}{\partial t} = \frac{1}{R} \frac{\partial}{\partial R} R K(b) \frac{\partial b}{\partial R} \quad (8)$$

where  $R$  is the distance from the axial centre. A solution is achieved by assuming a steady rate situation, i.e. the rate of water content decrease  $\partial \theta / \partial t$  is assumed to be independent of radial distance:

$$\frac{\partial \theta}{\partial t} = -S_r = -\frac{T_p}{Z_{root}} \quad (9)$$

where  $Z_{\text{root}}$  is the thickness of the root zone. A solution of Eq. (8) can be derived in terms of the matric flux potential, which is defined as:

$$\Phi = \int_{h_w}^b K(x) dx = \int_{\theta_w}^{\theta} D(x) dx \quad (10)$$

where  $\Phi$  is the matric flux potential ( $\text{cm}^2 \text{ d}^{-1}$ ),  $K$  the soil hydraulic conductivity ( $\text{cm d}^{-1}$ ),  $D$  the hydraulic diffusivity ( $\text{cm}^2 \text{ d}^{-1}$ ),  $h_w$  the pressure head at wilting point and  $\theta_w$  the corresponding water content. Combining Eqs. (8), (9) and (10), the partial differential equation to be solved becomes:

$$\frac{1}{R} \frac{\partial \Phi}{\partial R} + \frac{\partial^2 \Phi}{\partial R^2} = -S_r \quad (11)$$

The boundary conditions used are: a given value for the matric flux potential at the root surface:

$$R = R_0, \Phi = \Phi_0 \quad (12)$$

and a flux condition at the root surface following from the required uptake rate:

$$R = R_0, \frac{\partial \Phi}{\partial R} = \frac{R_1^2}{2R_0} S_r \quad (13)$$

The solution of Eq. (11) with Eqs. (12) and (13) is:

$$\Phi = \Phi_0 + \frac{S_r}{4} \left( R_0^2 - R^2 + 2(R_0^2 + R_1^2) \ln \left( \frac{R}{R_0} \right) \right) \quad (14)$$

Equation (14) is thus the solution when the uptake rate is constant. It is assumed that the uptake proceeds according to the potential transpiration as long as the matric flux potential at the surface of the root ( $\Phi_0$ ) is higher than that corresponding to permanent wilting point ( $\Phi_w$ ). If that is not the case, the flux boundary condition Eq. (13) is replaced by a potential boundary condition:

$$R = R_0, \Phi_0 = \Phi_w = 0 \quad (15)$$

Then for any uptake rate  $S$ , Eq. (14) is generalized:

$$\Phi(R) = \Phi_0 + \frac{S}{4} \left( R_0^2 - R^2 + 2(R_0^2 + R_1^2) \ln \left( \frac{R}{R_0} \right) \right) \quad (16)$$

The potential  $\Phi_0$  is either the matric flux potential corresponding to wilting point or has a value higher than wilting point.

Finally Eq. (16) is written with the value of  $\Phi(R)$  corresponding to the average value of water content in the soil cylinder. By numerical simulation, this value was found to be proportional to  $R_1$  with proportionality factor  $a$ . Making the uptake rate explicit one gets:

$$S = \frac{4(\bar{\Phi} - \Phi_0)}{R_0^2 - a^2 R_1^2 + 2(R_0^2 + R_1^2) \ln\left(\frac{aR_1}{R_0}\right)} = w_{mi}(\bar{\Phi} - \Phi_0) \quad (17)$$

where  $w_{mi}$  is given by:

$$w_{mi} = \frac{4}{R_0^2 - a^2 R_1^2 + 2(R_0^2 + R_1^2) \ln\left(\frac{aR_1}{R_0}\right)} \quad (18)$$

For commonly observed values of the root length density (0.1 - 5 cm cm<sup>-3</sup>) and root radius (0.01 - 0.05) of arable crops,  $R_1 \gg R_0$ . So  $w_{mi}$  can be given by (using  $R_1^2 = 1/\pi L_{rv}$ ):

$$w_{mi} \approx \frac{4}{-a^2 R_1^2 + R_1^2 \ln\left(\frac{a^2 R_1^2}{R_0^2}\right)} = \frac{4\pi L_{rv}}{-a^2 + \ln\left(\frac{a^2}{\pi L_{rv} R_0^2}\right)} \quad (19)$$

So  $w_{mi}$  is almost proportional to root length density as the numerator of the RHS of Eq. (19) changes much faster with change in  $L_{rv}$  than the denominator.

The highest possible uptake rate occurs when the pressure head at the root surface is that at wilting point. In that case the matric flux potential at the root surface is then zero by definition, see Eq. (10). If the corresponding uptake rate is greater than the required uptake rate the actual uptake rate is equal to the required uptake rate, else it equals the highest possible uptake rate. So the actual uptake rate of a single layer can be formulated as:

$$S_a = \min(S, S_r) = \min\left(w\bar{\Phi}, \frac{T_p}{L}\right) \quad (20)$$

For a root system Eqs. (14) and (17) apply to each layer:

$$S_i = \frac{4(\bar{\Phi}_i - \Phi_{0,i})}{R_{0,i}^2 - a_i^2 R_{1,i}^2 + 2(R_{0,i}^2 + R_{1,i}^2) \ln\left(\frac{a_i R_{1,i}}{R_{0,i}}\right)} = w_{mi,i}(\bar{\Phi}_i - \Phi_{0,i}) \quad (21)$$

The influence of root radius and proportionality factor  $a$  on  $w_{mi,i}$  was found (by sensitivity analysis, see also Eq. (19)) to be quite small, and therefore both were assumed to be the same for all layers. Accordingly:

$$w_{mi,i} = \frac{4}{R_0^2 - a^2 R_1^2 + 2(R_0^2 + R_{1,i}^2) \ln\left(\frac{aR_{1,i}}{R_0}\right)} \quad (22)$$

By numerical simulations, de Jong van Lier et al., (2006) found for factor  $a$  the median value 0.53 (-). Another assumption is that the matric flux potential at the root surface has the same value in every layer. The total maximum transpiration rate is calculated as the sum of uptake of each layer when the root surface matric flux potential is zero:

$$T_{\max} = \sum_{i=1}^n \Delta z_i w_i \bar{\Phi}_i \quad (23)$$

If the sum in Eq. (23) is smaller than or equal to the potential transpiration,  $\Phi_0 = 0$  and the uptake in each layer is calculated with Eq. (21). If, on the other hand,  $T_{\max} > T_p$ ,  $\Phi_0$  is greater than zero and can be calculated from:

$$T_p = \sum_{i=1}^n \Delta z_i w_i (\bar{\Phi}_i - \Phi_0) \rightarrow \Phi_0 = \frac{\sum_{i=1}^n \Delta z_i w_i \bar{\Phi}_i - T_p}{\sum_{i=1}^n \Delta z_i w_i} \quad (24)$$

Next equation Eq. (20) is used to calculate the extraction rate at each node. In this way an automatic redistribution of extraction rates is simulated: soil water is extracted at those depths that are most favorable with regard to root length density and matric flux potential.

The possibility exists that in one or more layers  $\Phi_0 > \Phi_i$  so that in those layers water flows from the root into the soil. Contrary to the water uptake routines of FUSSIM2 and RSWMS this so-called hydraulic lift is not allowed in SWAP-micro. The water uptake is set in these layers to zero, and the calculation is repeated with the remaining layers.

**Summarizing**, the water uptake routine in SWAP-micro is an extension of that in SWAP-macro. Next to the average soil pressure head SWAP-micro takes also into account the gradient around the root necessary to transport water to the root. Data input is limited to root length densities and plant wilting point. Compensation of root water extraction when certain parts of the root zone experience stress, is automatically accommodated. Due to linearization of the radial soil water flow equation with the matric flux potential, no iterations are required and the computational effort for the entire root zone is relatively small. SWAP-micro neglects the hydraulic gradients inside the root system itself, but assumes a constant pressure head at the soil-root interface, with a minimum at wilting point. In this way only the hydraulic resistance in the soil is considered.

### 2.2.3 FUSSIM2

The uptake routine in this model (De Willigen and Van Noordwijk, 1987; De Willigen 1990; De Willigen and Van Noordwijk 1991) is based on the results of a microscopic model where a single root is considered. In this model the flow of water into the root was assumed to consist of two components: flow from bulk soil to root surface and flow from root surface into the root. The first flow was calculated by an equation similar to Eq. (11), with boundary condition Eq. (12) but with a zero flux condition at the outer boundary of the soil cylinder viz.:

$$R = R_1, \frac{\partial \Phi}{\partial R} = 0 \quad (25)$$

The solution of Eq. (11) with Eqs. (12) and (25) is:

$$\Phi = \Phi_0 + \frac{S}{4} \left( R_0^2 - R^2 + 2R_1^2 \ln \left( \frac{R}{R_0} \right) \right) \quad (26)$$

Note the difference between Eq. (26) and Eq. (16):

$$\frac{S}{4} \left( 2R_0^2 \ln \left( \frac{R}{R_0} \right) \right).$$

To relate the uptake rate to the average value of root water potential (or rather to the root water potential corresponding to the average pressure head in the soil cylinder), the average matric flux potential is calculated from (26) as:

$$\overline{\Phi} = \frac{\int_{R_0}^{R_1} 2R\Phi dR}{R_1^2 - R_0^2} = \Phi_0 + SR_0^2 G(\rho) \quad (27)$$

where  $\rho = R_1 / R_0$  and

$$G(\rho) = \frac{1}{2} \left( \frac{1-3\rho^2}{4} + \frac{\rho^4 \ln \rho}{\rho^2 - 1} \right) \quad (28)$$

The uptake rate can be made explicit from Eq. (27) yielding:

$$S = \frac{\overline{\Phi} - \Phi_0}{R_0^2 G(\rho)} = w(\overline{\Phi} - \Phi_0) \quad (29)$$

As mentioned in the context of Eq. (17)  $R_1 \gg R_0$ , so  $\rho^2 \gg 1$ , so that:

$$G(\rho) \approx \frac{-3\rho^2}{8} + \frac{\rho^2}{2} \ln \rho = \frac{-3}{8} \frac{R_1^2}{R_0^2} + \frac{R_1^2}{2R_0^2} \ln \left( \frac{R_1}{R_0} \right)$$

Thus

$$\begin{aligned} w_{Fus} &= \frac{1}{R_0^2 G(\rho)} \approx \frac{1}{\frac{-3}{8} R_1^2 + \frac{R_1^2}{2} \ln \left( \frac{R_1}{R_0} \right)} = \frac{1}{\frac{R_1^2}{4} \left( \frac{-3}{2} + \ln \left( \frac{R_1^2}{R_0^2} \right) \right)} = \\ &= \frac{4\pi L_{rv}}{\frac{-3}{2} + \ln \left( \frac{1}{\pi L_{rv} R_0^2} \right)} \end{aligned} \quad (30)$$

Note the similarity between Eq. (30) and Eq. (19). The constant in the second term of the denominator on the RHS of Eq. (19) is  $-\alpha^2 + \ln(\alpha^2) = -1.55$ , almost the same as -1.5 in Eq. (30).

The other flow component, viz. the flow of water from the root surface into the root is proportional to the difference between the pressure head at the root surface and that in the root xylem, the latter will be denoted as the root water potential:

$$U = L_n K_R (h_0 - h_R) \quad (31)$$

where  $K_R$  is the conductance of the root ( $\text{cm d}^{-1} = \text{cm}^3 \text{ water}/(\text{cm root length.cm pressure.d})$ ), and  $h_0$  and  $h_R$  denote the pressure head at the root surface and in the xylem respectively. The xylem water potential is assumed to be the same all over the root system. From the xylem water potential and the plant conductance the leaf water potential is calculated as:

$$h_L = h_R - \frac{T_a}{L_p} \quad (32)$$

Where  $h_L$  is the leaf water pressure head (cm),  $h_R$  is the root water pressure head (cm),  $T_a$  is the actual transpiration rate ( $\text{cm d}^{-1}$ ), and  $L_p$  is the conductance in the path root to leaf (d). Details are found in Appendix I. The actual transpiration is a function of the potential transpiration and the leaf water potential, we used the approach of Campbell (1985, 1991) proposed, i.e.:

$$T_a = \frac{T_p}{1 + \left( \frac{h_L}{h_{L,1/2}} \right)^q} \quad (33)$$

In this equation  $h_{L,1/2}$  the value of  $h_L$  where  $T_a = T_p/2$ , and  $q$  is a parameter. Figure 2 gives a graph of Eq. (33). So in total, in a one-layer system with thickness  $\Delta z$  cm, we have three equations, viz.

$$\frac{\bar{\Phi} - \Phi_0}{R_0^2 G(\rho)} = L_n K_R (h_0 - h_R) \quad (34)$$

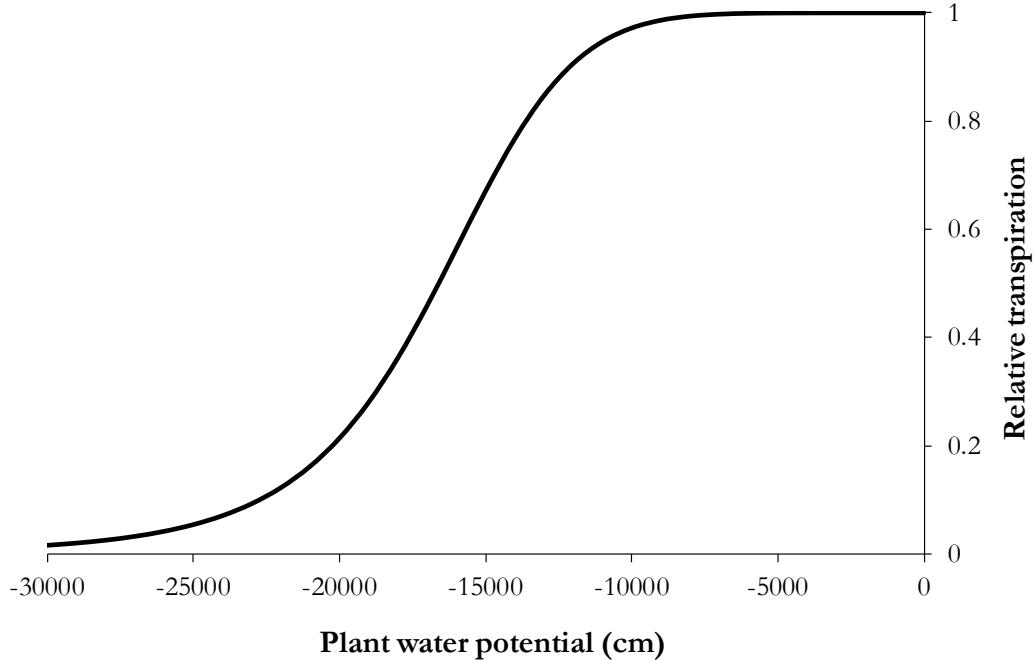
$$h_L = h_R + \frac{T_p}{K_p \left( 1 + \left( \frac{h_L}{h_{L,1/2}} \right)^q \right)} \quad (35)$$

$$L_n \Delta z K_R (h_0 - h_R) = \frac{T_p}{1 + \left( \frac{h_L}{h_{L,1/2}} \right)^q} \quad (36)$$

Equation (34) states that in the path soil - root surface - xylem there is no accumulation of water, Eq. (35) gives the relation between leaf and root potential, and Eq. (36) states that transport into the root equals actual transpiration. Because of the non-linearity of Eqs. (35) and (36) these equations have to be solved by iteration for the three unknowns  $h_0$  (from which  $\Phi_0$  follows)  $h_R$  and  $h_L$  for a given bulk pressure head  $h$  in the soil layer (from which  $\Phi$  follows).

The calculations for a multilayer system proceed along the same lines. Details can be found in Appendix 1.

**Summarizing:** the FUSSIM2 water uptake routine does not merely take the soil properties into account, but also the plant properties as radial conductance, and plant conductance. The actual transpiration is a function of the leaf water potential.



**Figure 2**

Relative transpiration as a function of plant water potential (Eq. (33)). Parameters:  $q = 0.7$ ,  $h_{L,1/2} = 16600$  cm.

## 2.2.4 RSWMS

The uptake model in RSWMS is obtained by coupling the Richards equation, which solves the soil water flow equation, to the Doussan equation (Doussan et al., 1998), which explicitly solves the water flow in a root system given its 3D architecture (the Doussan equation is explained in Appendix 2).

This coupling is necessary since the Richards equation (Eq. (1)) needs the 3D sink term distribution  $S(x,y,z)$  to be solved, while the root system solution depends on soil water potential distribution  $h$  around the roots. In the coupled model, the sink term for soil voxel  $j$  is defined as

$$S_j = \frac{\sum_{i=1}^{n_j} J_{r,i}}{V_j} \quad (37)$$

where the nominator represents the sum of all the radial fluxes of the  $n_j$  root nodes located inside a soil voxel  $J_{r,i}$  ( $\text{cm}^3 \text{ d}^{-1}$ ) and  $V_j$  is the volume of the  $j^{\text{th}}$  soil voxel ( $\text{cm}^3$ ). The radial flow rate from soil to a root node  $i$  is obtained by

$$J_{r,i} = K_{r,i}^* s_{r,i} \left[ \langle h_s \rangle_i - h_{x,i} \right] \quad (38)$$

where  $h_{x,i}$  is the xylem water potential for root node  $i$  (cm), obtained by solving the Doussan equation (see Appendix 2) and  $\langle h_s \rangle_i$  the averaged soil water potential around root node  $i$ .

To solve the Doussan root flow equation for the whole rooting system, the soil water potential around each root node  $\langle h_s \rangle_i$  is needed. This is defined as a weighed averaged of the soil pressure head  $h_{s,k}$  of the 8 nodes which surround the root node  $i$  as follow

$$\langle h_s \rangle_i = \frac{\left( \sum_{k=1}^8 \frac{1}{dist_k} h_{s,k} \right)}{\sum_{k=1}^8 \frac{1}{dist_k}} \quad (39)$$

where  $dist_k$  (cm) represents the spatial distance between the root node  $i$  and the soil node  $k$ .

For coupling the water flow in both the soil and root systems, we used an implicit iterative scheme. First the root flow system is solved given an initial estimate of the pressure head distribution in the soil. This generates a first estimate of the xylem pressure head  $H_x$  and water flow distribution (Eq. (38)). A 3D sink term distribution can thus be calculated from Eq. (37), which allows the numerical solution of the Richards equation (Eq. (1)). We iterate these two steps until the maximum change in root and soil pressure head at all the nodes does not exceed a minimum threshold value and there is no change in the total water uptake between consecutive iterations.

By default, the boundary condition (BC) for the root is a potential flux at the root collar (potential transpiration). As the flow equation within the root is explicitly solved, a pressure value is calculated for each root node at each time step, in particular at the root collar. When the pressure head at the root collar node reaches a limiting value  $h_{x,lim}$  it is considered that the potential flux cannot be sustained anymore (i.e. stomata close in order to keep a constant potential) and the root collar boundary switches from flux type condition (i.e. the potential transpiration) to head-type boundary condition (i.e., pressure head at the collar is equal to  $h_{x,lim}$ ).

From then on, the actual flux resulting from this BC is compared at each iteration to the potential flux.

When actual flux is higher than the actual flux, BC is switched back to flux-type.

**Summarizing**, RSWMS fully solves the water flow equation in the soil and in the root systems and estimate the 3D uptake distribution based on water potential gradient between each root node and the surrounding soil voxel. Therefore, no functional relationship between soil water potential and optimal transpiration (Feddes function) or between the plant water potential and the transpiration are needed.

### 3 Scenarios and parameter values

The root water uptake (WU) models described in Chapter 2 will be compared in several scenarios as described below. The WU models are part of larger models that solve the Richards equation (Eq. (1)). So, first we need to assure that the numerical solution of the Richards equation by the three basic models (SWAP, FUSSIM2 and RSWMS) yields similar results.

All scenarios share in common the dimension of the soil domain, the soil properties and the root architecture (or root length density distribution) when WU is modeled. The soil domain and resolution are given in Table 3. Three soil types were involved in the comparison, viz. Zandb3 (sand), Kleib11 (clay), Leemb13 (loam) (Wösten et al., 2001). The hydraulic relations are depicted in Figure 6 and the parameters given in Table 4.

**Table 3**

*Domain and resolution details of the four models.*

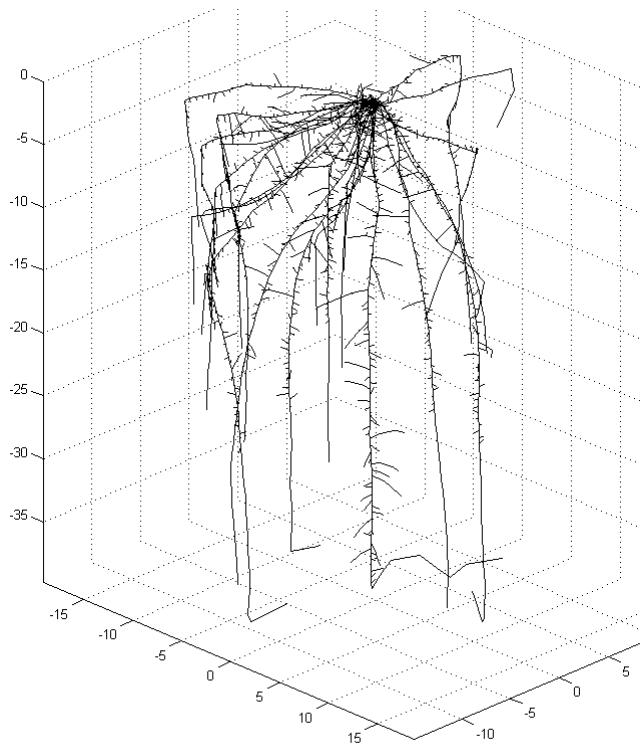
	<b>Resolution</b>	<b>Z domain</b>	<b>Y domain</b>	<b>X domain</b>
SWAP	$\Delta z=1$ cm	0-40 cm		
FUSSIM2	$\Delta x=\Delta z=1$ cm	0-40 cm	-12 to +12cm	
RSWMS	$\Delta x=\Delta y=\Delta z=1$ cm	0-40 cm	-12 to +12cm	-12 to +12cm

**Table 4**

*Mualem - van Genuchten parameters for three soils of the Dutch Staring series (Wösten et al., 2001).*

<b>Soil</b>	$\theta_r$	$\theta_s$	$K_s$	$\alpha$	$\lambda$	$n$
<b>Name</b>	<b>cm<sup>3</sup> cm<sup>-3</sup></b>	<b>cm<sup>3</sup> cm<sup>-3</sup></b>	<b>cm d<sup>-1</sup></b>	<b>cm<sup>-1</sup></b>	-	-
Zandb3	0.02	0.46	15.42	0.0144	-0.215	1.534
Kleib11	0.01	0.59	8.0	0.0195	-5.901	1.109
Leemb13	0.01	0.42	12.98	0.0084	-1.497	1.441

The root architecture (see Figure 3) corresponds to a 45-day old maize root grown in a closed box as simulated by the RootTyp software (Pagès et al., 2004). It consists in a root system of 2862 nodes and the corresponding root length density is given in Figure 5.



**Figure 3**  
Architecture of a 45-d old Maize root system.

### Soil water flow without water uptake

In the check scenario the Richards equation is solved without a sink term. Initially the soil water was in hydrostatic equilibrium with  $h = -1500$  cm at the bottom of a 40 cm deep soil layer. During the first day, rainfall of  $20 \text{ mm d}^{-1}$  is specified. At the soil surface evaporation is excluded (as all models have different evaporation sub-models), and a no-flow boundary at the bottom is applied. The simulation was run for 10 days in total.

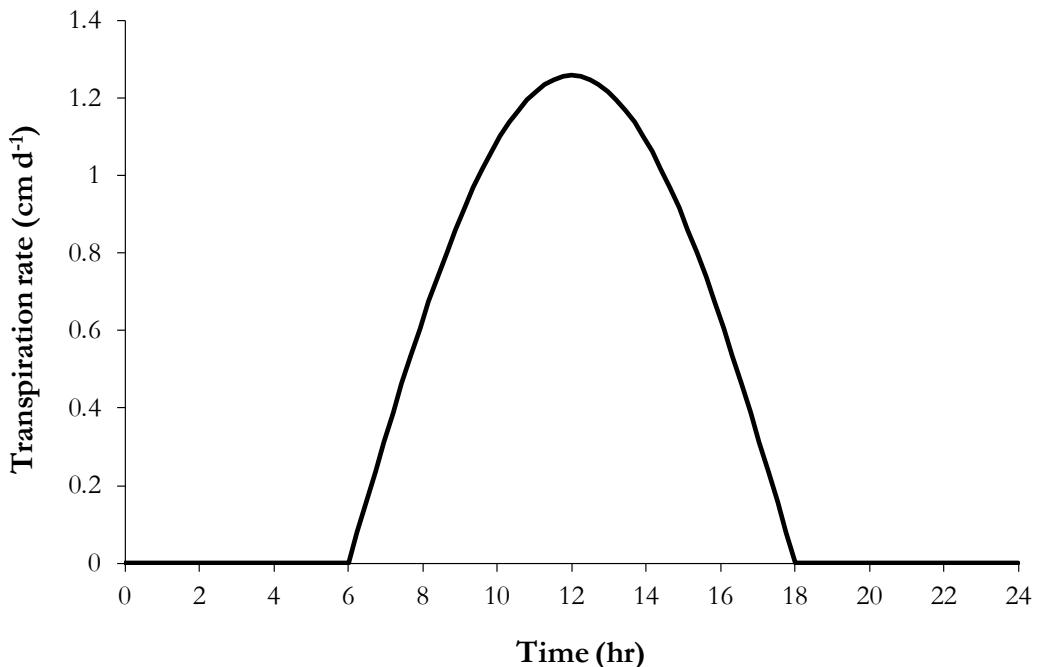
### Water uptake without transport of water in soil

The water uptake routines are compared both in case of a single layer and for a number of layers. In the first case the reduction of uptake by a single root in a single layer of soil as a function of average pressure head in the layer is studied. In the second case the focus is on the distribution of water uptake over the root system shown in Figure 3. In both cases the comparison was done for the three soil types.

### Root water uptake scenarios

**S1:** The first actual root water uptake scenario considers a 1D vertical soil column of 40 cm length, with a no-flow boundary at the bottom, no evaporation at the soil surface. The potential transpiration rate is  $4 \text{ mm d}^{-1}$  for 31 days, and one precipitation event at day 15 with a rate of  $20 \text{ mm d}^{-1}$  with a duration of one day. Initially the soil is at hydrostatic equilibrium with  $h = -700$  cm at the bottom. The same three soil types as mentioned in Table 4 will be considered. The amount of water corresponding to the initial pressure head distribution was quite different as follows from Figure 6: 58 mm for Zandb3, 177 mm for Kleib11, and 77 mm for Leemb13.

**S2:** The second root water uptake scenario is similar to S1, except that 1) precipitation did not occur, and 2) the transpiration during the day was distributed according to a sinusoidal pattern: 00:00 - 06:00, no transpiration; 06:00 - 18:00, transpiration following a (positive) sine curve (in total 4  $\text{mm d}^{-1}$ ); 18:00 - 24:00, no transpiration. This means that at 12:00 the potential transpiration demand is 12.6  $\text{mm d}^{-1}$ , much larger than the average demand of 4  $\text{mm d}^{-1}$  (Figure 4).



**Figure 4**

*Course of transpiration rate over the day for scenario S2.*

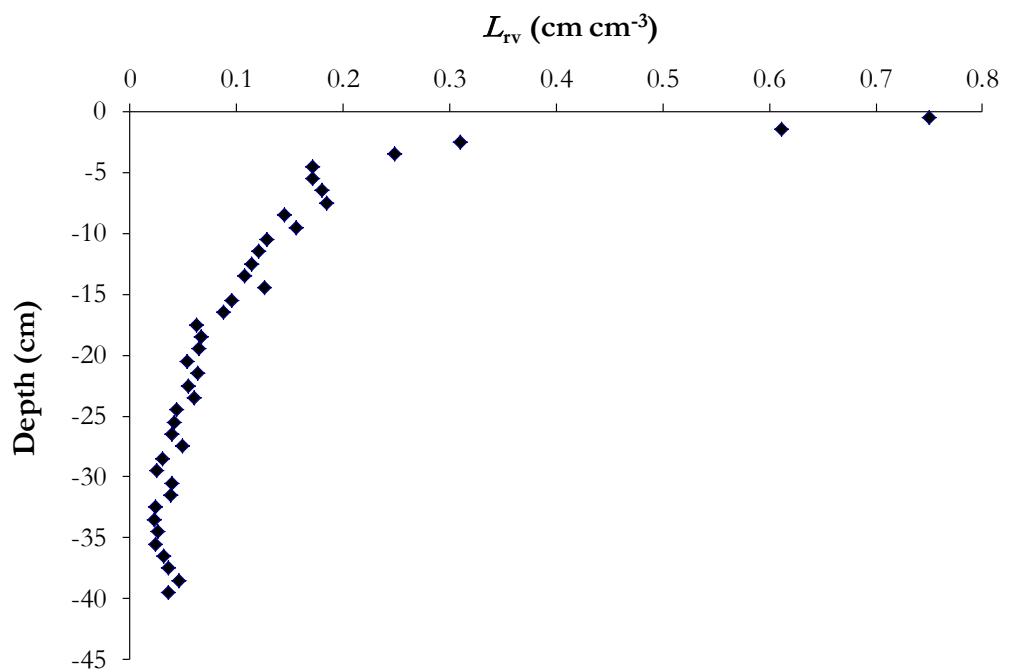
For scenarios S1 and S2 we considered the following output:

- cumulative transpiration in time;
- normalized sink term profile at  $t = 0.5 \text{ d}$ ,  $15.5 \text{ d}$  (or  $30.5 \text{ d}$  if simulated);
- water content and pressure head profiles at  $t = 0.5 \text{ d}$ ,  $15.5 \text{ d}$  (or  $30.5 \text{ d}$  if simulated);
- water potential in the xylem and at the interface profiles at  $t = 0.5 \text{ d}$ ,  $15.5 \text{ d}$  (or  $30.5 \text{ d}$  if simulated);
- relative root water uptake, i.e. the uptake from a certain layer divided by the uptake of the complete profile, versus relative root length density, i.e. the root length in a certain layer divided by the total root length in the soil profile; plots at  $t = 0.5 \text{ d}$ ,  $15.5 \text{ d}$  (or  $30.5 \text{ d}$  if simulated).

Table 5 lists the specific input data (parameters) of the four WU models. The parameters of SWAP-macro were chosen as to comply with the scenarios given above. Those of SWAP-micro are as mentioned by de Jong van Lier et al. (2008). In case of FUSSIM2 the radial root conductance was derived from the root conductivity given by Javaux et al. (2008) taken into account the value of the root radius used here. The half value of leaf water potential and the exponent of the reduction function were taken from Kremer et al. (2008).

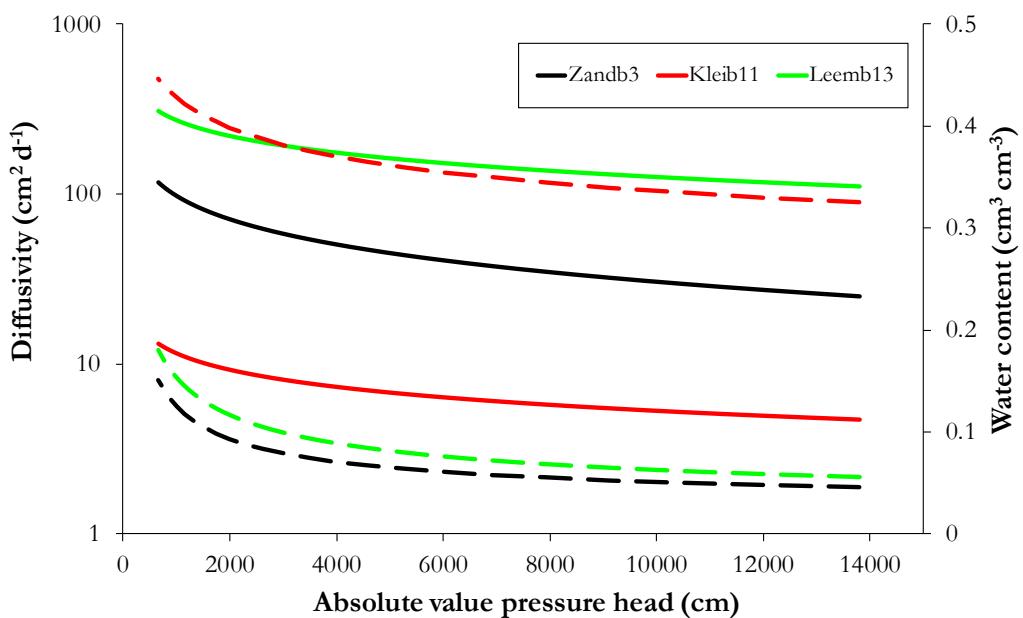
**Table 5**  
*Model specific input data with respect to root water extraction.*

Model	Input parameter	Symbol	Value
SWAP-macro	Critical soil water pressure head at $T_{\text{high}}$	$h_{3h}$	-600 cm
	Critical soil water pressure head at $T_{\text{low}}$	$h_{3l}$	-900 cm
	Wilting point	$h_4$	-15000 cm
	Level of high atmospheric demand	$T_{\text{high}}$	4 mm d <sup>-1</sup>
	Level of low atmospheric demand	$T_{\text{low}}$	1 mm d <sup>-1</sup>
	Minimum pressure head at interface soil-root	$h_w$	-15000 cm
SWAP-micro	Root radius	$R_0$	0.032 cm
	Relative radial distance of mean water content	$a$	0.53
	Root radial conductance	$K_R$	8.143E-5 cm d <sup>-1</sup>
FUSSIM2	Half value of leaf water potential	$h_{l,1/2}$	1.66E+4 cm
	Exponent reduction function	$q$	7 (-)
	Limiting collar xylem water potential	$h_{x,lim}$	-15000 cm
RSWMS	Xylem conductance	$Kh_x$	0.0432 cm <sup>3</sup> d <sup>-1</sup>
	Radial root conductivity	$L_r$	1.77728E-4 d <sup>-1</sup>



**Figure 5**

*Distribution of root length density with depth, as used in the calculations.*



**Figure 6**

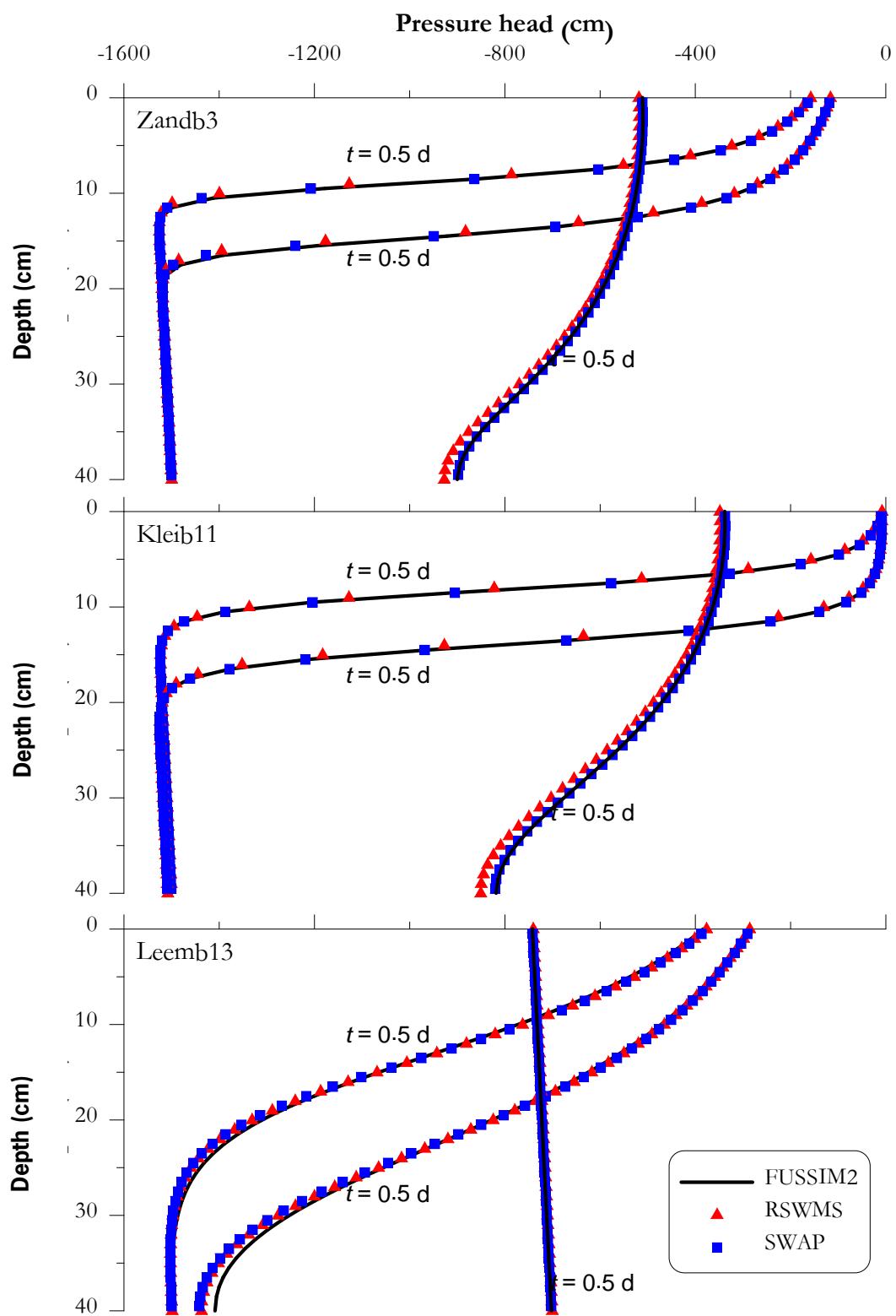
*Diffusivity (solid lines) and volumetric water content (broken lines) as a function of absolute pressure head.*



## 4 Comparison of results

### 4.1 Solution of Richards equation

The profile of pressure head for three points in time is shown in Figure 7. Although not exactly identical, the three models yielded very similar results. After 0.5 d, water infiltrated to a depth of 30 cm in the loam (Leemb13) soil, and to a depth of 12-13 cm in the clay (Kleib11) and sand (Zandb3) soil. From the high degree of similarity of the model results we conclude that model differences in the forthcoming water uptake scenarios should be attributed to differences in the uptake routines.



**Figure 7**

Scenari Check. Distribution of pressure head with depth at time = 0.5, 1 and 10 days. The lines pertain to FUSSIM2, the squares to SWAP and the triangles to RSWMS for the three soils Zandb3 (a), Kleib11 (b) and Leemb13 (c).

## 4.2 Water uptake routines

### 4.2.1 Reduction function

To compare the water uptake routines, the transpiration reduction (i.e. the ratio of actual and potential transpiration) was calculated as a function of soil pressure head for the three soils and two root length densities, viz. 1 and  $0.16 \text{ cm cm}^{-3}$ . The latter is the average root length density in the upper 20 cm of the root system shown in Figure 5. Other parameter values used for the calculation were potential transpiration ( $T_p = 4 \text{ mm d}^{-1}$ ), thickness root zone ( $Z_{\text{root}} = 20 \text{ cm}$ ), root radius ( $R_0 = 0.075 \text{ cm}$ ).

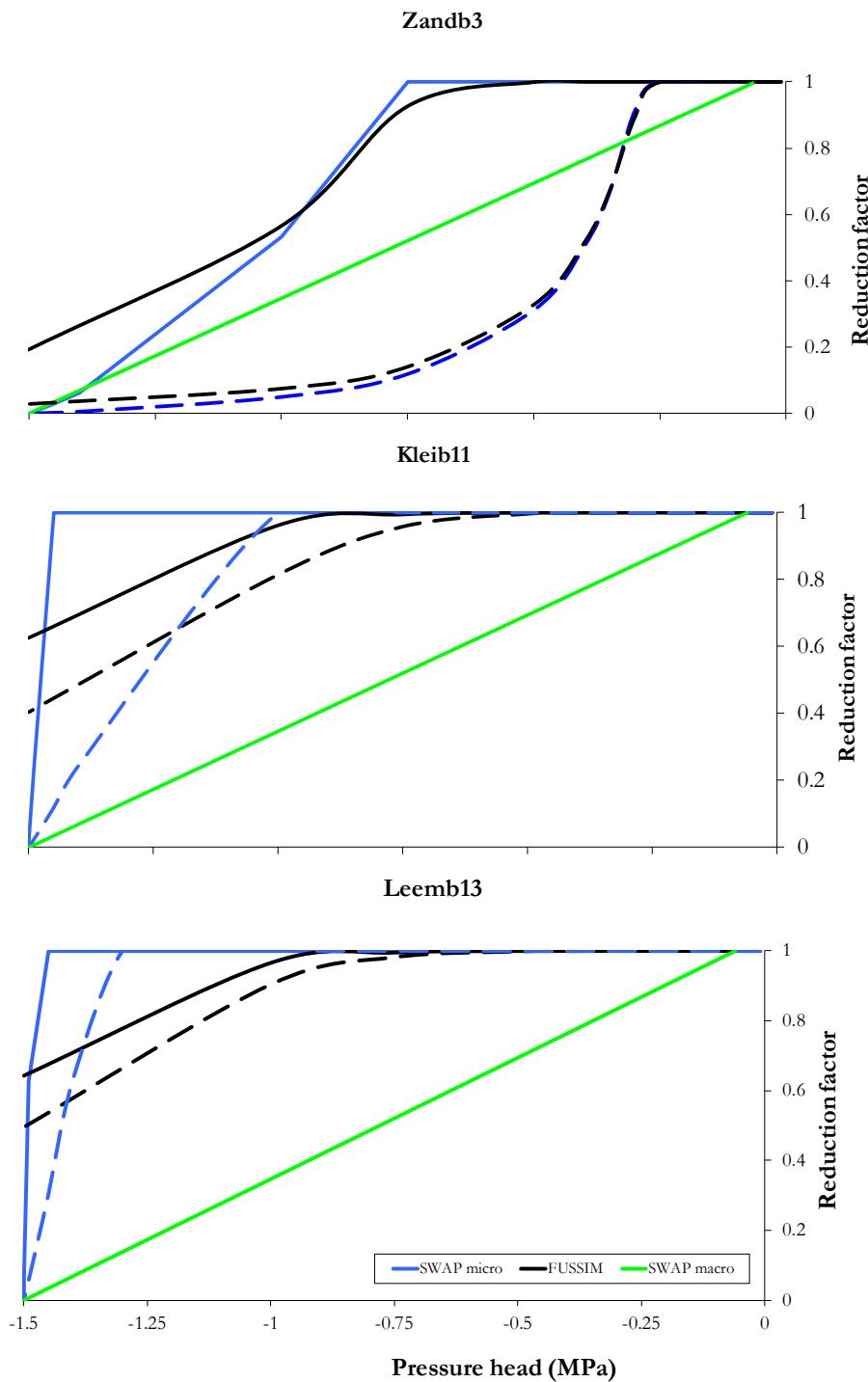
For SWAP-macro the function depicted in Figure 1 for high transpiration was used, with the parameter values given in Table 5. Neither absolute root length density nor soil type does play a role in the transpiration reduction of the SWAP-macro routine.

For SWAP-micro the calculation starts with computing the matric flux potential  $\phi$  corresponding to the pressure head in the soil with Eq. (10), where the pressure head at wilting point ( $h_w$ ) amounts to  $-15000 \text{ cm}$ . Here the soil properties are important. The relation between  $\phi$  and  $h$  depends on the hydraulic properties.

In FUSSIM2 the reduction function is found by solving Eqs. (34), (35) and (36). Additional parameters in case of FUSSIM2 were those used to calculate reduction as a function of leaf water potential, viz. the root water conductance ( $K_R = 8.14 \cdot 10^{-5} \text{ cm d}^{-1}$ ), the half value of leaf water potential ( $h_{L,1/2} = -16600 \text{ cm}$ ), and the exponent ( $q = 7$ ). Due to the low value of  $K_R$  the root water potential is considerably lower than  $h$  at the soil root interface, this leads to a stronger reduction at higher  $h$  than SWAP-micro shows.

In RSWMS, there is no explicit definition of the reduction function within the code. Reduction mechanism appears when the potential demand generates a water potential at the root collar lower than a limiting threshold value  $h_{lim}$ . The collar boundary condition (CBC)  $h_{collar}$  is then switched to a constant head condition where  $h_{collar} = h_{lim}$ . When the potential demand gets lower than the actual flux generated by this constant head CBC, the CBC is switched back to the potential demand again.

Figure 8 shows the reduction function for the three models and the three soils. As mentioned before in case of SWAP-macro the reduction function is independent of soil properties or root length density. For the sandy soil the reduction function of SWAP-micro and FUSSIM2 are very similar. For the two other soils the reduction starts at higher values of soil pressure head in case of FUSSIM2, but at wilting point the reduction factor is still considerable of the order 0.5-0.6. In fact the decrease in case of SWAP-micro begins at values close to wilting point. In the low pressure head range the transpiration is less reduced in case of FUSSIM2 compared to SWAP-micro. For both SWAP routines the uptake is zero when the pressure head is at wilting point ( $-15000 \text{ cm}$ ).



**Figure 8**

The reduction function of the water uptake routines for FUSSIM2, SWAP-micro and SWAP-macro respectively for three soils and two root length densities,  $1 \text{ cm cm}^{-3}$ (full lines) and  $0.16 \text{ cm cm}^{-3}$ (interrupted lines). Potential transpiration  $0.4 \text{ cm d}^{-1}$ , thickness root zone  $20 \text{ cm}$ , values of other parameters are found in Table 5. Note that the results of SWAP-macro do not depend on soil type, so these are identical for the three soils.

## 4.2.2 Critical value of the soil pressure head

Below a certain value of the soil pressure head the potential transpiration is reduced.

For SWAP-macro this value follows direct from the reduction function given in Table 5, it amounts to -900 cm for the low to -600 cm for high potential transpiration (but these values may differ from crop to crop).

For SWAP-micro the flow of water to the root is driven by the difference between the soil matric flux potential and the matric flux potential at the soil root interface ( $\Phi_0$ ) as given in Eq. (14) or (16). When the actual transpiration equals the potential transpiration the lowest possible value of  $\Phi_0$  is zero, i.e. the value corresponding to wilting point, then:

$$\overline{\Phi} = \frac{T_p}{wL} \quad (40)$$

The coefficient  $w$  is approximately proportional to root length density, as shown in Eq. (19).

For FUSSIM2 the situation is somewhat more complicated as more parameters and functions play a role.

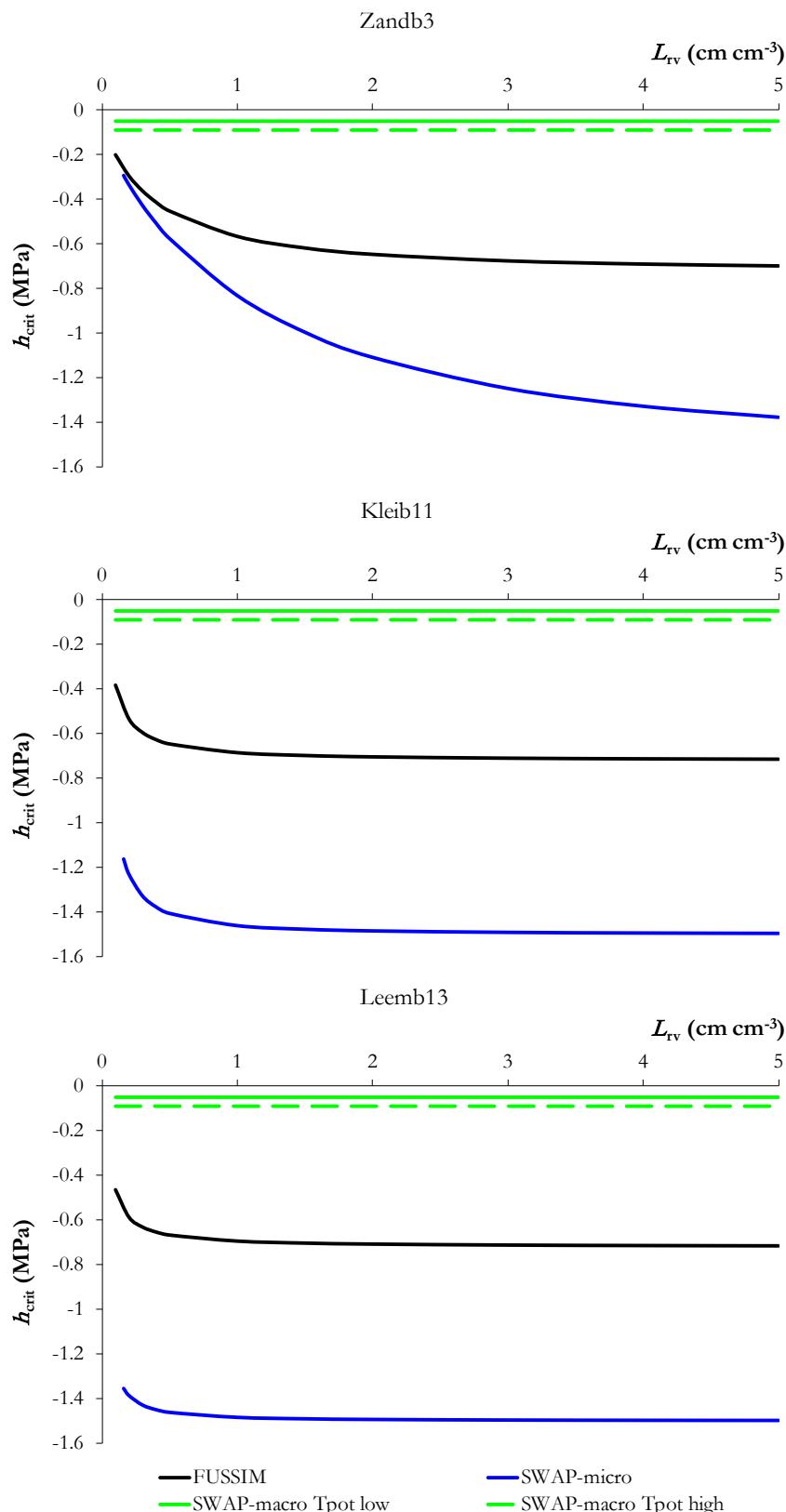
Denoting the reduction coefficient by  $\beta$ , from (33) it follows

$$\frac{T_a}{T_p} = \beta = \frac{1}{1 + \left( \frac{h_L}{h_{L,1/2}} \right)^q} \quad (41)$$

However, the reduction coefficient has the value 1 for the plant water potential being zero only. So the limiting value of plant water potential is defined for a value of  $\beta$  close to 1, say  $\beta = 0.95$ . Then using consecutively Eqs. (36), (35) and (34), the soil matric flux potential, and with that the soil pressure head, can be found.

In RSWMS there is a critical value for the collar pressure head  $h_{lim}$  beyond which it is assumed that the plant closes its stomata to prevent a lower value than this  $h_{lim}$ . This results in a decreased actual transpiration. So we do not have an explicit expression for the pressure head in the soil where transpiration reduction starts.

Figure 9 shows the critical value as a function of the pressure head for the models SWAP-macro, SWAP-micro and FUSSIM2. As mentioned before  $h_{crit}$  in case of SWAP-macro is constant. The critical values of the SWAP-micro routine are much lower than those of FUSSIM2. Even for a low value of root length density the reduction starts when almost all of the available water has been taken up, especially in case of the loam and clay soil. The difference in critical pressure head between SWAP-micro and FUSSIM2 seems quite substantial: the critical pressure head is about twice as high in case of SWAP-micro compared to FUSSIM2. The corresponding differences in water content, however, are quite modest: a factor 1.3 at the most.

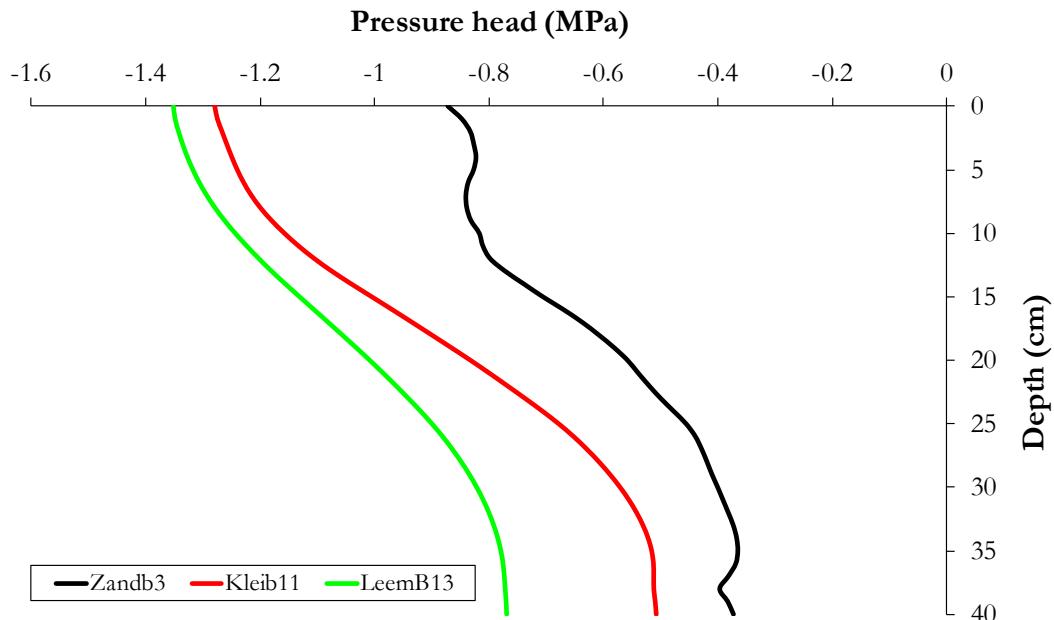


**Figure 9**

Critical value of the pressure head of the soil as a function of root length density.

#### 4.2.3 Distribution of root water uptake as a function of pressure head distribution

The previous two sections presented the different water uptake models in case of a single layer. It is also interesting to see how uptake is distributed over the root system for a given pressure head distribution. The model RSWMS was used to generate the pressure head profiles for the three soils after a dry period of 15.5 days, with a potential transpiration rate of  $4 \text{ mm d}^{-1}$ . This pressure head profile was used to calculate the corresponding water uptake distribution for the four models, employing the parameters given in Table 5. Figure 10 presents the pressure head profile for the three soil types and Figure 11 the computed relative root water uptake from the soil column. Note that only in the case of SWAP-macro the soils pressure head distribution has a direct relation to water uptake distribution. In the other three models the relation is indirect: in case of SWAP-micro via the pressure head at the soil-root interface (PHR), for FUSSIM2 via PHR, the root pressure head (PHX) and radial root resistance, and in RSWMS via PHR, PHX, root radial and axial resistance. The water uptake distribution of FUSSIM2 shows the largest differences between the three soils, which has to do with the fact that here in case of clay and loam hydraulic lift occurred in the upper 10-15 cm. The other models showed a similar pattern of uptake distribution for all three soils, especially in the case of RSWMS.



**Figure 10**

Pressure head distribution as calculated with RSWMS, after a dry spell of 15.5 days with a potential transpiration rate of  $4 \text{ mm d}^{-1}$ .

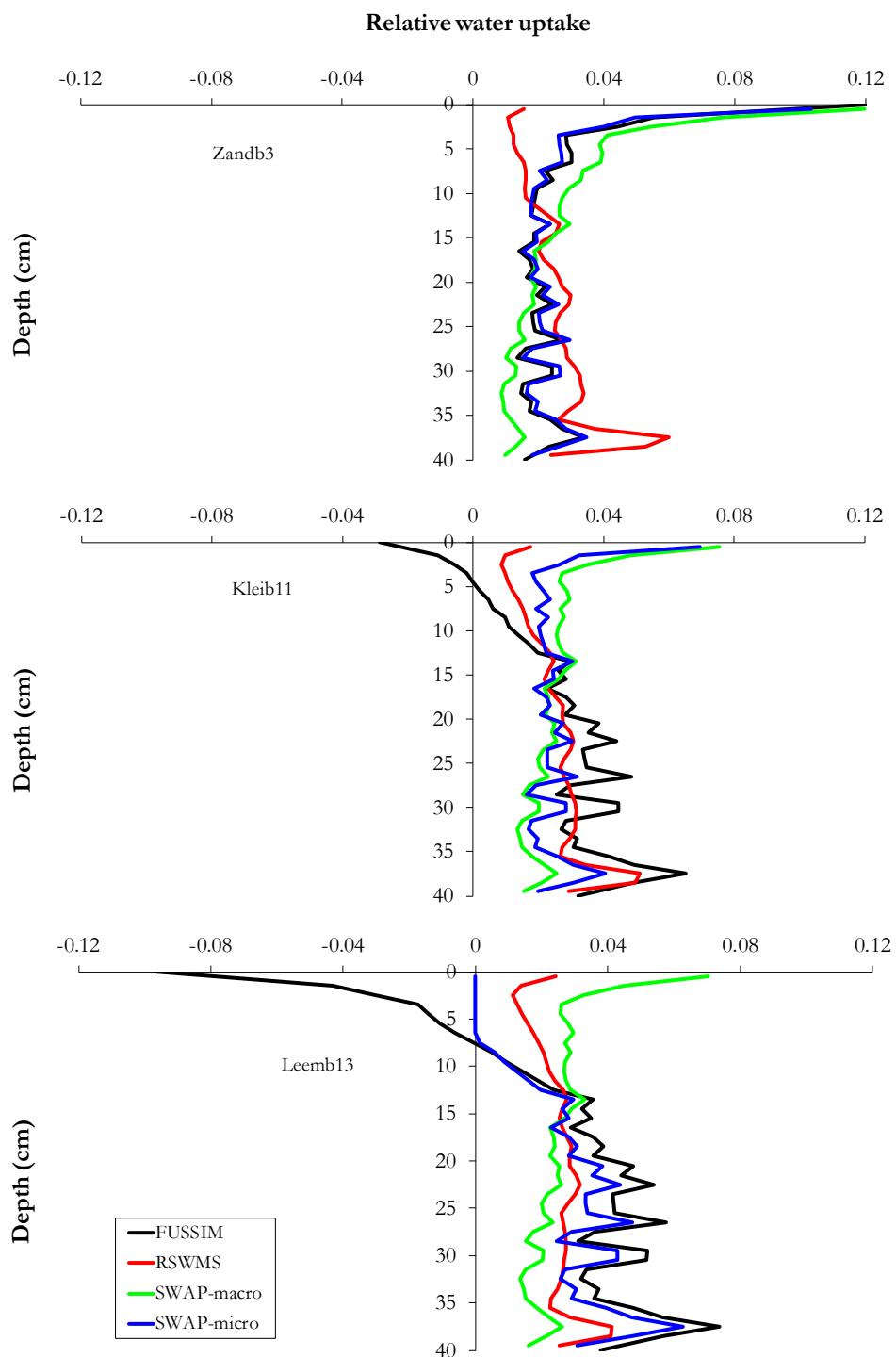
**Table 6**

*Total water uptake rate in cm d<sup>-1</sup> of the models corresponding to the pressure head distribution given in Figure 10.*

	<b>SWAP-macro</b>	<b>SWAP-micro</b>	<b>FUSSIM2</b>	<b>RSWMS</b>
Zandb3	0.212	0.0506	0.0757	0.0570
Kleib11	0.0117	0.4	0.210	0.0988
Leemb13	0.0846	0.4	0.191	0.0946

The total uptake rate of water is shown in Table 6. The differences are quite remarkable. SWAP-micro has the highest uptake in case of the sandy soil, the other models showed highest uptake for the clay and loamy soil. Another special point is the unhampered uptake in case of the SWAP-micro model on the clay and the loam soil.

The examples shown in Section 4.2 show clearly the differences in water uptake distribution as a consequence of the different mathematical description of the water uptake models. However, since these models are embedded in the Richards equation, the actual distributions of  $\lambda(z)$  for each model will differ from the ones assumed here as will be shown in 4.3 and 4.4.



**Figure 11**

Simulated relative root water uptake of the four models, corresponding to the pressure head distribution depicted in Figure 10, root densities depicted in Figure 5 and potential transpiration rate  $0.4 \text{ cm d}^{-1}$

## 4.3 Scenario S1

### 4.3.1 Cumulative transpiration and transpiration rate

In scenario S1 a dry spell of 15 days with a potential transpiration of  $4 \text{ mm d}^{-1}$  is followed by a day of heavy rain (intensity  $2 \text{ cm d}^{-1}$ ) and again a dry spell of 16 days. Initially the soil contained 5.8 cm (Zandb3), 17.7 cm (Kleib11), and 7.7 cm (Leemb13).

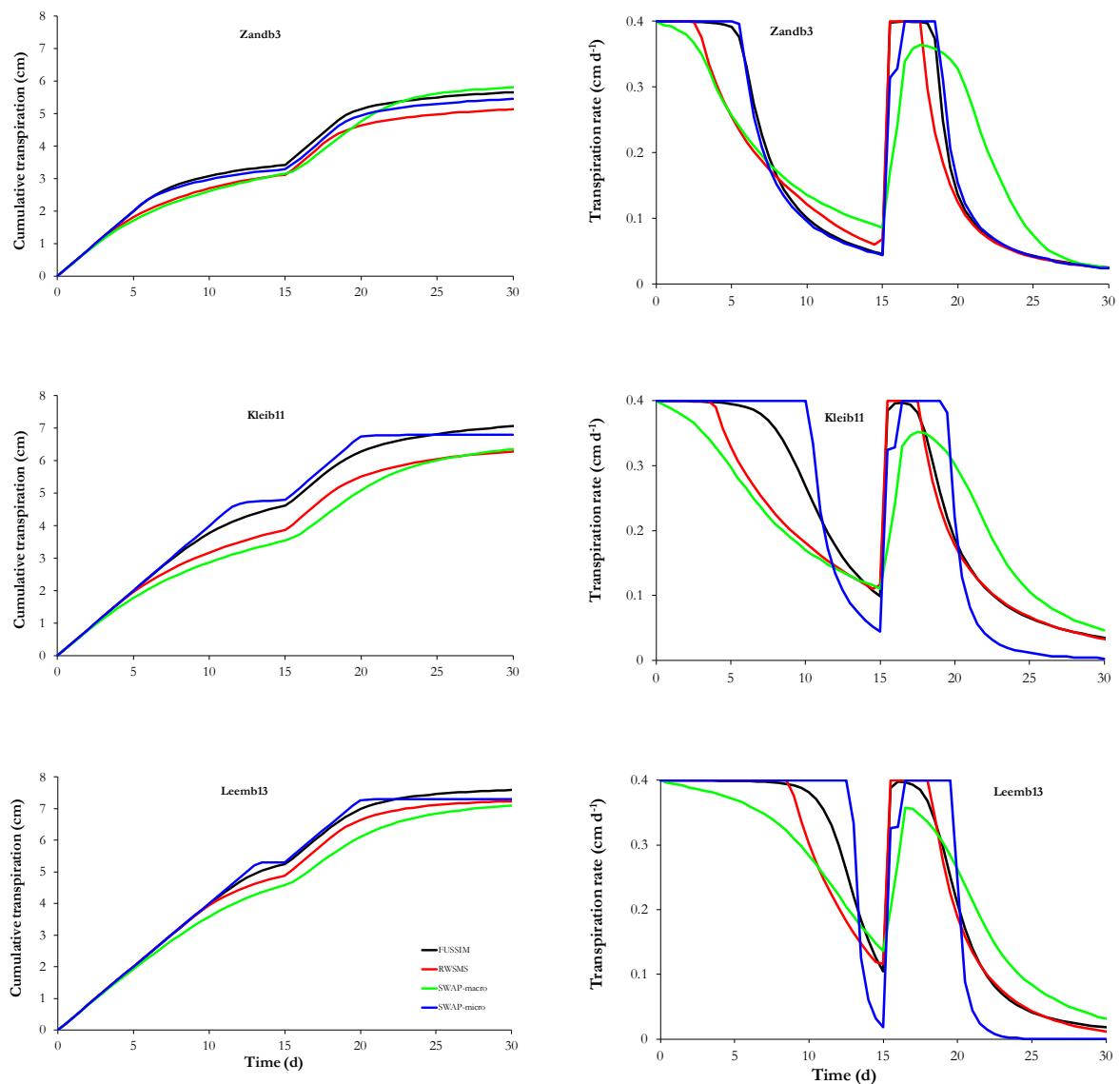
The courses of cumulative transpiration and transpiration rate are shown in Figure 12. In the SWAP-macro model no compensation occurs and the reduction of transpiration begins at a pressure head of -600 cm (see Figure 1), so with the initial conditions chosen here, with pressure heads between -700 and -740 cm, reduction starts immediately. Qualitatively, the other models yielded similar results, reduction started first for the Zandb3 soil, followed by the Kleib11, while Leemb13 was the last to show reduction. Quantitatively, as Table 7 shows, large differences exist in the time of onset of transpiration reduction, but differences in cumulative transpiration over the period of 30 days are small.

In case of SWAP-micro the onset of the reduction starts much later, but the difference in total transpiration realized between SWAP-micro and SWAP-macro is of the order of 2-6% only. For the sandy soil the results of FUSSIM2 and SWAP-micro are very similar, and the same is true for RSWMS and SWAP-macro, be it that SWAP-macro catches up with the other models after the precipitation at day 15. For the two other soils this is also the case though much less pronounced especially in the case of Leemb13.

**Table 7**

*Time of onset of the reduction period and the total transpiration realized in 30 d for the different models in scenario S1.*

<b>Model</b>	<b>Onset reduction period (d)</b>			<b>Total transpiration (cm)</b>		
	<b>Zandb3</b>	<b>Kleib11</b>	<b>Leemb13</b>	<b>Zandb3</b>	<b>Kleib11</b>	<b>Leemb13</b>
SWAP-macro	0.0	0.0	0.0	5.81	6.35	7.09
SWAP-micro	5.5	10.0	13.0	5.46	6.80	7.30
FUSSIM2	4.5	5.0	8.0	5.66	7.06	7.59
RSWMS	2.5	4.0	8.5	5.14	6.29	7.30



**Figure 12**

The time course of cumulative transpiration and transpiration rate for the three soils and scenario S1.

#### 4.3.2 Distribution of pressure head in soil, pressure head at soil root interface and relative water uptake

In Figure 13 through 15 the depth distribution of pressure head in soil (PHS), pressure head at the soil root interface (PHR) and relative water uptake (RWU, the water uptake from a certain layer relative to the total water uptake) is shown at days 0.5, 15.5 (i.e. half a day after the onset of rain), and 30.5. Notice that for RSWMS, these are the plane-averaged values which are given.

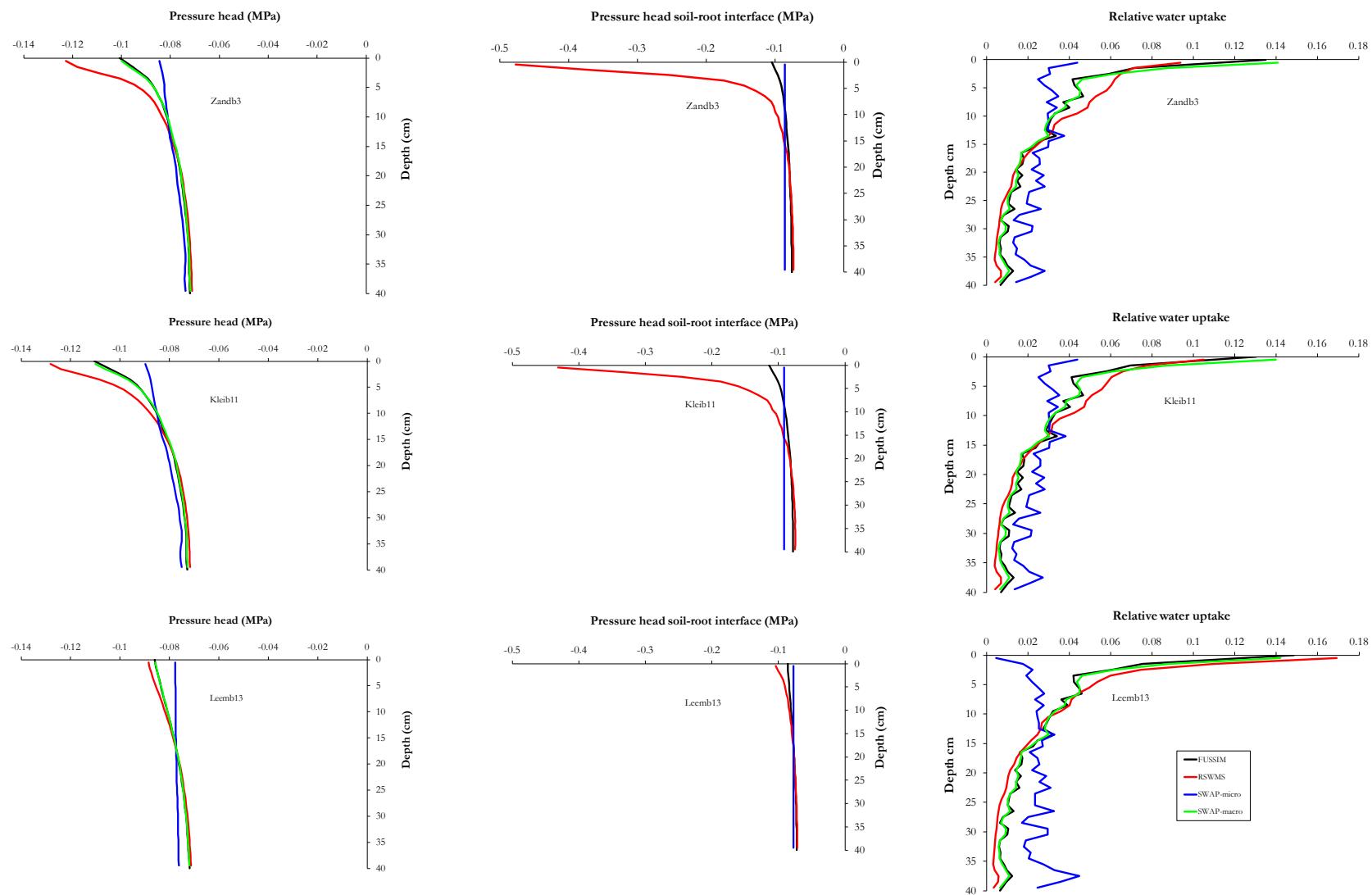
At  $t = 0.5$  d (Figure 13) the soil pressure head profile of SWAP-macro, FUSSIM2 and RSWMS show a sharp transition between the wet upper 5 cm and the lower layers, though there are some quantitative differences. A similar sharp transition is found in the profile of PHR for FUSSIM2 and RSWMS. SWAP-macro does not calculate PHR and SWAP-micro assumes a constant value over the complete root system as explained in Section 2.2.2. Most models extract water from the uppermost layer where the root density is highest and the moisture content is high. However, in case of SWAP-micro the difference between uptake in higher and lower layers is much less. This is also reflected in the small gradients of the pressure head calculated by this model. At  $t = 15.5$  d (Figure 14), the pressure head both in bulk soil as well as at the root surface show a sharp wetting front after half a day of rain. The uptake takes place almost exclusively in the upper 5 cm. In fact, in case of FUSSIM2 and RSWMS there is a water flow from the root into the soil (hydraulic lift) in the lower layers. As explained in section 2.2.2, in SWAP-micro hydraulic lift is set to zero and this leads to the situation that water is taken up exclusively from the uppermost layer. Attempts to implement hydraulic lift in SWAP-micro often lead to unrealistically high predictions of hydraulic lift, which is attributed to the lack of a radial root resistance in the SWAP-micro model.

At  $t = 30.5$  d (Figure 15), after an additional dry period of 15 days, in all models the maximum uptake shifts to lower layers. Note the low soil pressure heads, well below wilting point, that are calculated by FUSSIM2, see also Section 4.2.2. Again, the most extreme water uptake distribution is presented by SWAP-micro and the loamy soil, where no water uptake occurs in the upper 25 cm which is already at wilting point. For the clay soil, the water uptake distribution of FUSSIM2, SWAP-macro and RSWMS is to a large degree quite similar.

For the sand soil, SWAP-macro is the exception. For the loam soil, SWAP-micro is the exception.

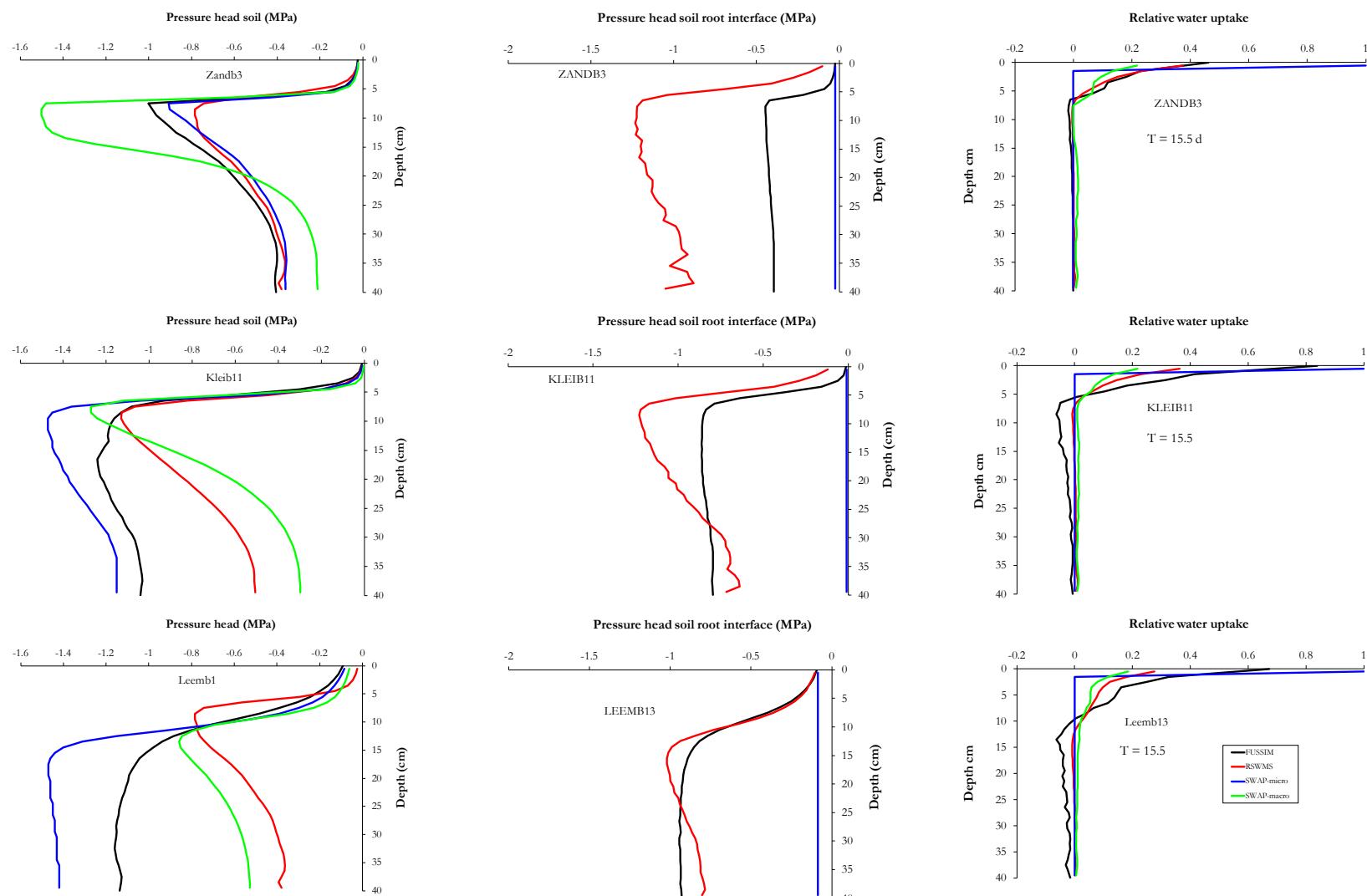
It is interesting to note that PHR and PHS are relatively different for RSWMS and FUSSIM2, but that both yield a comparable RWU profile. This is due to the fact that both models estimate the xylem water potential differently. RSWMS will generate a xylem water profile variable with depth and FUSSIM2 assumes it to be constant.

Because of that, even if PHR is different, both models can still have a comparable gradient between PHR and PHxylem, which will generate the same RWU profile. Figure 16 shows this, the differences between the results of RSWMS and FUSSIM2 are of the order of 6000 cm for PHR and PHX and less than 100 cm for PHR-PHX.



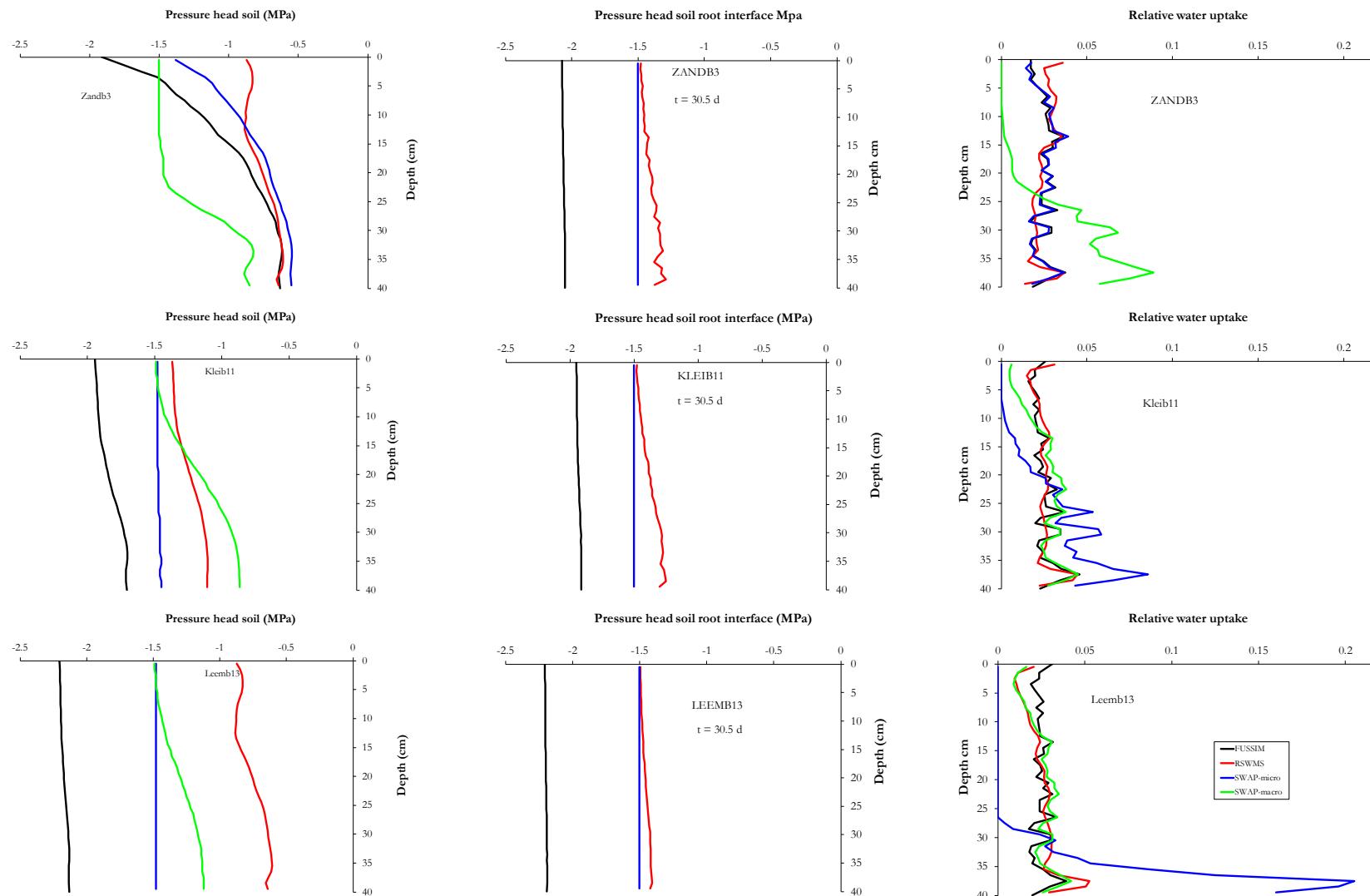
**Figure 13**

Distribution of pressure head of the soil, pressure head of the soil root interface and relative water uptake with depth at  $t = 0.5$  d.



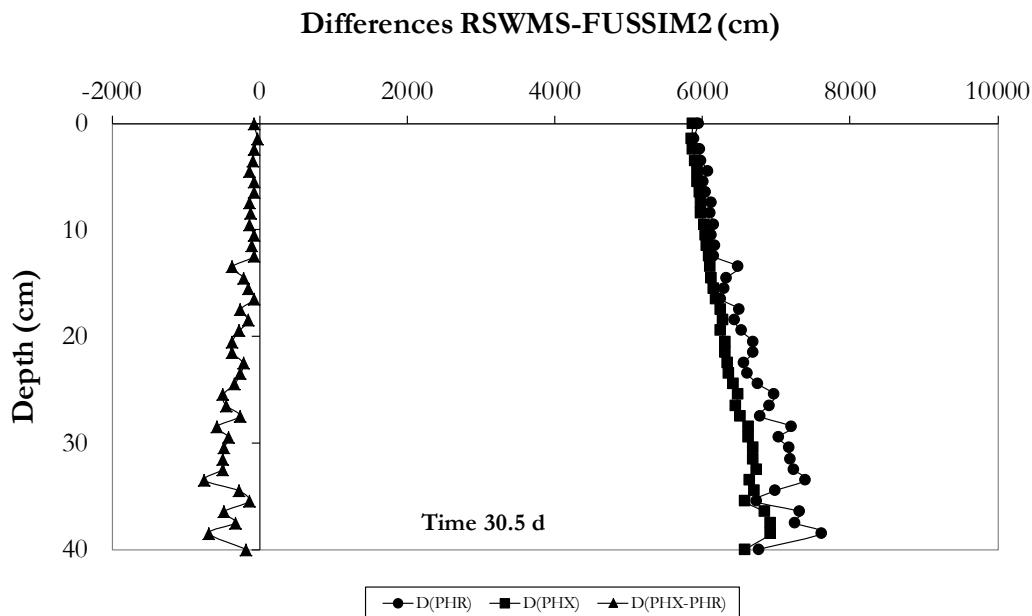
**Figure 14**

As Figure 13 for  $t = 15.5$ .



**Figure 15**

As Figure 13 for  $t = 30.5$  d.



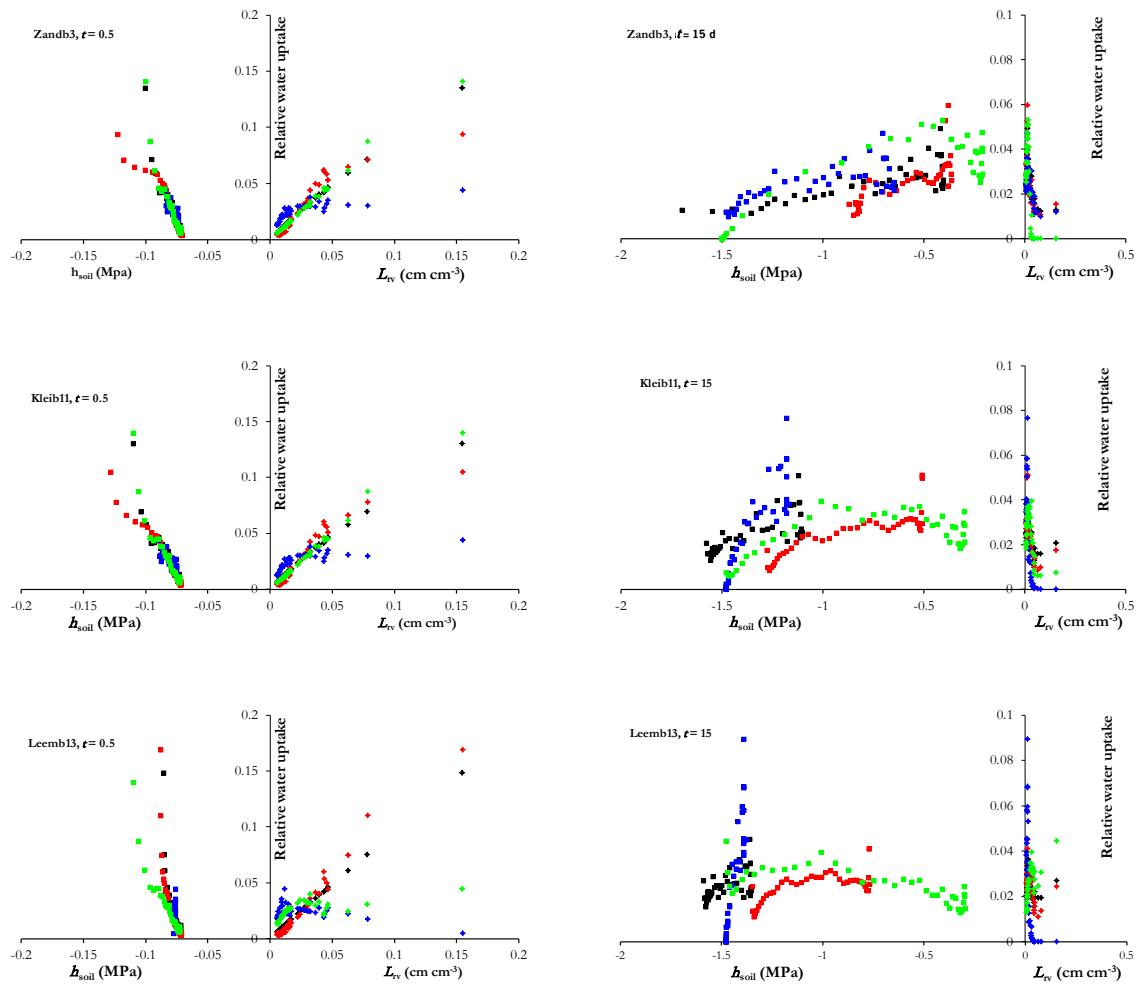
**Figure 16**

Differences in pressure head at root surface (PHR), in root xylem (PHX) and gradient of pressure head between root surface and xylem (PHX-PHR) between results of RSWMS and FUSSIM2.

#### 4.3.3 Relative water uptake in relation to root length density and soil wetness

In Figure 17 the relative water uptake is shown as a function of root length density and pressure head in the soil for two points in time:  $t = 0.5$  d and  $t = 15$  d. The latter depicts the situation just before the onset of rain.

The left column of Figure 17 gives the results at  $t = 0.5$  d. When the vertical pressure head gradients in soil are small - of the order of  $1 \text{ cm cm}^{-1}$  - the distribution of root water uptake follows that of root length density. The root water uptake is even larger at lower pressure heads (drier conditions), as the higher root length densities can compensate for the drier conditions. This is especially clear for SWAP-macro and FUSSIM2. The results of SWAP-micro in case of soil Leemb13 are somewhat different. Due to the very high matric flux potential of this soil, small differences in soil water pressure head cause large differences in root water uptake. The slightly lower soil moisture content of this layer has a larger impact on root water extraction than the higher root density.



**Figure 17**

Relative water uptake as a function of root length density and pressure head at  $t = 0.5$  d (left column) and  $t = 15$  d (right column).

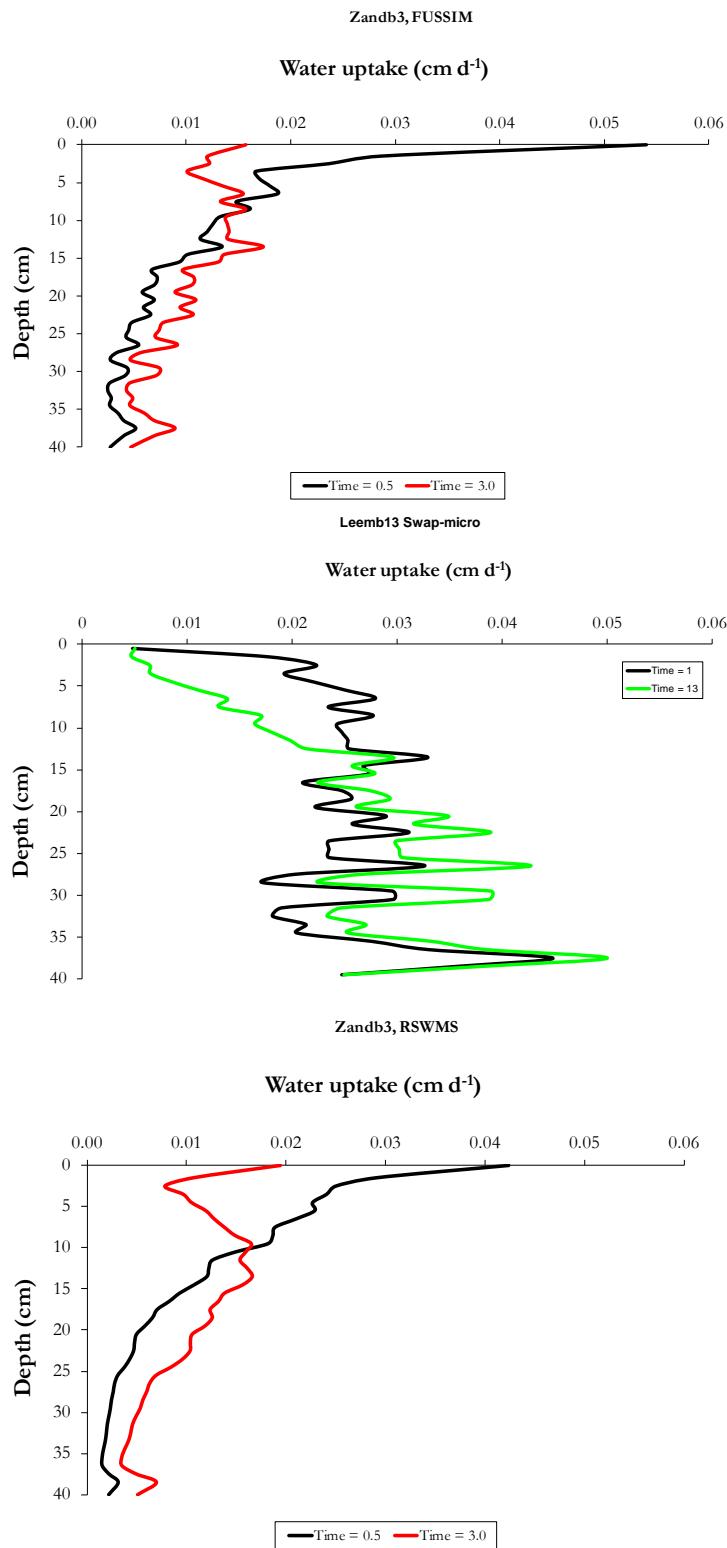
When the soil is dry, after a period of 15 days of transpiration without any rain, instead of root length density the soil wetness distribution governs the distribution of root water uptake (right column of Figure 17). The scatter is considerable but still it is clear that now - with vertical gradients of soil pressure head of the order of  $100-300 \text{ cm cm}^{-1}$  - there is a positive correlation between soil wetness and relative water uptake, and a negative correlation between water uptake and root length density. For clay and loam, SWAP-macro somewhat deviates in the relation between soil wetness and relative water uptake. Low water uptake occurs both at low pressure heads in the upper part of the root zone, and at high pressure heads with low root density in the lower part of the root zone. In SWAP-macro, water uptake linearly depends on both root density and soil water pressure head (see Section 2.2.1). Therefore the highest water uptake is found in this model in the middle part of the root zone with moderate soil wetness and root density.

#### 4.3.4 Compensation

As shown in Figure 15 relative uptake of water increases in the lower layers when the upper layers become dry. In the models SWAP-micro, FUSSIM2 and RSWMS the diminished uptake in dry layers can sometimes be fully compensated by enhanced uptake in wetter layers. An example is shown in Figure 18, where the decrease in uptake in the upper 5-10 cm is fully compensated by an increase in uptake in deeper layers, the total uptake being 4 mm d<sup>-1</sup> in all the three cases. The compensation in all three models occurs as a 'natural' consequence of the description of uptake, contrary to attempts to force compensation by postulation of empirical parameters, the value of which can only be obtained by curve fitting (Šimůnek and Hopmans, 2009; Jarvis, 2010).

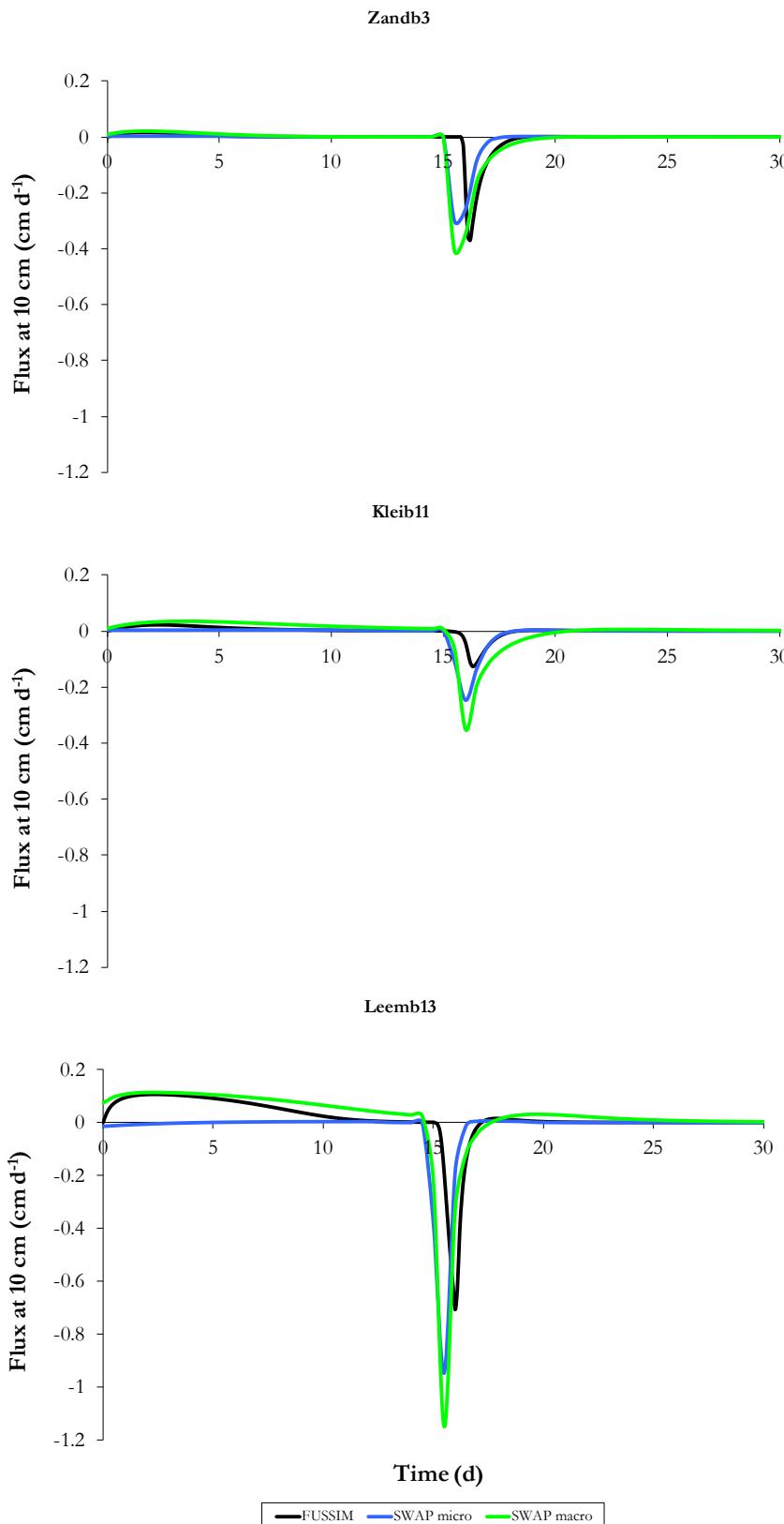
#### 4.3.5 Flux at 10 cm depth

Differences in root water uptake will affect the vertical soil water fluxes. In order to show some of the dynamics of the soil water fluxes, in Figure 19 the time course of the flux at 10 cm depth is depicted. SWAP-macro and SWAP-micro show the largest downward fluxes. Upward fluxes mainly occur in the loam soil, and are relatively small.



**Figure 18**

*Distribution of water uptake with depth at two times as calculated by FUSSIM2 for soil Zandb3, SWAP-micro for Leemb13 and RSWMS for Zandb3. At all times the total uptake was equal to the potential transpiration.*



**Figure 19**  
The flux at 10 cm depth as a function of time.

## 4.4 Scenario S2

### 4.4.1 Cumulative transpiration and transpiration rate

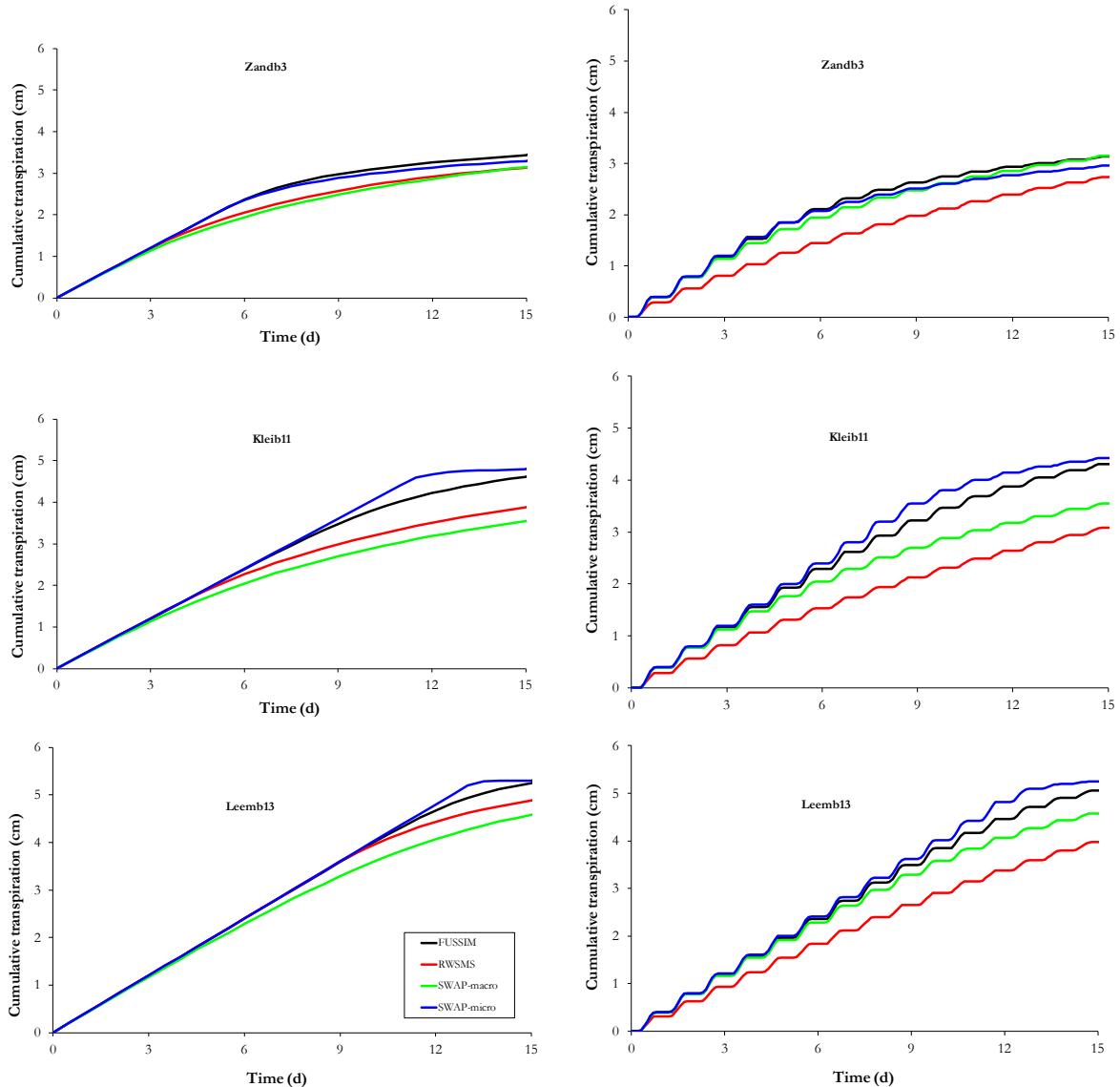
Figure 20 compares the time course of cumulative transpiration for scenario S1 and S2. Generally, the reduction starts earlier - for RSWMS almost immediately - and the total transpiration over a 15 day period is less in case of S2 (Table 8). The exception is SWAP-macro. In this model the critical pressure head  $h_3$  is affected by the daily atmospheric demand, not the instantaneous transpiration flux. Therefore the results of a uniform and of a sinusoidal transpiration rate are identical for this model. The differences between cumulative transpiration in S1 and S2 are the highest for RSWMS amounting to 20% in case of Leemb13.

It seems that RSWMS is more sensitive to the instantaneous flux than the other models. It is probably due to the three dimensions of RSWMS. Indeed, as soon as the potential demand is high, the local fluxes increase as well, which create a sudden drop of water content and conductivity in the voxels close to the root nodes. As the lateral redistribution is not instantaneous (as it is in 2D or 1D models, when the depth-averaged water potential is felt by the root), high flux may create more rapidly local low potentials, which generate stress during the middle of the day.

**Table 8**

Total transpiration (cm) after 15 days in scenario S1 and S2.

<b>Model</b>	<b>Total transpiration S2 (cm)</b>			<b>Total transpiration S1 (cm)</b>		
	<b>Zandb3</b>	<b>Kleib11</b>	<b>Leemb13</b>	<b>Zandb3</b>	<b>Kleib11</b>	<b>Leemb13</b>
SWAP-macro	3.15	3.55	4.58	3.15	3.55	4.58
SWAP-micro	2.96	4.43	5.25	3.29	4.64	5.29
FUSSIM2	3.13	4.31	5.05	3.43	4.61	5.25
RSWMS	2.74	3.08	3.98	3.16	3.87	4.88

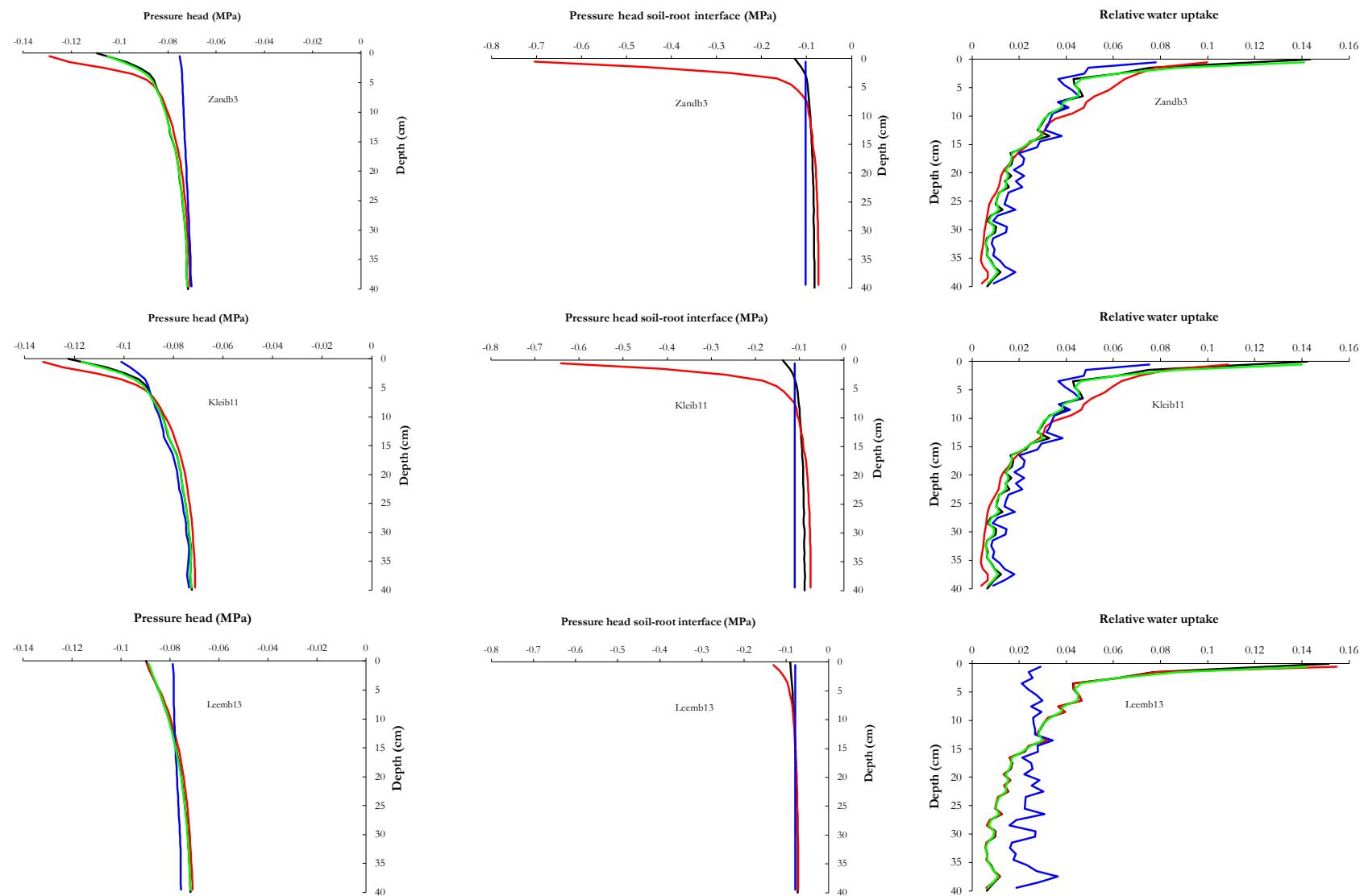


**Figure 20**

Time course of cumulative transpiration for S1 (left column) and S2 (right column).

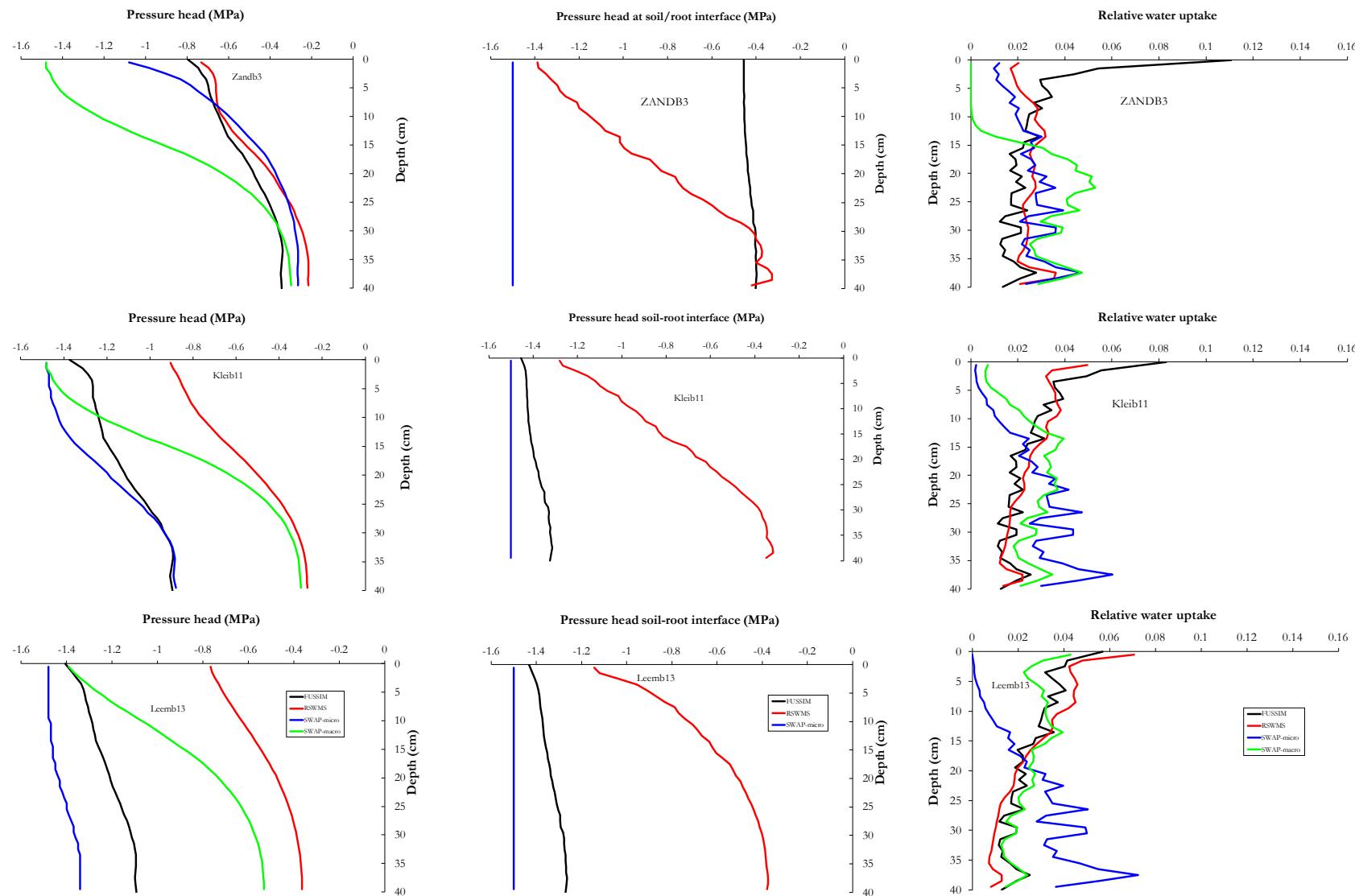
#### 4.4.2 Distribution of pressure head in soil, pressure head at soil root interface and relative water uptake

Figure 21 and Figure 22 show the depth distribution of pressure head in soil, pressure head at the soil root interface and relative water uptake at day 0.5 and 15.5, respectively. The gradients in PHS and PHR are larger for RSWMS than for the other models, especially in case of the sand and clay soil. Again, this is probably related to the fact that RSWMS generates a 3D xylem water pressure distribution in the root.



**Figure 21**

*Distribution of pressure head of the soil, pressure head of the soil root interface and relative water uptake with depth at  $t = 0.5$  d for scenario S2.*



**Figure 22**

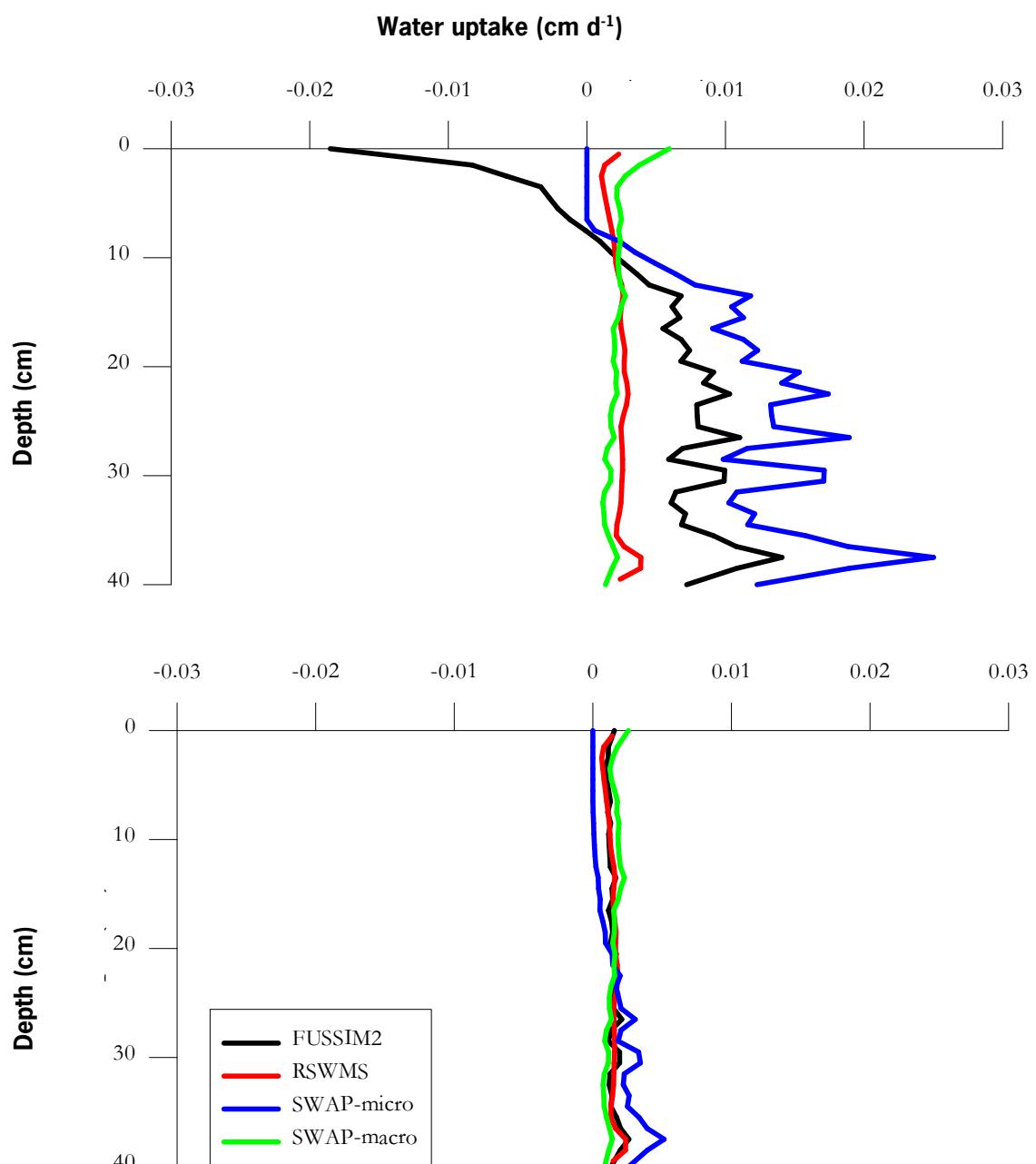
Distribution of pressure head of the soil, pressure head of the soil root interface and relative water uptake with depth at  $t = 15.5$  d for scenario S2.

## 5 Discussion

In this report we studied four water uptake models, that were all embedded in a greater model dealing with transport of water in (an unsaturated) soil.

Our analysis started with considering the soil water flow and the water uptake routine separately. Without the sink term the models yielded very similar results (Section 5.1, Figure 7), what is to be expected as they all solve Richard's equation (Eq. (1) without the sink term) in essentially the same way.

Next, the water uptake routines were compared. In three models (SWAP-macro, SWAP-micro and FUSSIM2) the sink term was derived from a single root model which was scaled up to a root system. When these single root models were compared considerable differences appeared when the effects of soil pressure head (Figure 8) and root length density (Figure 9) were evaluated. This is also the case for the depth distribution of root water uptake (Figure 11) as a function of a given depth distribution of pressure head (given in Figure 10). But when the depth distribution of the pressure head was generated by the water flow model in combination with the appropriate the water uptake routine, the pattern of water uptake distribution differs not so much between the models, an example being given in Figure 23. This is caused by feedback mechanisms: the tendency of the soil to aim at equilibrium of total head and consequently at evening out of differences in total head, and secondly by the fact that in all water uptake routines the uptake in a certain layer depends directly or indirectly on the pressure head in that layer, where lower values of pressure head lead generally to lower uptake. In case of SWAP-macro uptake is completely determined by the local pressure head, for the other three models the uptake in a certain layer is also determined by the uptake possibilities in other layers. This can lead to total compensation, where uptake in some layers can make up for uptake deficit in others (Section 5.3.4, Figure 18).



**Figure 23 a and b**

The depth distribution of water uptake as a function of pressure head distribution. In figure 23a the same pressure head distribution was used for all models (given in Figure 11), in 23b the pressure head distribution was calculated with the corresponding water flow model.

To show the effect of different compensation mechanisms on pressure head distribution and realized transpiration some additional calculations were done with FUSSIM2. These pertain to the soil Zandb3, with a profile depth of 40 cm, consisting of 20 layers with a root length distribution as we used before and subject to a potential transpiration of 4 mm d<sup>-1</sup>. Three cases are considered:

1. Water uptake from a layer completely determined by the soil pressure head in that layer, no compensation whatsoever. The relation between water uptake and pressure head was as given in Figure 8 (Zandb3, FUSSIM2, for a root length density of 0.16 cm cm<sup>-3</sup>) in our report. There is no transport of water between the layers, each layer is separated from its neighbors by an impermeable membrane.
2. As 1) but the uptake from a certain layer is also determined by the uptake possibilities of other layers in the way FUSSIM2 does, i.e. by assuming a similar root water potential in each layer. Again no exchange of water between the layers.
3. Water uptake and transport as normally calculated by FUSSIM2.

Results are given in Figure 24 a and b. In Figure 24a the depth distribution of pressure head after 10 days is shown. Clearly, the gradient in pressure head are much greater when exchange of water between the layers is absent (Case 1). When transport of water is possible this leads to a decrease in gradients (Case 2), and this is more pronounced when compensation in uptake occurs (Case 3). The effects of compensation is also reflected in the course of cumulative transpiration shown in Figure 24b , thanks to compensation the realized cumulative transpiration is larger.

In extreme situations this can in case of FUSSIM2 and RSWMS lead to the phenomenon of hydraulic lift (Figure 14) which lead to evening out of differences in soil pressure head by transport through the root system followed by flow of water from roots to soil. So the large differences in local water uptake between the models do not necessarily lead to large differences in simulated transpiration and distribution of water over a period of time. However, even small differences in the water uptake distribution in the rooted zone will cause differences in pressure head distribution in the rooted zone (Figure 14). This may then lead to differences in water fluxes at the local scale, and thus in leaching fluxes to below the rooted zone. So, despite the fact that several models may result in similar total water uptake, their prediction of leaching, especially leaching of solutes, may be different. This aspect was not further investigated in this study, and needs future attendance.

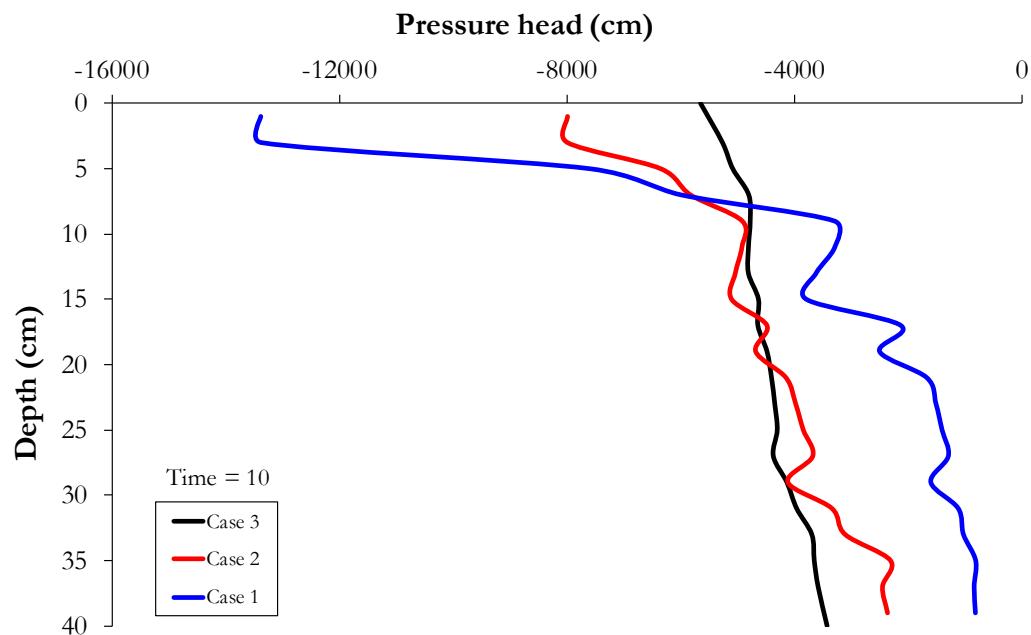
A model, by definition, is a simplification of part of the real world. In making a model one tries to leave out as much as possible, with the intent to include only the processes which really do matter for the phenomena one wants to study. It is therefore difficult to give a general recommendation as to which of the models discussed here can best be used, this depends on the purpose of the user and the data available. For instance if one is interested in simulation of the transpiration in the growing season and data on distribution of root length density are not available SWAP-macro seems a suitable choice. At the other end of the spectrum one finds the model RSWMS that is more flexible and by which subtleties of differences in radial and axial conductance can be investigated.

Another example is the actual flow pattern in the root zone. If this flow pattern is predominantly vertical, as in close, uniform covered cultivated soils, a one-dimensional approach as used by SWAP-macro and SWAP-micro may suffice. However, at two-dimensional or radial symmetric flow patterns for instance in case of drip irrigation, FUSSIM2 might be more suitable. In case of three-dimensional patterns analysis by RWSMS seems more justified.

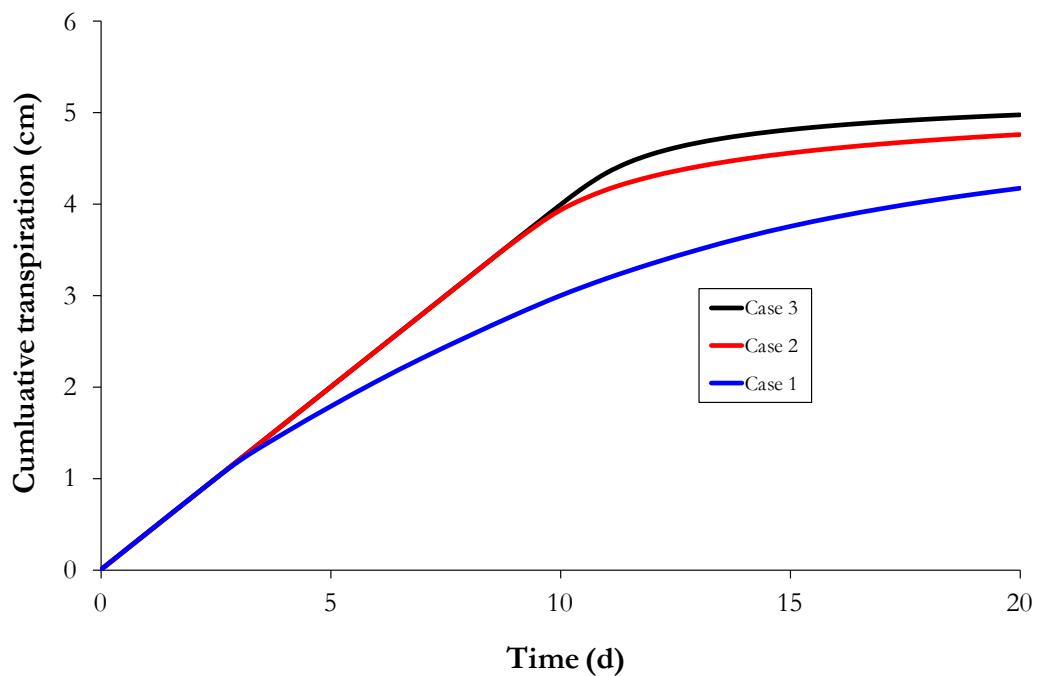
The depicted root water extraction patterns for two scenarios and four clearly different models may serve as a reference for other, alternative root water uptake modeling concepts.

Unfortunately, within the given time we had no opportunity to compare the four models to an actual root water extraction data set. This would be an interesting analysis and will be the subject of a next publication.

a)



b)

**Figure 24**

a) Pressure head distribution after 10 days for the three cases considered, and b) cumulative transpiration for the three cases considered.

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# Appendix 1 Mathematical details of the root water uptake model of FUSSIM2

## Assumptions

The basic assumptions used in derivation of the water uptake in FUSSIM2 already mentioned in Paragraph 2.2.3 will be repeated here:

1. The flux of water from bulk soil to root surface can be described adequately by a steady rate profile of the matric flux potential. The flux from root surface to root xylem is described as a steady state situation.
2. In the path soil - root surface - root xylem there is no accumulation of water, which implies that transport rate from bulk soil to root surface equals transport rate from root surface to root xylem.
3. The xylem water potential has the same value in the root system.
4. Total water uptake equals total transpiration.
5. Actual transpiration is a function of potential transpiration and between leaf water potential.

## Derivations

The soil domain in FUSSIM2 is a rectangle with length  $L$  and thickness  $Z$  cm consisting of layers and columns, together forming a grid of so-called control volumes. Within a control volume the root length density is uniform. Every layer has its own thickness  $\Delta z$ , subdivided in compartments with length  $\Delta x$ , and width  $\Delta y = 1$  cm. The number of layers is denoted by  $N$  and the number of compartments per layer by  $M$ .

In every control volume the flux to the root surface is given by an equation similar to (29):

$$V_{I,J} = S_{I,J} (\bar{\Phi}_{I,J} - \Phi_{0,I,J})$$

where  $S_{I,J} = \frac{\Delta z_J}{R_{1,I}^2} \frac{\rho_{I,J}^2 - 1}{G(\rho_{I,J})} \text{ cm}^{-1}$ ,  $G(\rho) = \frac{1}{2} \left( \frac{1-3\rho^2}{4} + \frac{\rho^4 \ln \rho}{\rho^2 - 1} \right)$  whereas  $\rho = \frac{R_1}{R_0}$ ,  $R_1 = \sqrt{\pi L_n}$ ,  $R_0$

the radius of the root in cm and  $\Phi$  the matric flux potential defined as:

$$\Phi = \int_{h_{ref}}^h K(x) dx,$$

$K$  being the soil water conductivity,  $h_{ref}$  a reference value, and  $h$  the relevant pressure head. For convenience and in agreement with earlier studies (De Willigen and Van Noordwijk (1987), De Willigen (1990), De Willigen and Van Noordwijk (1991)) we use here the absolute value of the pressure head denoted by the symbol  $P$ , so  $P = |h| = -h$ , as we only consider unsaturated conditions. The matric flux potential in terms of  $P$  is thus:

$$\Phi = \int_P^{P_{rf}} K dP$$

It follows then that:

$$\overline{\Phi} - \Phi_{rs} = \int_{\overline{P}}^{P_{rf}} K dP - \int_{P_{rs}}^{P_{rf}} K dP = \Delta\Phi = \int_{\overline{P}}^{P_{rs}} K dP$$

The flux from the root surface to the root xylem is given by the steady state equation:

$$U_{I,J} = Q_{I,J}(P_R - P_{0,I,J})$$

where  $Q_{I,J} = L_{r,I,J}K_R$ ,  $P_R = -b_R$ ,  $P_{0,I,J} = -b_{0,I,J}$

Because of assumption 2 in every individual control-volume it holds:

$$V_{I,J} = U_{I,J} \quad (A1-1)$$

The water uptake from control volume (I,J) per unit surface is:

$$U_{I,J} = \Delta x_J Q_{I,J}(P_R - P_{0,I,J}) \frac{\text{cm}}{\text{d}}$$

Total water uptake is

$$\Delta y \sum_{J=1}^N \sum_{I=1}^M \Delta x_I U_{I,J} = \Delta y \sum_{J=1}^N \sum_{I=1}^M \Delta x_I \Delta x_J L_{r,I,J} K_R (P_R - P_{0,I,J}) \frac{\text{ml}}{\text{d}}$$

Total transpiration is  $\Delta y \left( \sum_{i=1}^M \Delta x_I \right) T_a = \Delta y L T_a \frac{\text{ml}}{\text{d}}$ , so it follows that:

$$\sum_{J=1}^N \sum_{I=1}^M \Delta x_I \Delta x_J L_{r,I,J} K_R (P_R - P_{0,I,J}) = L T_a \quad (A1-2)$$

The actual transpiration  $T_a$  is a function of the leaf water potential  $h_L$  and the (known)  $T_p$ :

$$T_a = \frac{T_p}{1 + \left( \frac{h_L}{b_{L,1/2}} \right)^q} = \frac{T_p}{1 + \left( \frac{P_L}{P_{L,1/2}} \right)^q} = \frac{T_p}{1 + \left( \frac{P_R + \Delta P}{P_{L,1/2}} \right)^q} \quad (A1-3)$$

For a given transpiration rate the leaf water potential can be given as:

$$b_L = b_R - \frac{T_p}{L_p} \text{ or equivalently } P_L = P_R + \frac{T_p}{L_p}$$

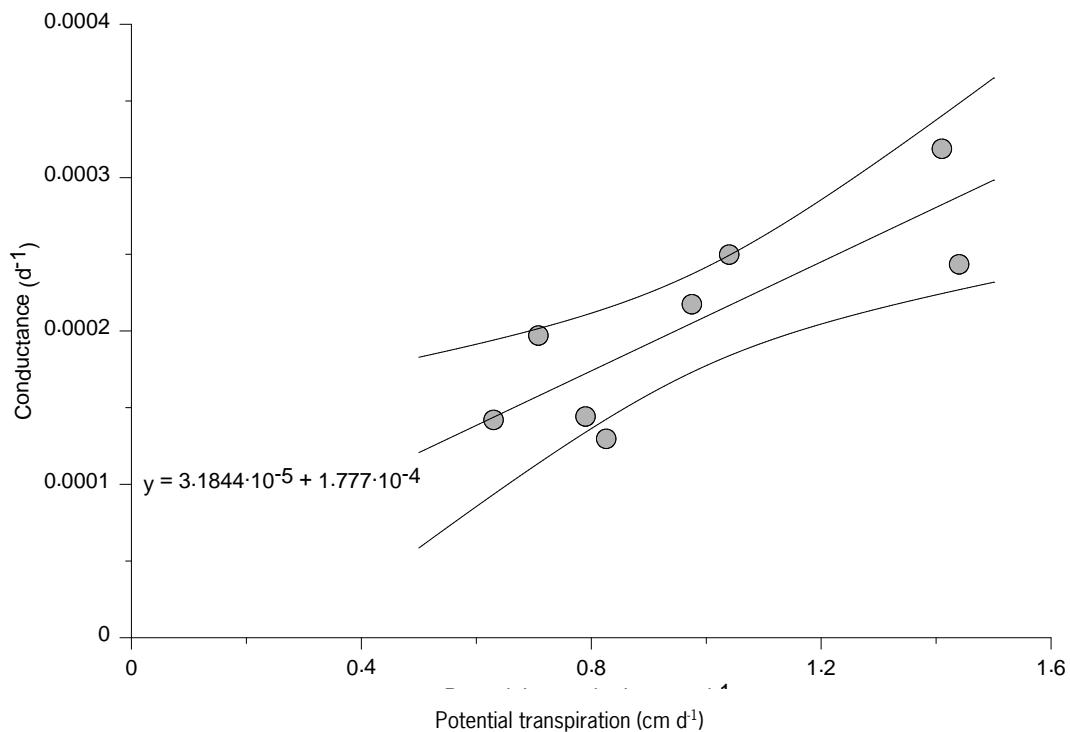
$L_p$  being the conductance (d) in the path root – leaf.

According to the study of Zhuang et al. (2001) the conductance in a maize plant in the path root - leaf is a function of the potential transpiration (Figure A-1). So the leaf water potential can be calculated as:

$$P_L = P_R + \frac{T_p}{a_1 T_p + a_0}$$

Thus:

$$\Delta P = P_L - P_R = \frac{T_p}{L_p} = \frac{T_p}{a_1 T_p + a_0}$$



**Figure A-1**

Relation between the conductance in the path root - leaf for maize and potential transpiration. Data of Zhuang et al. (2001).

### Solution

We have  $M \times N$  equations of the form (A1-1), and one given by (A1-2). The unknowns are the  $M \times N$  values of  $h_{0,I,J}$ , and the value of  $h_R$ . At any time the pressure head of the control volumes are known (and thus also the matric flux potential), these follow from macroscopic calculations of flow of water. If we for convenience set  $m = M \times N$ , and  $n = m+1$  then we want to find the solution for  $m$  equations of the form:

$$f_i = 0, \text{ where} \\ f_i = U_i - V_i = Q_i(P_R - P_{0,i}) - S_i \Delta \Phi_i, i = 1, 2, \dots, m \quad (A1-4)$$

And one equation of the form:

$$f_n = \sum_{J=1}^N \sum_{I=1}^M \Delta x_I Q_I (P_R - P_{0,I,J}) - L T_a \quad (A1-5)$$

$T_a$  being given by (A1-3). Following Press *et al.* (1992) we use the Newton-Raphson method for multiple dimensions. The unknowns are denoted by a vector  $\mathbf{X}$  with, in our case, dimension  $n = M \times N + 1$ . The components of  $\mathbf{X}$ :  $x_1, x_2, \dots, x_n$  are equal to  $P_{0,1}, P_{0,2}, \dots, P_{0,m}, P_R$ . Essentially in this method an estimated solution is improved by using the corrections  $\delta \mathbf{X}$ , which is the solution of the matrix equation:

$$\mathbf{A} \delta \mathbf{X} = \mathbf{B} \quad (A1-6)$$

The components of the matrix  $\mathbf{A}$  are the partial derivatives with respect to the unknowns evaluated at the values of the current integration step. It holds that:

$$\alpha_{ij} = \frac{\partial f_i}{\partial x_j}$$

The matrix  $\mathbf{A}$  is a sparse matrix, which means that the majority of its elements are zero, only the diagonal and the last row and column are filled with non-zero values. Generally for dimension  $n$  there are  $n \times n$  elements, of which  $3n/2$  are non-zero.

The  $i$ th element of the vector  $\mathbf{B}$  is given by  $\beta_i = -f_i$ . After solving (A1-6) for  $\delta \mathbf{X}$ , the new values are calculated as:

$$x_i^{new} = x_i^{old} + \delta x_i, i = 1, \dots, n$$

## Appendix 2 The Doussan equation in RSWMS

Doussan et al. (1998) proposed an algorithm to solve water flow within the whole root system in function of the static soil water status. They simplified the root architecture as a series of interconnected nodes in which radial (soil to root) and longitudinal (along xylem vessels) flow take place. Assuming the osmotic potential gradient as negligible, the radial water flow [ $L^3 T^{-1}$ ] between the soil-root interface and the root xylem can be written as

$$J_r = K_r^* s_r [H_s(z) - H_x(z)] \quad (A2.1)$$

where  $H_s$  and  $H_x$  are the total water potential (written on weight basis) at the root surface and in the xylem [ $L$ ],  $K_r^*$  is the intrinsic radial conductivity [ $T^{-1}$ ] and  $s_r$  is the root-soil interface area [ $L^2$ ]. Note that the total water potential is  $H = h + z [L]$ , where  $h$  is the matric (in soil) or the hydrostatic (in root) potential. Longitudinal water flow in the xylem [ $L^3 T^{-1}$ ] is defined as

$$J_x = K_x^* A_x \frac{dH_x(z)}{dl} = K_x \left[ \frac{dh_x(z)}{dl} + \frac{dz}{dl} \right] \quad (A2.2)$$

with  $H_x$  the total water potential  $A_x$  the xylem cross sectional area [ $L^2$ ],  $dl$  an infinitesimal segment length [ $L$ ],  $K_x^*$  the intrinsic axial conductivity [ $L T^{-1}$ ] and  $K_x = K_x^* A_x [L^3 T^{-1}]$  the xylem conductance. Negative  $J_x$  refer to fluxes toward the root collar.

When using finite differences instead of differentials in Eqs. (A2.1) and (A2.2), we can write the water mass balance for a given root node  $i$  as:

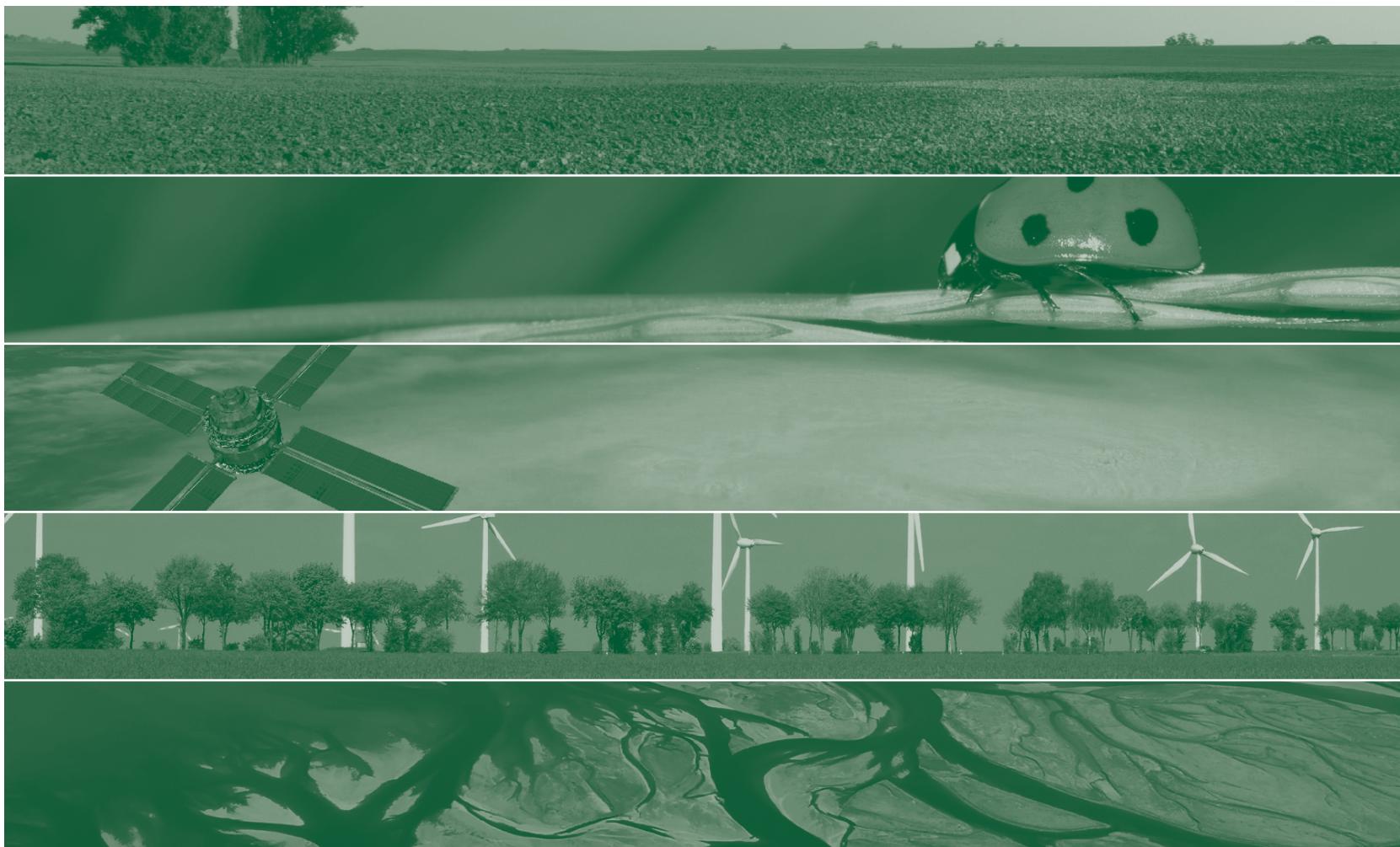
$$K_{x,i:i-1} \frac{(H_{x,i} - H_{x,i-1})}{l_{i:i-1}} = K_{x,i+1:i} \frac{(H_{x,i+1} - H_{x,i})}{l_{i+1:i}} + K_{r,i}^* s_{r,i} (H_{s,i} - H_{x,i}) \quad (A2.3)$$

where the right-hand side term refer to the water flow from node  $i$  to node  $i-1$  (mother node) through the segment  $i:i-1$  with a length  $l_{i:i-1}$  and a root xylem conductance  $K_{x,i:i-1}$  while the subscripts  $i+1:i$  refer to the segment between the nodes  $i+1$  and  $i$  (upstream root segment).

When generalized to all the nodes of a root system, the water potential distribution in the xylem is obtained by solving a system of simple linear equations like Eq. (A2.3), which writes in matrix notation (Doussan et al., 1998),

$$\mathbf{C} \cdot \mathbf{H}_x = \mathbf{Q} \quad (A2.4)$$

where  $\mathbf{C}$  (dimensions  $n_p \times n_p$  with  $n_p$  the number of root nodes) is called the “conductance matrix”,  $\mathbf{Q}$  (dimensions  $n_p \times 1$ ) contains the soil factors and  $\mathbf{H}_x$  (dimensions  $n_p \times 1$ ) is the xylem water potential vector. Following the type of boundary conditions which is applied at the root collar (head or flux-type), matrix  $\mathbf{C}$  and vector  $\mathbf{Q}$  are slightly affected (see Appendix 1 in Javaux et al. (2008)). Due to the large size of the system, these matrices are stored under a sparse format to reduce memory consumption. A bi-conjugate gradient method is used to solve the non-symmetric linear system (Press et al., 1992). Note that solving Eqs. (A2.3-4) requires the assessment of the soil water potential in the vicinity of each root node  $H_{s,r}$



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