## **Author's Response**

We are thankful for the critical reading, comments and suggestion made by N. Jarvis and Referee#2. Their suggestions were implemented in the manuscript. We also replied the questions and comments made by referee#2 in the following.

## **Anonymous Referee #2**

Abstract: If you briefly mention what is behind the 'alternative empirical models' that are proposed, I think that the abstract could be improved. How do they differ from the Feddes and Jarvis models?

#### We added how, in general, all empirical models are defined.

P6 ln 2-3: Maybe before going to De Jong van Lier et al. (2013) where the reader can find information about the algorithm, I think it would be helpful to explain how an equation with three unknowns Ta, hl and h0 can be solved in general. First, I think you need to write that in equation 8, there are only two unknowns: either h0 and hl or h0 and Ta. In order to solve the equation for the two unknowns, additional equations are required. After formulating equations for h0's at different depths, Eq 1, making use of Eq. 6, can be used to solve for Ta (or hl) and the distribution of h0 with depth in the soil profile.

#### We rewrote this part of the manuscript according to your suggestions

P6 Figure 2: I am afraid that I still do not understand figure 2 and its caption. What I suppose that is shown in Figure 2 is the sink term for the case that the root length density and the soil water potential are uniform in the root zone (i.e. they do not change with depth in the root zone). As a consequence, also the sink term is uniform in the root zone and the transpiration rate is simply the sink term multiplied by the root zone thickness. So I do not understand that the plant transpiration was set to 1 mm d-1.

The caption of Fig. 2 was corrected. The root water uptake (RWU) is not calculated considering a homogeneous root length density (RLD) down to a depth of 50 cm. It corresponds to the RWU for any soil layer having a given RLD (three values are shown in Fig. 2) belonging to a certain RLD distribution. Thus, Fig. 2 shows the RWU in a given soil layer (with a certain RLD) when a plant adjusts its  $h_l$  to achieve a transpiration rate of 1 mm d<sup>-1</sup> for different soil water conditions. The true value of  $h_l$  will depend on the RLD distribution and soil moisture distribution over the root zone.

#### With the corrected caption, we think it is now what we intend to show in Fig. 2.

P7 and P8: Comparison of the Jarvis model and the De Jong van Lier model and Figure 5. In my previous comments on the paper, I posed the question whether the analogy between the two models relies on the assumption that when stress occurs the water potential the root surface is every the same in the root zone. I also asked whether the model of De Jong van Lier only predicts stress when the water potential at the root surface is everywhere equal to the wilting point. If the De Jong van Lier model can predict that stress may also occur even when in parts of the root zone the surface water potential at the root surface is still above the wilting point, then the De Jong van Lier and Jarvis models may also deviate under stress conditions. I think that the main problem in the description here is that the authors are not fully consistent in defining the stress conditions: Eq. 14 is not the same as Eq. 10. In Eq. 14, it is assumed that the main loss of pressure head between the bulk soil and the leaves is in the soil when stress occurs. Under this assumption, it can be stated that the pressure head at the soil root interface is everywhere in the root zone equal to the wilting point. However, when pressure head losses in the root system become important, the pressure head at the soil root interface can be in some parts of the root system well above the wilting point. To check this, another Tpmax can be defined which is the maximal uptake when the leaf water potential is equal to the critical leaf water potential, hwl and the water potentials at the soil root interface, h0, are everywhere in the root system equal to the bulk soil water potential hs. When this Tpmax is smaller than the Tpmax that is obtained assuming that the water potentials at the soil root interface are everywhere equal to the wilting point, then pressure head losses in the root system are more important.

In Eq. 14, there are no plant conductivities. Therefore, Tpmax as defined in Eq. 14 must be different from Tpmax in Figure 5. In figure 5, the effect of Kroot and Ll on Tpmax is evaluated. But it is not clear to me what exactly the boundary conditions were to calculate Tpmax. I think the authors should explain how they defined Tpmax and try to use a consistent definition.

The analogy between the models relies on the assumption of uniform  $h_0$  at the onset of drought stress

The De Jong van Lier et al. (2008) model indeed assumes that  $h_0 = h_w$  over the root zone at stress onset. The comparison of the Jarvis (1989) model with the De Jong van Lier et al. (2008) model (Jarvis, 2011) is also based on the assumption of  $h_0 = h_w$  over the root zone. It is also shown that the models differ in unstressed conditions. This information can be found in the last version of the manuscript. However, possibly referee#2 did not clearly distinguish between the De Jong van Lier et al. (2008) and De Jong van Lier et al. (2013) models. As shown in section 2.2.1, we are comparing the Jarvis (1989) model to the De Jong van Lier et al. (2008) model — a physical model that does not account for plant hydraulic resistances. We mention in section 2.1 that this model was extended to take this into account, leading to the De Jong van Lier et al. (2013) model. Thus, when stating that "If the De Jong van Lier model can predict that stress may also occur even when in parts of the root zone the surface water potential at the root surface is still above the wilting point, then the De Jong van Lier and Jarvis models may also deviate under stress conditions", he is referring to the De Jong van Lier et al. (2013) model, and not to the De Jong van Lier et al. (2008) model, which we are discussing and making the comparison in the current section.

Defining the stress condition: eq. 14 versus eq. 10

The stress conditions are defined differently by the De Jong van Lier et al. (2008) and De Jong van Lier et al. (2013) models — eq. 14 and eq. 10, respectively. In the De Jong van Lier et al. (2008) model at the stress onset,  $h_0 = h_w$  over the root zone and it is correlated to the Jarvis (1989) model (Jarvis, 2011). Whereas, in the De Jong van Lier et al. (2013) model, when stress occurs,  $h_l = h_{wl}$ . Notice that  $h_{wl} < h_w$ , and means that when  $h_l = h_{wl}$ ,  $h_0$  over the root zone must approach  $h_w$  due to pressure head loss, but it is not necessarily equal to  $h_w$ , as it is assumed in the De Jong van Lier et al. (2008) model.

We tried to make all this clearer by including in section 2.1 how  $T_{p,max}$  is defined in the De Jong van Lier et al. (2013) model and stressing the difference with  $T_{p,max}$  for the De Jong van Lier et al. (2008) model. We think it is now clearer how both models define stress, i.e. plant transpiration reduction: the De Jong van Lier et al. (2013) defines transpiration reduction in terms of plant leaf potential (eq. 10), which is an improvement of the De Jong van Lier et al. (2008) model that defines it in terms of the pressure at the root surface, considered constant with depth (eq. 14).

P10 section 2.2.5: I made the comment that besides the pressure head, also the potential transpiration rate plays a role in the definition of the stress function. Instead of making an extra section about it, I would suggest to include how the different model concepts deal with the dependence of the stress function on the potential transpiration. I would propose to include in Eq. 3 also Tp in the stress function:  $\alpha(z)$ ,Tp). In the physical model, the maximal uptake rate is calculated and this maximal uptake rate depends on the soil water potential. That means that if a stress function would be defined for the physical model as Ta/Tp(h), it would also depend on Tp since for a lower Tp, the pressure head at which the maximal uptake is equal to Tp is lower. The authors already mention for the Jarvis model, that the dependence of the stress function on Tp should be different from the dependence that is derived for the Feddes model. It is interesting that in the comparison between the Jarvis model and the physical model, they determine a stress function (Eq. 18) that is independent of the potential transpiration rate (neither M nor Mmax depend on Tp).

In the case of the dependence of the stress function on  $T_p$ , it should be noticed that  $\alpha$  in eq. 3 already takes  $T_p$  in to account by setting  $h_3$  for two levels of  $T_p$ : low (1 mm d<sup>-1</sup>) and high (5 mm d<sup>-1</sup>) level. In the manuscript we proposed to make the optimizations for these two levels of  $T_p$  aiming to provide  $h_3$  for the respective  $T_p$  levels. In that way, the dependence of  $h_3$  on  $T_p$  can be taken into account.

As commented by referee#2, we did mention the dependence of  $\alpha$  on  $T_p$  is different in Jarvis and Feddes model. It can be seen that we made this statement on the grounds of the  $h_3$  values in both models.

All the evaluated empirical models make use of the Feddes reduction function or a modified version, at which the dependence of  $\alpha$  on  $T_p$  is taken into account by the value of  $h_3$ .

P 18 Eq. 32: The authors included now the Aikake's information criterion. I think this is a very suitable parameter but in this context, I am wondering whether it would not be better to investigate the performance of a model that uses the same vegetation parameters for different soils and transpiration conditions could be used. The problem now is that for the same properties of the vegetation (root density and root hydraulic conductivities) different 'root water uptake parameters' must be used depending on the soil and potential ET conditions. Therefore, although the empirical models do not have that many parameters, they need to be adjusted for different soil conditions and climate (potential transpiration). My question is therefore whether the de Jong van Lier model requires that many more parameters than the empirical models. Root length density can be measured and the root conductivities could be fitted as well. In the end, this might result in less parameters that need to be determined when the model is to be used in different soils and for different transpiration rates. This problem may be even more relevant when considering that soils often have layers with different hydraulic properties. I do not suggest that the authors refit now the models to the different cases they considered using only one parameter set for the different cases (soils and potential transpiration) but I would propose including this in the conclusion and discussion section.

#### 15 To address this, as comment was added to the conclusion.

P20: The authors concluded that one drying experiment would be sufficient to parameterize the model and use it to run root water uptake during a growing season. I am just wondering whether one drying experiment would be enough. How can the dependence of the stress parameters on the transpiration rate be defined then? Maybe, this dependence is not so important for simulations over an entire growing season as long as a drying period with a relevant transpiration rate for the entire growing season is chosen. But this could maybe be taken up in the discussion section. Furthermore, the authors used daily averaged transpiration rates and made the stress function dependent on the daily transpiration rates. But this means that in the model, the transpiration rates should not be resolved within one day since otherwise, different stress functions will have to be used that consider the peak transpiration rates during midday (which are about a factor 8 higher than the daily average transpiration rate).

This part must be rephrased. The dependence of  $\alpha$  on  $T_p$  is accounted for by the parameter values derived for the two levels of  $T_p$  in the drying-out experiment. By setting a constant  $T_p$  over the drying-out period, the optimized parameters are therefore defined for this  $T_p$  level. Parameter values in between can be obtained by linear interpolation as we did in section 4.2, and explained in section 3.4.

P21: The authors concluded that for cases with low root water uptake compensation, which correspond with cases of low root length density, the Feddes models perform pretty well. Can this be explained by the fact that for low root density, the resistance to water water flow from the soil to the leaves is mainly dominated by the resistance to flow in the soil? When the soil dries out at one depth, the resistance to the flow at another depth and therefore flow will not change since this resistance is dominated by the soil conditions and is hardly influenced by changing conditions in the roots.

Higher root hydraulic resistances will increase root water uptake "compensation". As this mechanism is enhanced, the Feddes models will not perform well. However, in our simulations we kept plant hydraulic resistances constant and varied only the root length density. Thus, the performance of the Feddes models when varying R is not related to the increase/decrease of plant hydraulic resistances. Increasing  $K_{root}$ , for instance, as R increases will enhance the deviations.

# Benchmarking test of empirical root water uptake models

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**Abstract.** Detailed physical models describing root water uptake (RWU) are an important tool for the prediction of RWU and crop transpiration, but involved hydraulic parameters are hardly-ever available, making them less attractive for many studies. Empirical models are more readily used because of their simplicity and the associated lower data requirements. The purpose of this study is to evaluate the capability of some empirical models to mimic the RWU distribution under varying environmental conditions predicted from numerical simulations with a detailed physical model. A review of some empirical models used as sub-models in ecohydrological models is presented, and alternative empirical RWU models are proposed. All these empirical models are analogous to the standard Feddes model, but differ in how RWU is partitioned over depth or how the transpiration reduction function is defined. The parameters of the empirical models are determined by inverse modelling of simulated depthdependent RWU. The performance of the empirical models and their optimized empirical parameters depend on the scenario. The largely used empirical RWU model by Feddes standard empirical Feddes model only performs well in scenarios with low root length density R, i.e. for the seenarios of scenarios with low RWU "compensation". For medium and high R, the Feddes RWU model cannot mimic properly the root uptake dynamics as predicted by the physical model. The RWU model by Jarvis only provides good predictions only for low and medium R scenarios. For high R, the Jarvis model it cannot mimic the uptake patterns predicted by the physical model. Incorporating a newly proposed reduction in the Jarvis model improved RWU predictions. Regarding the ability of the models in predicting plant transpiration, all models that accounts for compensation have accounting for compensation show good performance. The AIC information Akaike information criteria (AIC) indicates that JMII, which has with no empirical parameters to be estimated, is the "best model". The proposed models are more capable of predicting similar RWU patterns by better in predicting RWU patterns similar to the physical model. The statistical indices point them as the best alternatives to mimic RWU predictions by of the physical model.

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#### 1 Introduction

The rate at which a crop transpires depends on atmospheric conditions, the shape and properties of the boundary between crop and atmosphere, the root system geometry, and crop and soil hydraulic properties. The study and modelling of the involved interactions is motivated by the importance of transpiration for global climate and crop growth (Chahine, 1992) as well as by the role of root water uptake (RWU) plays in soil water distribution (Yu et al., 2007). The common modelling approach introduced by Gardner (1960), referred to as microcoscopic or mesoscopic (Raats, 2007), is not readily applicable to practical problems due to the difficulty in describing the complex geometrical and operational function of the root system and its complex interactions with soil (Passioura, 1988). However, it gives insight into the process and allows developing upscaled-physical macroscopic models (De Willigen and van Noordwiik, 1987; Heinen, 2001; Raats, 2007; De Jong van Lier et al., 2008, 2013).

In many one- and two-dimensional problems, macroscopic RWU is modelled as a sink term in the Richards equation, whose dependency on water content or pressure head is usually represented by simple empirical functions (ex. Feddes et al. (1976, 1978); Lai and Katul (2000); Li et al. (2001); Vrugt et al. (2001); Li et al. (2006)). Most of these models are derived from the Feddes et al. (1978) model, which consists of partitioning potential transpiration over depth according to root length density and applying a stress reduction function of piecewise linear shape — defined by five threshold empirical parameters — to account for local uptake reduction. Results of experimental studies (Arya et al., 1975b; Green and Clothier, 1995, 1999; Vandoorne et al., 2012) and the development of physically based-models (De Jong van Lier et al., 2008; Javaux et al., 2008) have helped in understanding increased the understanding of the mechanism of RWU as a non-local process affected by non-uniform soil water distribution in the rhizosphere (Javaux et al., 2013). Accordingly, a plant can increase water uptake in wetter soil layers in order to compensate for uptake reductions in dryer layers to keep transpiration rate at potential rate or mitigate transpiration reduction. Several empirical approaches have been developed over the years to account for this so-called compensation mechanism (Jarvis, 1989; Li et al., 2002, 2006; Lai and Katul, 2000). These models have been incorporated into larger hydrological models and tested at site-specific environments, showing improved predictions an improvement of predictive quality for, e.g., soil water content and crop transpiration (ex. Braud et al. (2005); Yadav et al. (2009); Dong et al. (2010)). Comparisons with physicallybased models (Jarvis, 2011; de Willigen et al., 2012) implicitly accounting for compensation showed that models that do not account not accounting for compensation, like Feddes et al. (1978), are under some circumstances (e.g. high root length density) less accurate with respect to crop transpiration and soil water content predictions under some circumstances, e.g. at high root length density.

Recently, De Jong van Lier et al. (2013) developed a mechanistic model for predicting water potentials along the soil-root-leaf pathway, allowing the prediction of RWU and crop transpiration. This model was incorporated in the eco-hydrological model SWAP (Van Dam et al., 2008) by employing a piece-wise function between leaf pressure head and relative transpiration, reducing the number of empirical parameters compared to other relations (ex. Fisher et al. (1981)). Besides parameters describing soil hydraulic properties and root geometry, this new model requires information about root radial hydraulic conductivity,

xylem axial conductance and a limiting leaf water potential. Although conceptually interesting, the difficulty to obtain the required input parameters makes the model less attractive for routine applications.

Other physical RWU models also exist varying from the simpler model but include the Couvreur et al. (2012), comparable to the De Jong van Lier et al. (2013)model to, as well as more complex three-dimensional models (e.g. Javaux et al. (2013)), which accounts account for the full root architecture, requiring more input parameters and a higher computational effort. Specifically, the De Jong van Lier et al. (2013) differ model differs from the previous mentioned models on by the fact the RWU is based on matric flux potential with an equation derived from the microscopic RWU approach (De Jong van Lier et al., 2008), whereas in other models RWU is based on water pressure head. Note that De Jong van Lier et al. (2013) model does not include the gravimetric potential, as this component is considered of minor importance in dry conditions. The osmotic potential is not included in current analysis, but straightforward can also be included in the model see (de Jong van Lier et al., 2009).

Empirical RWU models are more readily used because of their relative simplicity and lower data requirements. On the other hand, their empirical parameters do not have a clear physical meaning and cannot be independently measured. Their limitations under varying environmental conditions are not well established. For the case of the Feddes et al. (1978) transpiration reduction function, indeed, threshold values are available in literature (Taylor and Ashcroft, 1972; Doorenbos and Kassam, 1986) for some crops and some levels of transpiration demand. Nevertheless, experimental (Denmead and Shaw, 1962; Zur et al., 1982) and theoretical (Gardner, 1960; De Jong Van Lier et al., 2006) studies indicate that these parameters do not depend only on crop type and atmospheric demand, but are also determined by root system parameters and soil hydraulic properties. Furthermore, there are only a few analyses of the validity of these values threshold values are hardly ever validated, and they cannot be used for other models (ex. the Jarvis (1989) model) due to differences in model concepts conceptual differences. Therefore, more accurate values for crops accounting for more environmental factors are necessary in order to apply these models in for a wider range of scenarios. Due to the great number of models developed over the years, it is paramount to investigate some of these models before attempting to determine their parameters.

The general purpose of this study is to evaluate the capability of some empirical models to mimic the dynamics of RWU distribution under varying environmental conditions performed in numerical experiments with a detailed physical model (De Jong van Lier et al., 2013) proposed by De Jong van Lier et al. (2013). The detailed physical model accounts for resistances from the soil to the leaf. We first review some empirical RWU models that have been employed in ecohydrological models and suggest some alternatives. By determining the parameters of the empirical models by inverse modelling of simulated depth-dependent RWU, it becomes clear to which extent the empirical models can mimic the dynamic patterns of RWU.

#### 2 Theory

RWU and crop transpiration are linked through the continuity principle principle of mass conservation for water flow in the soil-plant-atmosphere pathway:

$$T_a = \int_{z_{--}} S(z) dz \tag{1}$$

where  $T_a$  (L) is the crop transpiration and S (L<sup>3</sup>L<sup>-3</sup>T<sup>-1</sup>) is the root water uptake, dependent on crop properties and soil hydraulic conditions, a function of soil depth z (L), and  $z_m$  (L) the maximum rooting depth. Eq. 1 neglects the change of water storage in the plant, which is justified for daily scale predictions, assuming that plants rehydrate to the same early morning water potentials on successive days (Taylor and Klepper, 1978).

In a macroscopic modelling approach, RWU is calculated as a sink term S in the Richards equation, which for the vertical coordinate is given by:

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z} \left[ K(\theta) \left( \frac{\partial h}{\partial z} + 1 \right) \right] - S \tag{2}$$

where  $\theta$  (L<sup>3</sup> L<sup>-3</sup>) is the soil water content, h (L) the soil water pressure head, K (L T<sup>-1</sup>) the soil hydraulic conductivity, t (T) the time and z (L) the vertical coordinate (positive upward). To apply eq. 2, an a functional expression for S is needed. Physical equations in analogy to Ohm's law have been suggested (see the review of Molz (1981) for examples) as well as expressions derived by upscaling microscopic models (De Willigen and van Noordwijk, 1987; Feddes and Raats, 2004; De Jong van Lier et al., 2008, 2013). Alternatively, simple empirical models requiring less information about plant and soil hydraulic properties have also been proposed and are more commonly used. Most of these models use the Feddes approach (Feddes et al., 1976, 1978), formulated as:

$$S(z) = S_p(z)\alpha(h[z]) \tag{3}$$

where  $\alpha(h)$  is the RWU reduction function, defined by Feddes et al. (1978) as a piece-wise linear function of h (Fig. 1). According to this approach, a reduction in S due to  $\alpha(h[z]) < 1$  directly implies a transpiration reduction, making  $\alpha(h)$  to be called as a transpiration reduction function.  $S_p$  is the potential RWU, which is determined by partitioning potential transpiration  $T_p$  over depth. Several ways to estimate  $S_p$  have been proposed (Prasad, 1988; Li et al., 2001; Raats, 1974; Li et al., 2006), but it is most common to distribute  $T_p$  according to the fraction of root length density R (L L<sup>-3</sup>):

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$$S_p(z) = \frac{R(z)}{\int\limits_z R(z) dz} T_p = \beta(z) T_p$$
 (4)

where  $\beta$  (L<sup>-1</sup>) is the normalized root length density.

Different functions to calculate expressions for  $\alpha$  have been suggested, normally considering  $\alpha$  a function of  $\theta$  (ex. Lai and Katul (2000); Jarvis (1989)), of h (ex. Feddes et al. (1978)) or of a combination of both (Li et al., 2006). Comparing to  $\theta$ , h seems to be more feasible because of its relation to soil water energy and the fact that obtained parameters of such a function would be more likely applicable to different soils. Some reduction functions, generally associated to reservoir models for soil water balance, correlates RWU to the effective saturation. Regarding the shape of the reduction curve, they can be smooth nonlinear functions constrained between wilting point and saturation or piece-wise linear functions, but they all have more than one empirical parameter. The parameters of the smooth non-linear functions allow easy curve fitting, whereas in the piece-wise functions they stand for the threshold at which RWU (or crop transpiration) is reduced due to drought stress, which has been an important parameter in crop water management.

Metselaar and De Jong van Lier (2007) showed that for a vertically homogeneous root system the shape of  $\alpha$  is linearly related nor not linearly related to soil water content neither to pressure head. A linear relation to the matric flux potential, a composite soil hydraulic function defined in eq. 5, is physically more plausible and was experimentally shown corroborated by Casaroli et al. (2010). Matric flux potential is defined as

$$M = \int_{h_{vv}}^{h} K(h) \, \mathrm{d}h \tag{5}$$

where  $h_w$  is the soil pressure head at wilting point. Accordingly, a more suitable expression for  $\alpha$  would be a piece-wise linear function of M (Fig. 1). RWU can then be calculated by the Feddes model (eq. 3) by replacing its reduction function for water deficit by the alternative illustrated in Fig. 1.

## 2.1 Physically based root water uptake model

By upscaling earlier findings (De Jong Van Lier et al., 2006; Metselaar and De Jong van Lier, 2007) of water flow towards a single root in the microscopic scale disregarding plant resistance to water flow, De Jong van Lier et al. (2008) derived the following expression for *S*:

$$S(z) = \rho(z)(M_s(z) - M_0(z)) \tag{6}$$

where  $M_s$  is the bulk soil matric flux potential,  $M_0$  the value of M at root surface and  $\rho(z)$  (L<sup>-2</sup>) a composite parameter, depending on R and root radius  $r_0$ :

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$$\rho(z) = \frac{4}{r_0^2 - a^2 r_m^2(z) + 2[r_m^2(z) + r_0^2] \ln[ar_m(z)/r_0]}$$
 (7)

where  $r_m (= \sqrt{1/\pi R})$  (L) is the rhizosphere radius — defined as the half distance between neighbouring roots— and a the relative distance from  $r_0$  distance relative to  $r_m - r_0$  where water content equals bulk the average soil water content. In De Jong van Lier et al. (2013), this model is extended by taking into account the hydraulic resistances to water flow within the plant.

Dividing water transport within the plant into two physical domains (from root surface to root xylem to leaf), assuming no water changes within the plant tissue and by coupling eq. 6 for water flow within the rhizosphere, they derived the following expression relating water potentials and  $T_a$ :

$$h_0(z) = h_l + \varphi(M_s(z) - M_0(z)) + \frac{T_a}{L_l}$$
(8)

where  $h_0$  and  $h_l$  (L) are the pressure heads at the root surface and leaf, respectively, and  $L_l$  (T<sup>-1</sup>) is the overall conductance over the root xylem-to-leaf pathway. Notice that S can be calculated by eq. 6 upon solving eq. 8., and  $\varphi$  (T L<sup>-1</sup>) is defined as:

$$\varphi(z) = \frac{\rho r_m^2(z) \ln \frac{r_0}{r_x}}{2K_{root}} \tag{9}$$

where  $K_{root}$  (L T<sup>-1</sup>) is the radial root tissue conductivity (from over the pathway from the root surface to the root xylem), and  $r_x$  (L) is the xylem radius.  $T_a$  is An analytical solution of eq. 8 for  $h_0$  or  $M_0$  depends on the  $M_0(h_0)$  expression. For a particular case of Brooks and Corey (1964) soils a solution is provided by De Jong van Lier et al. (2013). For van Genuchten-Mualem type soils, eq. 8 has to be solved numerically or by using a semi-analytical solution of eq. 5 (De Jong van Lier et al., 2009). In any case, application of eq. 8 requires a function between  $T_a$  and  $h_l$ . De Jong van Lier et al. (2013) defined  $T_a$  by a function of  $h_l$ , which was defined piece-wisely by piece-wise function imposing a limiting value  $h_{wl}$  on  $h_l$ :

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$$T_r = \begin{cases} 1 & : h_l > h_{wl} \\ 0 \le T_r \le 1 & : h_l = h_{wl} \\ 0 & : h_l < h_{wl} \end{cases}$$
 (10)

where  $T_r$  (=  $T_a/T_p$ ) is the relative crop transpiration. Crop-Because  $T_a$  and  $h_l$  are unknowns and  $T_a$  is undefined when  $h_l = h_{wl}$ , the equation system cannot be solved analytically. An iterative solution was provided in De Jong van Lier et al. (2013) by defining a maximum possible transpiration rate  $T_{p,max}$ , corresponding to  $T_a$  (eq. 8) for  $h_l = h_{wl}$ . The system of equations is then solved by defining plant stress in terms of  $T_{p,max}$ , according to the following boundary conditions:

$$\begin{cases} \text{unstressed conditions}: T_{p,max} > T_p : T_a = T_p, \ h_l > h_{wl} \\ \text{stressed conditions}: \quad T_{p,max} < T_p : h_l = h_{wl}, \ T_a < T_p \end{cases}$$

In the De Jong van Lier et al. (2013) model, crop water stress, a condition for which  $T_a < T_p$ , is defined at the crop level (Tardieu, 1996) and onsets when  $h_l = h_w$ . Because  $T_a$  and  $h_l$  are unknowns, S can be calculated using eq. 6 by solving eq. 8 and 10 cannot be solved directly, but an efficient algorithm is described in De Jong van Lier et al. (2013), along with a particular analytical solution for Brooks and Corey (1964) soils, with  $h_0$  (so  $M_0$ ) variable over the root zone and controlled by plant hydraulic properties and soil hydraulic conditions.

Fig. 2 helps to understand how RWU is distributed over depth.  $h_l$  can be regarded as a crop level measure of water deficit stress over the whole root zone: as soil gets drier water is depleted,  $h_l$  is reduced, which increases thus increasing the driving

force for RWU(see RWU for the. Fig. 2 shows RWU for several values of  $h_l$  in Fig. 2). As soil pressure head  $h_s$  decreases, high uptakes are only achieved by lower  $h_l$ . For a <u>eertain-given</u>  $h_l$  value, RWU is substantially reduced as  $h_s$  decreases. If  $h_l$  is not reduced as while  $h_s$  gets lowerdecreases, S becomes negative (negative S is not shown in Fig. 2, but it is part of an the extension of each curve) and water will flow from root to soil, a <u>phenomena phenomenon</u> called hydraulic lift or hydraulic re-distribution (Jarvis, 2011)<sup>Ref#1,point 4</sup>. This situation occurs when parts of the root zone are wetter and RWU from these parts satisfies transpiration demand, and hence  $h_l$  is not reduced.

Fig. 2 also shows that RWU is sensitive to both R and  $h_s$ , and that it can be locally balanced by the R and soil water content. Under homogeneous soil water distribution, RWU is partitioned proportionally to R. For heterogeneous conditions, RWU for lower R ean and higher R may be the same as for higher R depending on the stress level (indicated by  $h_l$ ) and the  $h_s$  (see Fig. 2). This is in agreement with experimental results reported by several authors (Arya et al., 1975b, a; Green and Clothier, 1995; Verma et al., 2014) who found less densely-rooted but wetter parts of the root zone to correspond to a significant portion of RWU when more densely-rooted parts of the soil are were drier, allowing the crop to maintain transpiration at potential rates. Due to empirical model concepts that employ only only use R for predicting RWU distribution over depth (for nonstressed under non-stressed conditions), these results have been interpreted as due to a mechanism labelled "compensation" by which uptake is "increased" from wetter layers to compensate the "reduction" in the drier layers (Jarvis, 1989; Šimůnek and Hopmans, 2009). Clearly, It is clear however, that this compensation concept is based found on a reference RWU distribution based on R and it only needs to be explicitly addressed in empirical models. In physical models, discriminating compensation is not necessary since in such models "compensation" follows implicitly from the RWU mechanism Refill, point 5.

In order to account for RWU pattern changes due to heterogeneous soil water distribution (the so-called "compensation"), several empirical models have been developed over the years. These models follow the general framework of the Feddes et al. (1978) model given by eq. 3. Below we review these models and present a new empirical alternative.

## 2.2 Empirical root water uptake models accounting for compensation

#### **2.2.1** The Jarvis (1989) model

Jarvis (1989) defined a weighted-stress index  $\omega$  ( $0 \le \omega \le 1$ ) as

25 
$$\omega = \int_{z_m} \alpha(z)\beta(z)dz$$
. (11)

where, differently from Feddes et al. (1978),  $\alpha$  was defined as a function of the effective saturation Ref#1, point 6. Whereas Feddes et al. (1978) assume the RWU reduction directly to reflect in crop transpiration reduction, the Jarvis (1989) approach employs a so-called "whole-plant stress function" given by:

$$\frac{T_a}{T_p} = \min\left\{1, \frac{\omega}{\omega_c}\right\} \tag{12}$$

where  $\omega_c$  is a threshold value of  $\omega$  for the transpiration reduction. Substituting eq. 3 and 4 into eq. 1 (the continuity mass conservation principle) and combining with eq. 12, results in:

$$S(z) = S_p \alpha(z) \alpha_2$$
, where  $\alpha_2 = \frac{1}{\max\{\omega, \omega_c\}}$  (13)

where  $\alpha_2$  is called the compensation factor of RWU, distinct from the Feddesmodel Feddes'  $\alpha$  (eq. 3) and which can be derived by defining  $T_a$  by eq. 12. In the Jarvis (1989) model,  $\alpha$  accounts for local reduction of RWU and transpiration reduction is computed by eq. 12. When  $\omega=1$ , there is no RWU reduction ( $\alpha=1$  throughout the root zone) and the model prediction is equal to the Feddes model. For  $\omega_c < \omega < 1$ , uptake is reduced in some parts of the root zone (as computed by  $\alpha < 1$ ) but the plant can still achieve potential transpiration rates by increasing RWU over the whole root zone by the factor  $\alpha_2$ . When  $\omega < \omega_c$ , even though the uptake is still-increased by the factor  $\alpha_2$  but, the potential transpiration rate cannot be met. The threshold value  $\omega_c$  places a limit on the plant's ability to deal with soil water stress. When  $\omega_c$  tends to zero, eq. 12 tends to 1, and the plant can fully compensate uptake and transpire at the potential rate provided that  $\alpha > 0$  at some position within the root zone.

In principle, any definition of  $\alpha$  is applicable in eq. 11, and usually commonly the Feddes et al. (1978) reduction function is used instead of the original Jarvis (1989) reduction function, as it is used in e.g. in the HYDRUS model (Simunek et al., 2009) for instance. This modified version of the Jarvis (1989) model, hereafter named referred to as JMf, will be further analysed Ref#1. point 6. Nevertheless, one should be careful in setting up and interpreting the threshold parameters of JMfRef#1. point 8. The Feddes et al. (1978) model does not account for compensation, and the threshold pressure head value below which RWU is reduced ( $h_3$ ) also represents the value below which transpiration is reduced, making  $h_3$  values from literature usually to refer to this interpretation. Instead, at in the JMf the transpiration reduction only takes place when  $\omega < \omega_c$ , and soil pressure head in some layers is already supposed to be more negative than  $h_3$ , which means that  $h_3$  in JMf is less negative than the its equivalent in the Feddes model. In that sense,  $h_3$  for the JMf is hard to determine experimentally. Inverse modelling by An option to do so would be by inverse modelling, optimizing outcomes of soil water flow models with measured values of field experiments is an option experimental data.

The Jarvis-type model

## Comparison to the De Jong van Lier et al. (2008) model

The physical basis of Jarvis (1989), defined by eq. 11 to 13 with using any  $\alpha$ , has been well criticized. Nevertheless, this model can to a certain extent be compared to the De Jong van Lier et al. (2008) physical model as shown by Jarvis (2011), which is shortly described below.

#### Comparison to the De Jong van Lier et al. (2008) model

The Jarvis (1989) model was shown to be "conceptual" identical to De Jong van Lier et al. (2008) physical model, but only under limiting hydraulic conditions (Jarvis, 2010, 2011). We briefly review this similarity and its implications on the empirical concept of questioned (Skaggs et al., 2006; Javaux et al., 2013). However, the Jarvis (1989) model Jarvis model has, to some extent, a physical basis, and a comparison with the physically-based model of De Jong van Lier et al. (2008) can be made, as demonstrated in Jarvis (2010, 2011). This is described in the following.

De Jong Van Lier et al. (2006) derived eq. 6 for describing RWU. Crop transpiration is obtained by integrating eq. 6 over  $z_m$  as defined in eq. 1, leaving two unknowns:  $M_0$  and  $T_a$ . In order to  $T_a$  solve for these, De Jong van Lier et al. (2008) defined  $T_a$  as a piece-wise function as follows:

$$\frac{T_a}{T_p} = \min\left\{1, \frac{T_{p_{\text{max}}}}{T_p} \frac{T_{p,max}}{T_p}\right\} \tag{14}$$

where  $T_{p_{\text{max}}}T_{p,max}$  (L T<sup>-1</sup>), differently from the definition in the De Jong van Lier et al. (2013) model, is the maximum possible transpiration rate attained when reached when the root surface pressure head is constant over depth and equal to a limiting value  $h_w$ . For such a condition  $M_0 = 0$ , then  $T_{p,max}$  is given by:

$$T_{\underline{p_{\max}}p,\max} = \int_{z_{m}} \rho(z)M(z) dz. \tag{15}$$

From eq. 14 when  $T_{p_{\text{max}}} < T_p T_{p,max} < T_p$ , drought stress occurs and  $T_a = T_{p_{\text{max}}} T_a = T_{p,max}$ . Under this condition, pressure head at the root surface reaches  $h_w \to M_0 = 0$  and S(z) becomes:

$$S(z) = \rho(z)M(z). \tag{16}$$

When  $T_{p_{\text{max}}} > T_p T_{p,max} > T_p$ ,  $T_a = T_p$  (no drought stress) and  $M_0$  (> 0) is given by:

$$M_0 = \frac{\int_{\rho(z)} M(z) dz - T_p}{\int_{z_m} \rho(z) dz}$$
(17)

Jarvis (2011) observed the similarities between eq. [14] and [12] of the models. Notice also the algebraic similarity between  $\omega$  (eq. 11) and  $T_{p_{max}}$  (eq. 15). Thus, Jarvis (2010) showed that both models provide the same results for the stressed phase under drought stress if  $\alpha$  and  $\beta(z)$  are defined as follows:

$$\alpha = \frac{M}{M_{max}} \tag{18}$$

$$\beta = \frac{\rho(z)}{\int\limits_{z_m} \rho(z) dz} \tag{19}$$

where  $M_{max}$  is the maximum value of M (i.e., at h=0). By substituting eq. [18] and [19] into eq. 15 and comparing eq. 12 with eq. 14,  $\omega_c$  is found to be equal to:

$$\omega_c = \frac{T_p}{M_{max} \int \rho(z) \, \mathrm{d}z} \tag{20}$$

Substitution of eq. [18] to [20] into eq. [12] and [11] results in eq. 16 of De Jong van Lier et al. (2008) model for stressed condition. Consequently, both models provide the same numerical results. For unstressed condition, analogous substitution results in:

$$S(z) = \rho(z)M(z)\frac{T_p}{T_{p_{max}}} = \frac{\rho(z)M(z)}{\int \rho(z)M(z)\,\mathrm{d}z}T_p \tag{21}$$

Eq. 21 is different from eq. 6 and, therefore, the models cannot be correlated for these conditions. The Jarvis (1989) model predicts RWU by a weighting factor between  $\rho$  and M throughout rooting depth. Defining  $\alpha$  and  $\beta$  by eq. 18 and 19, respectively, allowed to correlate both models only for stressed conditions. These definitions and the resulting model will be further analysed.

#### 2.2.2 The Li et al. (2001) model

Li et al. (2001) proposed to distribute potential transpiration over the root zone by a weighted stress index  $\zeta$ , being a function of both root distribution and soil water availability:

15 
$$\zeta(z) = \frac{\alpha(z)R(z)^{l_m}}{\int\limits_{z} \alpha(z)R(z)^{l_m} dz}$$
 (22)

where  $\alpha$  (-) and R (L L<sup>-3</sup>) were previously defined and the exponent  $l_m$  is an empirical factor. Originally, the  $l_m$  values were based on experimental works, but in principle it modifies the shape of RWU distribution over depth. For  $0 < l_m < 1$ , the RWU in sparsely rooted soil layers is increased in the attempt to mimic compensation. For  $l_m > 1$ , which has no maximum, the uptake in more densely rooted soil layers increases. Thus,  $S_p$  is given by:

$$S_p = \zeta(z)T_p \tag{23}$$

and RWU is calculated by substituting eq. 23 into eq. 3, following the Feddes approach.

Defining As an alternative to Jarvis (1989) model,  $S_p$  can be defined as function of root length density and soil water availability distribution is an alternative to the Jarvis (2011) model. Compensation is directly accounted for by the weighted stress index in

eq. 22. However, the choice of using  $\alpha$  to represent soil water availability in eq. 22 does not mimic properly the compensation mechanism. Compensation may take place before transpiration reduction. Using  $\alpha$  in eq. 22 means that compensation will only take place after the onset of transpiration reduction when  $\alpha$  in one or more layers is less than unity. smaller then 1. The  $l_m$  parameter may also be interpreted as to account for compensation under non-stressed condition. Compensation, however, and shape of However, compensation as well as the shape of the RWU distribution are likely to change as soil dries. A constant  $l_m$  can not account for that.

## 2.2.3 The Molz and Remson (1970) and Selim and Iskandar (1978) models

Decades before Li et al. (2001), Molz and Remson (1970) and Selim and Iskandar (1978) had already suggested to distribute potential transpiration over depth according to root length density and soil water availability. Instead of using  $\alpha$  to account for soil water availability, they used soil hydraulic functions. The weighted stress index was defined as

$$\zeta(z) = \frac{\Gamma(z)R(z)}{\int \Gamma(z)R(z)dz}$$
(24)

where  $\Gamma$  is a soil hydraulic function to account for water availability. Molz and Remson (1970) used soil water diffusivity D ( $L^2T^{-1}$ ), and Selim and Iskandar (1978) used soil hydraulic conductivity K ( $LT^{-1}$ ) for  $\Gamma$  in eq. 24. RWU is then calculated by substituting eq. 24 into eq. 23 and then into eq. 3 following the Feddes approach.

These models may better represent RWU and compensation than the Li et al. (2001) model. The compensation is implicitly accounted for by means of  $\Gamma$  in  $\zeta$ . Since  $\Gamma$  decreases as soil dries outwater is depleted, in a heterogeneous soil water distribution  $\zeta$  in wetter layers is relatively increased because the overall  $\int \Gamma R dz$  is reduced due to the reduction of  $\Gamma$  in drier, more densely rooted soil layers. Differently from the Li et al. (2001) model, this change in RWU distribution can occur before the onset of transpiration reduction. Heinen (2014) compared different types of  $\Gamma$  in eq. 24 such as the relative hydraulic conductivity ( $K_r = K/K_{sat}$ ), relative matric flux potential ( $M_r = M/M_{max}$ ) and others. He found that using different forms of  $\Gamma$  provides very different patterns of RWU, but did not indicate a preference for a specific one.

## 2.2.4 Proposed empirical model

In describing soil water availability, the matric flux potential M may be a better choice than K or D, since it integrates K and h or D and  $\theta$  (Raats, 1974; De Jong van Lier et al., 2013). We propose a new weighted stress index, defined as:

25 
$$\zeta_m(z) = \frac{R^{l_m} M(h)}{\int R^{l_m} M(h) dz}$$
 (25)

The exponent  $l_m$  provides additional flexibility on distribution of  $T_P$  over depth as was shown by Li et al. (2001). The proposed model differs from Li et al. (2006) only on the hydraulic property to account for soil water availability. The  $\alpha$  function used in Li et al. (2006) can not only alter RWU distribution before after the onset of transpiration reduction, as commented earlier. Whereas Contrastingly, M accounts allows for compensation before transpiration reduction, while it integrates ingrates the effects integrating the effect of both K and h.

The RWU can then be obtained by inserting eq. 25 into eq. 23  $(S_p)$  and multiplied by any reduction function, such as the Feddes et al. (1978) and proposed reduction functions. In other words, it follows the Feddes approach, which computes RWU by the two mentioned steps, differing only how with respect to the way  $S_p$  is obtained: eq. 25 (times multiplied by  $T_p$ ) versus eq. 4.

#### 0 2.2.5 Relationship between plant transpiration empirical parameters

This was suggested by the Referee2. I have just started this and I will be brief. Although I am in doubt whether this is really necessary (See Point i).

#### 3 Material and Methods

## 3.1 Applied models

Table 1 summarizes the empirical RWU models evaluated in this study. They all follow the original Feddes model (eq. 3), but differing in how RWU is partitioned over rooting depth or how  $\alpha$  is defined. For each model, except for Jarvis (2010), we defined a modified version by substituting the Feddes reduction function by the proposed reduction function (Fig. 1b), and these modified versions were also evaluated. The threshold values of the Feddes et al. (1978) reduction function for anoxic conditions ( $h_1$  and  $h_2$ ) were set to zero. The value of the parameter  $h_4$  was set to -150 m. The other parameters of the models were obtained by optimization as described in section 3.3.

All these models were embedded as sub-models into the ecohydrological model SWAP (Van Dam et al., 2008) in order to solve eq. 2 and to apply it different scenarios of root length density, atmospheric demand and soil type (described in section 3.2) in order to analyse the behaviour and sensitivity of the models. Simulation results of SWAP in combination with each of the RWU models were compared to the SWAP predictions in combination with the physical RWU model developed by De Jong van Lier et al. (2013).

The values of the De Jong van Lier et al. (2013) model parameters used in the simulations are listed in Table 2. The values of  $K_{root}$  and  $L_l$  are within the range reported by De Jong van Lier et al. (2013).

#### 3.2 Simulation scenarios

#### 3.2.1 Drying-out simulation

Boundary conditions for these simulations were no rain/irrigation and a constant atmospheric demand (potential transpiration) over time. The simulation continued until simulated crop transpiration by the physical RWU model approached zero. Soil evaporation was set to zero making soil water to depleted only due to RWU or bottom drainage. Free drainage (unit hydraulic gradient) at the maximum rooting depth was the bottom boundary condition. The soil was initially at hydrostatic equilibrium with a water table located at 1 m depth. We performed simulations for two levels of atmospheric demand given by potential transpiration  $(T_p)$  of 1 and 5 mm d<sup>-1</sup>. We also considered three soil types and three levels of root length density, as described in the following.

#### 10 **3.2.2** Soil type

Soil data for three top soils from the Dutch Staring series (Wösten et al., 1999) were used. The physical properties of these soils are described by the Mualem-van Genuchten functions (Mualem, 1976; Van Genuchten, 1980) for the  $K - \theta - h$  relations:

$$\Theta = [1 + |\alpha h|^n]^{(1/n) - 1} \tag{26}$$

$$K = K_{sat} \Theta^{\lambda} [1 - (1 - \Theta^{n/(n-1)})^{1 - (1/n)}]^{2}$$
(27)

where  $\Theta = (\theta - \theta_r)/(\theta_s - \theta_s)$ ;  $\theta$ ,  $\theta_r$  and  $\theta_s$  are water content, residual water content and saturated water content (L<sup>3</sup> L<sup>-3</sup>), respectively; h is pressure head (L); K and  $K_{sat}$  are hydraulic conductivity and saturated hydraulic conductivity, respectively (L T<sup>-1</sup>); and  $\alpha$  (L<sup>-1</sup>), n, and  $\lambda$  are empirical parameters. The parameter values for the three soils are listed in Table3. These soils are identified in this text as clay, loam and sand.

#### 3.2.3 Root length density distribution

Three levels of root length density were used, according to the range of values normally found in the literature. We considered low, medium and high root length density for average crop values equal to 0.01, 0.1 and 1.0 cm cm<sup>-3</sup>, respectively. For all cases, we set the maximum rooting depth  $z_{max}$  equal to 0.5 m. Root length density over depth z was described by the exponential function:

$$R(z_r) = R_0(1 - z_r) \exp^{-bz_r}$$
(28)

where  $R_0$  (L L<sup>-3</sup>) is the root length density at the soil surface, b (-) is a shape-factor parameter and  $z_r$  (=  $z/z_{max}$ ) is the relative soil root depth. The term  $(1-z_r)$  in eq. 28 guarantees that root length density is zero at the maximum rooting depth.

The parameter  $R_0$  is hardly ever determined, whereas the average root length density of crops  $R_{\text{avg}}$  is usually reported in the literature. Assuming R of such a crop given by eq. 28, it can be shown that:

$$\int_{0}^{1} R_0(1 - z_r) \exp^{-bz_r} dz_r = R_{\text{avg}}$$
(29)

Solving eq. 29 for  $R_0$  and substituting into eq. 28 gives:

5 
$$R(z_r) = \frac{b^2 R_{\text{avg}}}{b + \exp^{-b} - 1} (1 - z_r) \exp^{-bz_r}$$
 (b > 0)

Fig. 3 shows  $R(z_r)$  calculated from eq. 30 for different values of b and  $R_{\text{avg}} = 1 \text{ cm cm}^{-3}$ . As b approaches zero, eq. 30 tends to become linear, however it is not defined for b = 0. In our simulations b was arbitrarily set equal to 2.0.

## 3.3 Optimization

The parameters of the empirical RWU models were estimated by solving the following constrained optimization problem:

minimize 
$$\Phi(\mathbf{p}) = \sum_{i=1}^{n} \sum_{j=1}^{m} [S_{i,j}^* - S_{i,j}(\mathbf{p})]^2$$
subject to 
$$\mathbf{p} \in \Omega$$
(31)

where  $\Phi(\mathbf{p})$  is the objective function to be minimized,  $S_{i,j}^*$  is the RWU simulated by SWAP model together with the De Jong van Lier et al. (2013) model at time i (time interval of one day) and depth j (of each soil layer) and  $S_{i,j}(\mathbf{p})$  is the corresponding RWU predicted by SWAP in combination with one of the empirical models shown in Table 1.  $\mathbf{p}$  is the model parameter vector to be optimized, constrained in the domain  $\Omega$ . Both  $\mathbf{p}$  and  $\Omega$  vary depending on the empirical RWU model used. Table 4 shows the parameters of each empirical RWU model that were optimized and their respective constraints  $\Omega$ . m and n are the number of soil layers (50 soil layers of 1 cm thickness) and days of the simulation, respectively. The Jarvis (2010) model has no empirical parameters and therefore requires no optimization.

Eq. 31 was solved using the PEST (Parameter ESTimation) tool (Doherty et al., 2005) coupled to the adapted version of SWAP. PEST is a non-linear parameter estimation program that solves eq. 31 by the Gauss-Levenberg-Marquardt (GLM) algorithm, searching for the deviation, initially along the steepest gradient of the objective function and switching gradually the search to Gauss-Newton algorithm as the minimum of the objective function is approached. Upon setting PEST parameters we made reference runs of SWAP with each empirical model using random values of **p** and assessed the ability of PEST for retrieving **p**. These reference runs allowed to properly set up PEST for our case. For highly non-linear problems as in eq. 31, the optimized parameters set depends on the initial values of **b**. We used five random sets of initial values for **p** in order to guarantee that GLM encountered the global minimum and also to check the uniqueness of the solution. Runs led to the same minimum in most cases, but if not, the minimum was compared and a fit run was run again.

The optimizations were performed for the drying-out simulation only. This guaranteed that RWU predictions from SWAP corresponded to the best fit of each empirical model to the De Jong van Lier et al. (2013) model. This analysis aimed to investigate the capacity of the empirical RWU models to mimic the RWU pattern predicted by the De Jong van Lier et al. (2013) model. These optimized parameters were subsequently used to evaluate the models in an independent growing season scenario.

## 3.4 Growing season simulation

5

The models were evaluated by simulating the transpiration of grass with weather data from the De Bilt weather station, the Netherlands ( $52^{\circ}06^{\circ}$  N;  $5^{\circ}11^{\circ}$ E), for the year 2006. The same root system distribution as in the drying-out simulations was used, i.e. a crop with roots exponentially distributed over depth as eq. 30 (b=2.0) down to 50 cm below soil surface. We also performed simulations for the same three types of soils and root length densities. In all cases the crop fully covered the soil with a leaf area index of 3.0. Daily reference evapotranspiration  $ET_0$  was calculated by SWAP using the FAO Penman-Monteith method (Allen et al., 1998). In SWAP model, a potential crop evapotranspiration  $ET_p$  is obtained by multiplying  $ET_0$  by a crop factor, which for the grass vegetation was set to 1 (Van Dam et al., 2008).  $ET_p$  was partitioned into potential evaporation  $E_p$  and  $E_p$  using parameter values for common crops given in SWAP model (see Van Dam et al. (2008) for details).

The values of the empirical parameters of each RWU model corresponding to the type of soil and root length density were taken from the optimizations performed in the drying-out experiment. Each parameter was estimated for two levels of  $T_p$  (1 and 5 mm d<sup>-1</sup>) and was linearly interpolated for intermediate levels of  $T_p$ . For  $T_p > 5$  mm d<sup>-1</sup> or  $T_p < 1$  mm d<sup>-1</sup>, the values estimated for these highest or lowest  $T_p$  values were used.

The bottom boundary condition was the same as in the drying-out simulations (free drainage). Initial pressure heads were obtained by iteratively running SWAP starting with the final pressure heads of the previous simulation until convergence.

#### 4 Results and Discussion

## 4.1 Drying-out simulation

#### 4.1.1 Root water uptake pattern: De Jong van Lier et al. (2013) model

In this section we first focus on the behaviour of the De Jong van Lier et al. (2013) model in predicting RWU for the evaluated scenarios in the drying-out experiment. Fig. 4 shows the RWU patterns for the case of clay soil for the three evaluated root length densities R and the two levels of potential transpiration  $T_p$ . It can be seen how R and  $T_p$  affect RWU distribution and transpiration reduction as soil dries out. The onset and shape of transpiration reduction is affected by the RWU pattern. For low

R, the low amount number of roots in deeper layers is not sufficient to supply high RWU rates. When the upper layers become drier, transpiration reduction follows immediately. Under medium and high R, the RWU front moves gradually downward as water from the upper layers is depleted. For high R, the RWU front goes even deeper compared to medium R, and transpiration is sustained maintained at potential rates for a longer time (Fig. 4). Accordingly, the plant exploits the whole root zone and little water is left when transpiration reduction onsets, causing an abrupt drop in transpiration. Regarding  $T_p$ , the RWU patterns are very similar for both evaluated rates, differing only in time scale: for high  $T_p$  the onset of transpiration reduction and the shift in RWU front occur earlier. The patterns for the sand and loam soil (not shown here) show very similarfeatures are very similar. However, for sand soil transpiration prolonged the sand soil potential transpiration is maintained a bit longer at potential rates and more water was is extracted at deeper layers. Whereas, for For the loam soil, the onset of transpiration reduction started earlier.

The leaf pressure head  $h_l$  over time shown in Fig. 4 illustrates how the model adapts  $h_l$  to R and  $T_p$  levels and soil drying. Initially all scenarios have the same water content distribution and lower  $h_l$  values are required for low R or high  $T_p$  scenarios to supply potential transpiration rates. As soil becomes drier,  $h_l$  is decreased in order to increase the pressure head gradient between bulk soil and root surface<del>and</del>, thus maintaining RWU corresponding to the potential demands demand. Therefore, uptake in wetter layers become becomes more important. Transpiration reduction only onsets when  $h_l$  reaches the limiting leaf pressure head  $h_{wl}$  (= -200 m), after significant changes in the RWU patterns, characterized by increased uptake in from deeper layers.

For the high  $T_p$ -low R scenarios, transpiration reduction starts at the first day of simulation although the soil is relatively wet. This is a case of transpiration reduction under non-limiting soil hydraulic conditions due to high atmospheric demand (Cowan, 1965). For such conditions, the high water flow within the plant required to meet the atmospheric demand cannot be supported by the root system with a low R and hydraulic parameters given in Table 2. Higher atmospheric demand (here represented by  $T_p$ ) leads to faster reduction of  $h_l$  caused by the hydraulic resistance to water flow within the plant, and the transpiration rate and RWU are a function of  $h_l$ . The physical model assumes a parsimonious relationship (eq. 10) between transpiration and  $h_l$ : transpiration rate is only reduced when  $h_l$  reaches a limiting value  $h_{wl}$ , which corresponds to a maximum possible transpiration rate  $T_{p,max}$  allowed by the plant for the current soil hydraulic and atmospheric conditions. Under non-limiting soil hydraulic conditions,  $T_{p,max}$  is a function of root system properties and plant hydraulic parameters only (Table 2) are the major determining factors for  $T_{p,max}$ , whereas soil hydraulic conditions play a minor role. Fig. 5 shows  $T_{p,max}$  as a function of  $K_{root}$  for some values of  $L_l$  with a constant soil pressure head in the root zone of -1 m for the in the root zone for low R in the sandy soil. It can be seen that In this scenario,  $K_{root}$  is limiting the crop transpiration and that  $L_l$  becomes important only when  $K_{root}$  increases. The potential transpiration can be achieved by raising  $K_{root}$  up to about  $10^{-7}$  m d<sup>-1</sup>. This can also be achieved by decreasing  $h_{wl}$  (not shown in Fig. 5).

In the field, transpiration rate and root length density are related to each other: a high transpiration rate only occurs at high leaf area and a high leaf area implies a high root length density. Thus, even in very dry and hot weather conditions, a crop with a

low R may not be able to realize high transpiration rate. Furthermore, crop transpiration depends on the stomatal conductance. In the De Jong van Lier et al. (2013) model, this is implicitly taken into account by the simple relationship between  $h_l$  and  $T_a$ . However, stomatal conductance is relatively complex and depends on several environmental factors such as air temperature, solar radiation and  $CO_2$  concentration. Thus Thefore, high potential transpiration rate may not be achieved because of the stomatal conductance reduction due to temperature or solar radiation. These results can be enhanced by the coupling of the De Jong van Lier et al. (2013) model to stomatal conductance models, such as the Tuzet et al. (2003) model.

#### 4.1.2 Root water uptake pattern predicted by the empirical models

In this section, we evaluate the empirical RWU models (models and their abbreviations are listed in Table 1) based on the comparison of RWU patterns and transpiration reduction over time with the respective predictions from the De Jong van Lier et al. (2013) model (VLM). All empirical model predictions are performed with respective optimized parameters as shown in Table 5 and are discussed in section 4.1.4, thus representing the best fit with VLM.

The RWU patterns simulated by VLM and the empirical models for the scenario of sandy soil and high R are shown in Fig. 6 and 7 for low and high  $T_p$ , respectively. Both versions of the Feddes model (FM and FMm) predicted enhanced RWU from the upper soil layers. When the soil pressure head  $(h_s)$  (for FM) or soil matric flux potential  $(M_s)$  (for FMm) is greater than the threshold value for uptake reduction, these uptake patterns are equivalent to the vertical R distribution. For conditions drier than the threshold value (when  $\alpha_f$  and  $\alpha_m$  are less than 1), the predicted RWU patterns by the models become different (Fig. 6 and 7).

After a period of reduced RWU, the length of which depends on R,  $T_p$  and  $h_3$ , RWU from the upper soil layers predicted by FM rapidly decreases to zero. This zero-uptake zone expands downward as soil dries out. On the other hand, the uptake predicted by FMm is substantially reduced right after the onset of transpiration reduction, proceeding at lower rates and a much longer time until approaching zero. These features become evident by comparing the shape of both reduction functions (Fig. 8).  $\alpha_m$  is linear with M after  $M > M_c$ , but it is concavely-shaped as a function of h— as also shown by Metselaar and De Jong van Lier (2007) and De Jong van Lier et al. (2009). Thus, This makes  $\alpha_m$  is abruptly reduced to reduce abruptly for  $M > M_c$ , causing substantial reduction a substantial decrease in RWU even when h is slightly below the threshold value. Therefore, RWU proceeds at low rates for a longer time. Conversely, due to the linear shape of  $\alpha_f$ , RWU predicted by FM remains higher for a longer time after  $h < h_3$ . No abrupt change in RWU patterns is predicted by this model, especially when  $T_p$  is low (Fig. 6). When h comes close to  $h_4$ ,  $\alpha_f$  is still relatively high and RWU continues, making h to rapidly approach  $h_4$ . Another diverging feature between  $\alpha_f$  and  $\alpha_m$ , also shown in Fig. 8, is that the shape of  $\alpha_m$  varies with soil type (regardless the value of its threshold parameter  $M_c$ ), whereas  $\alpha_f$  does not. These different features of the reduction functions also affect the matching values of the parameters as discussed below. The choice of the reduction function, however, affects transpiration eury-e-over time only slightly, but RWU patterns are strongly affected (Fig. 6 and 7).

The RWU patterns predicted by JMf and JMm models can be very different, as shown by Fig. 6 for the high R-low  $T_p$  scenario. In fact, the JMf model did not predict any compensation at all because the optimal  $\omega_c$  was equal to unity equalled 1 (Table 5) — thus becoming identical to FM — and the optimal  $h_3$  for JMf and FM were similar. In Fig. 6, although  $h_3$  values for FM and JMf ( $\omega_c = 1$ ) are close to zero, the plant transpiration is elose to near  $T_p$  for a prolonged time due to a small reduction of  $\alpha$ . These high R-low  $T_p$  scenarios with a high R in deep soil layers allow RWU at higher rates when surface soil layers becomes drier (as predicted by VLM). Then, reducing  $\omega_c$  in an attempt to predict compensation with JMf makes the RWU pattern to deviate even more from the VLM pattern. This is illustrated in Fig. 6 and by the optimal  $h_3$  and  $\omega_c$  values shown in Table 5. In order to mimic the VLM uptake patterns, the value of  $h_3$  for all soil types in this scenario was equal or close to zero. Decreasing  $h_3$  or  $\omega_c$  in order to simulate compensation makes JMf predicting higher uptake from upper layers, increasing the discrepancy between the models. The optimal  $\omega_c$  for all soil types was equal to 1 (in other words: no compensation). RWU in the upper layers predicted by VLM is substantially reduced within a few days, whereas reducing  $\omega_c$  in JMf model to predict compensation causes also an increase of uptake in upper layers. The model, therefore, cannot mimic the scenarios with compensation evaluated here. Conversely, the JMm was able to reproduce considerably well the VLM pattern for these scenarios due to the shape of  $\alpha_m$  as discussed above. As soon as  $M > M_c$  in the upper layers, RWU decreased at a higher rate, compensated by increasing uptake from the wetter, deeper layers. This agrees more closely to VLM predictions.

For high  $T_p$  (Fig. 7), the JMf model can predict compensation ( $\omega_c < 1$ ), however its predicted RWU pattern is very different from JMm and VLM. JMf predicts a higher RWU near the soil surface for a longer period than the other models that account for compensation. This makes soil water depletion to be more intense and RWU from these layers will cease sooner when  $h_s$  becomes lower than  $h_4$ . At this point,  $T_a$  is predicted to continue equal to  $T_p$  because of the low optimal  $\omega_c$  (= 0.19), which increases RWU from the deeper layers where h is close or equal to  $h_4$ . JMm behaved very differently with uptake over the first few days (when  $M_s > M_c$ ) in accordance with R distribution. After  $M < M_c$  in upper soil layers,the RWU pattern started to change gradually and RWU increased at lower depths.

The proposed models (PM and PMm ) are capable of predicting similar RWU patterns as VLM. For the low  $T_p$ -high R scenario (Fig. 6), RWU is more uniformly distributed over depth than in the VLM model for the first days and uptake from upper layers is lower than that predicted by VLM model. For high  $T_p$  (Fig. 7), these models better represent RWU patterns and, in general, there is not much difference in predictions of RWU between the proposed models. The shape of the transpiration reduction over time however, is smoother than the VLM model. Concerning the relative transpiration curve, the proposed models appear to be less precise than the other models that account for RWU compensation.

JMII does not mimic well the RWU pattern predicted by VLM for the high R-low  $T_p$  scenarios. It overestimates uptake from surface layers for the first days. Before the onset of transpiration reduction, uptake from upper layers becomes zero, but is compensated by a higher uptake from deeper layers. The model is very sensitive to both R and M. For the high R-high  $T_p$  scenarios, JMII provides better uptake pattern predictions (Fig. 7). However, the model does not perform well in the other scenarios of with low and medium R (data not shown here).

Comparing RWU predictions from JMf and JMIIit is clear, it is seen that the Jarvis-type models are affected by the definition of  $\alpha$ . This becomes more evident by analysing Fig. 9 which shows  $\alpha$  of JMII (eq. 18) as a function of  $h_s$  and  $\omega_c$  (eq. 20) for different soil types, expressed by  $M_{max}$ . Focussing first on the  $\alpha$  function, it can be seen that despite the fact that even though the soil resistance should increase continuously as soil dries, defining  $\alpha$  by eq. 18 does not seem very realistic. In this case  $\alpha$  is suddenly reduced even when the soil is near saturation. When  $h_s = 1$  m, for instance,  $\alpha$  is much lower than 0.5. Such a behaviour is not expected for the  $\alpha$  concept. The  $\omega_c$  values are also extremely low. The low  $\alpha$  values are, however, balanced by high  $\alpha_2$  values (due to low  $\omega$  and  $\omega_c$  values), leading to suitable values of RWU in a given soil layer. Nevertheless, the magnitude of  $\alpha$  and  $\omega_c$  are conceptually questionable. Therefore, we conclude that: i) the  $\omega_c$  value in Jarvis-type models, which sets the compensation level, depends on the  $\alpha$  definition. For instance, for the original Jarvis (1989) model,  $\omega_c = 0.5$  corresponds to a moderate level of compensation. Surely, it does not hold if  $\alpha$  is defined by eq. 18; ii) Comparing Jarvis (1989) to the Jarvis (1989) to the De Jong van Lier et al. (2008) model led to a rather unrealistic  $\alpha$  function, and its behaviour does not properly represent the  $\alpha$  concept. This behaviour might be is possibly due to the fact that the De Jong van Lier et al. (2008) model does not take into consideration the plant hydraulic resistances. This might explain the rapid decline of  $\alpha$  near saturation. The threshold type functions like the other ones evaluated in this paper seems seem to be more feasible.

The fact that JMII is more sensitive to both R and M, as stated above, when compared to the other M-based models is attributed to the  $\alpha$  function and the derived equations to express their parameters (eq. 19 and 20). It can be seen from Fig. 9(c) that  $\beta$  defined by eq. 19 ( $\beta$  of JMII) tends to be higher when R increases and lower when R decreases compared to  $\beta$  of JMf and JMm. Thereby, for the first days of simulations when the soil hydraulic conditions tend to be rather uniform over depth, JMII overestimates RWU compared to VLM predictions. This becomes more important for the high R-low  $T_p$  scenarios. For such conditions, the RWU over depth predicted by the VLM tends to be more uniform, which is reasonable since seems reasonable as the low transpiration demand can be met by any small R that can be found in deeper soil depths. After some period of time, the discrepancies between VLM and JMII tend to increase, since the higher RWU in the upper layers reduces h; thus, because of the  $\alpha$  shape of JMII RWU in the upper layers are suddenly reduced towards zero. These are the main reasons why JMII does not predict well in the high R-low  $T_p$  scenarios.

## 25 4.1.3 Statistical indices

The performance of the empirical models was analysed by the coefficient of determination  $r^2$  and the model efficiency coefficient E (Nash and Sutcliffe, 1970) calculated by comparing to the RWU and relative transpiration predicted by VLM. For the low R-high  $T_p$  scenarios, the VLM predicts water stress ( $T_a < T_p$ ) since the beginning of the simulation as discussed in section 4.1.1. The empirical models (except for JMf and JMm by setting  $\omega_c > 1$ ) are not able to reproduce these results, thus these scenarios are not taken into account when analysing the performance of the models.

These statistical indices for the evaluated scenarios of each model are concisely shown by the boxplots in Fig. 10. The width of whiskers indicates the range of the statistical indices for each model used in the evaluated scenarios. The outliers indicate

whether a model had different performance at some scenarios than its overall performance. Focusing first on RWU, it can be easily seen the better performance of the proposed models. The performance of PM was just a bit poorer than PMm's, shown by the presence of an outlier and lower median. JMm performed as good as the proposed models, and only in two scenarios it had a bad performance as shown by the outliers in Fig. 10. The wider whiskers and presence of outliers of the others models confirm their poorer performances.

Among the models that account for RWU compensation, JMf and JMII had the poorest performances. These models had very low performances in the high R-low  $T_p$  scenarios and in general their performances were poorer for medium R scenarios, especially for low  $T_p$ . Thus, the use of  $\alpha_m$  in Jarvis-type models promotes substantial improvements, especially from medium to high R scenarios. For low R scenarios all models performed well and the highest values of the boxes in Fig. 10 usually refer to this scenario.

On predicting transpiration all models accounting for compensation performed well, except JMf. It can be noticed that JMII performed much better on predicting transpiration than RWU. Similarly as for the RWU predictions, all models had their poorest performance. All models performed poorest in the high R scenarios, similar to what was shown for RWU predictions.

As the evaluated models differ regarding the number of empirical parameters (from 0 to 2), it is important to use a statistical measure that penalizes the models with more parameters. The Akaike's information criteria (AIC) is a suitable measure for such a model comparison. The selection of the "best" model is determined by an AIC score, defined as (Burnham and Anderson, 2002):

$$AIC = 2K - \log(\mathcal{L}(\hat{\theta}|y)) \tag{32}$$

where K is the number of fitting parameters and  $\mathcal{L}(\hat{\theta}|y)$  is the log-likelihood at its maximum point. The "best" model is the one with the lowest AIC score. Table 6 lists the best models for every scenario based on AIC score. Overall, the AIC supports the above descriptive statistical analyses, indicating that the proposed models are the best models in predicting RWU estimated by VLM, specially from medium-high R scenarios. For the low R scenarios JMm is the best model. On predicting  $T_r$  by VLM, the above analyses indicated that in general most models had similar performance. The AIC indicated similar results, but overall JMm was the best model. The proposed models (PM or PMm) were the best models for high R-low  $T_p$  scenarios.

## 25 4.1.4 Relation of the optimal empirical parameters to R and $T_p$ levels

The optimal values of the empirical parameters of all models (except for JMII that has no empirical parameters) for all scenarios (except for the high  $T_p$ -low R scenario) are shown in Table 5. The threshold reduction transpiration parameters  $h_3$  and  $M_c$  (for FM and FMm, respectively) stands for the soil hydraulic conditions from which the crop cannot meet its potential transpiration rate. Conceptually, the more the roots, the lower is  $h_3$  or  $M_c$  due to the larger root surface area for RWU, i.e. the crop can extract water in drier soil conditions. Similarly, lower  $h_3$  and  $M_c$  are expected for low  $T_p$ . This can also be deduced from Fig. 6 and 7 by means of the predictions of relative transpiration and RWU by VLM.

The optimal  $h_3$  and  $M_c$  values (Table 5) for FM and FMm, respectively, increase as R increases, contradicting their conceptual relation to R. For  $T_p$ , there is no specific relationship for these parameters: whether they increase or decrease with  $T_p$  depends on the value of R. In drying-out scenarios, soil water from top layers depletes rapidly due to the higher initial uptake. As a result, uptake from these layer starts to decrease whereas RWU in deeper, wetter layers increases. The higher the R, the more intense is this process as seen by the VLM predictions in section 4.1.1. Because FM and FMm do not account for this mechanism, decreasing  $h_3$  or  $M_c$  in search for conceptually meaningful values would make these models to predict higher RWU at upper layers (in accordance with R distribution) for a longer period, increasing the discrepancy with VLM predictions. Therefore, their best fitted values are physically without meaning due to the model assumptions.

In order to interpret the parameters in Table 5 for JMf, one should first recall that  $\alpha$  in JMf stands for the local RWU reduction due to soil resistance. Thus, its  $h_3$  parameter refers to the local soil pressure at which RWU starts to reduce. It may be argued that RWU reduction occurs in drier soil conditions as R increases, that is  $h_3$  is more negative for higher R (similarly as for FM and FMm). However, since JMf accounts for compensation, RWU is interpreted as a non-local process, i.e. uptake in one layer depends on water status and root properties from other layers (Javaux et al., 2013). Thus, JM's  $h_3$  parameter is affected by other parts of the root zone. Predictions by VLM show that RWU reduction from the upper layers starts at less negative soil pressure head as R increases. Therefore,  $h_3$  in JMf should increase as R increases. The values of  $h_3$  for JMf shown in Table 5 agrees to this conceptual meaning. The JMm's  $M_c$  parameter can be interpreted likewise.

The JMf's  $\omega_c$  parameter values for the high R-low  $T_p$  scenarios equal 1, thus contradicting its conceptual meaning: as in these scenarios the compensation mechanism is more intense,  $\omega_c$  should be less than one for the medium and high R scenarios. The reason for  $\omega_c = 1$  was discussed in section 4.1.2. Conversely,  $\omega_c$  values for JMm follow the conceptual meaning.

The optimal parameters of the proposed models follow the logical relation to R and  $T_p$ . The  $l_m$  values for both models are very close. The optimal  $l_m$  values are less sensitive to soil types and more sensitive to R.

High correlation parameters might result in uncertainties and nonunique solution of the optimization problem. In general, the correlation parameter coefficients were low, except in some scenarios in which high correlation coefficients between  $\omega_c$  and  $h_3$  (or  $M_c$ ) were found. These high correlations might be due to model structure rather than to the data used for fitting the models, since the correlation for PM and PMm parameters were considerably low (absolute correlation coefficient below 0.53).

## 4.1.5 Optimization using $T_r$

In order to To evaluate the empirical models and find their empirical parameters, the empirical models were only fitted to RWU, since we are primarily interested on the capability of the models in predicting the RWU patterns under different scenarios. This is a great advantage of using physical RWU models, since RWU is not easily obtained in real conditions. Nevertheless, plant transpiration is one of the main outputs in RWU models and it is more easily obtained. Thus, one might consider to fit the

models to the temporal course of (relative) plant transpiration or to fit the models simultaneously to both plant transpiration and RWU, at which a rather complicated optimization scheme is required.

We addressed this issue by fitting the models to the course of relative transpiration for some scenarios. The procedure was the same as explained in Section 3.3, but substituting  $S_{i,j}$  in eq 31 by  $T_{r_i}$ . The results for some models in two contrasting scenarios of R is shown in Fig 11. It can be seen that the models who Models that account for "compensation" can predict  $T_r$  quite reasonably even when fitted to RWU only. The models who that do not account for "compensation" can do not mimic well  $T_r$  course for the high R scenario predicted by VLM, even when they are fitted to  $T_r$ , and the predictions worsen predictive quality decreases when fitted to RWU. The most important aspect shown in Fig 11 is that fitting the models to  $T_r$  can improve  $T_r$  predictions but impairing considerably their RWU predictions, specially especially for high R. Conversely, if a model can fit fits well to RWU, they it can provide suitable transpiration predictions. This can also be seen by the analysis of Section 4.1.3, when the proposed models and JMm had good performance in predicting  $T_r$  as well.

#### 4.2 Growing season simulation

By evaluating the RWU models under real weather conditions during a relatively dry year and considering the same soil types and crop characteristics as for the drying-out experiment, it was possible to use the respective soil type and root length density specific calibrated parameters. We did not evaluate the models for the low R scenario because the empirical models (except JMf and JMm) were not not not able to mimic those conditions for high  $T_p$  (section 4.1.1) . This evaluation is also important to analyse-when analysing whether calibration of an empirical model with a single drying-out experiment type results in consistent behaviour in other circumstances.

Fig 12 shows the time course of cumulative actual transpiration simulated by SWAP using all the RWU models, together with rain rainfall and  $T_p$  throughout the growing season period. It can be seen that right after Following the first dry spell,  $T_{ac}$  by FM and FMm, who do not account not accounting for "compensation", starts to be lower than that by other models. Two or three more dry spells occur in the evaluated period. The magnitude of this the underestimation, however, varies with soil type and R. For the medium R-loam soil scenario, for instance, the  $T_{ac}$  for all models are quite similar. The  $T_{ac}$  at the end of the evaluated period predicted by VLM for low R (not shown in Fig. 12) was much lower and approximately equal for the three soil types (40.45, 40.05 and 40.08 cm for clay, loam and sand soil, respectively). In fact, a higher R resulted in an increasing difference of cumulative transpiration between soil types. Most water is extracted from the clay soil, followed by sand and loam. Little difference of cumulative transpiration is found between medium and high R: for sand and clay soil, the cumulative transpiration was slightly higher for high R and practically identical for the loam soil.

Comparing cumulative  $T_a$  predicted by the empirical models with VLM predictions shows that the models that do not account for compensation underestimate cumulative  $T_a$  from 2.0 % (medium R –sand soil scenario) to 13.9 % (high R–clay soil

scenario). Overall, the highest underestimates occurred for high R. All other models predict similar values. Therefore, for total actual transpiration any of the evaluated models accounting for compensation might be suitable after calibration.

An overall analysis of the models performance is shown in Fig. 13 and a list of the "best" model for each scenario based on AIC is shown in Table 7. The best performances are from the models that account for compensation. An improvement of JMf by using the proposed reduction function can be observed. Among the models that account for compensation, JMf had the worst performance. JMII also was poor in predicting RWU, but showed good performance in estimating plant transpiration. Overall, the best performances were also obtained by the proposed models (PM and PMm) and by the modified Jarvis (1989) model (JMm) in predicting RWU. These results also indicate that the strategy of designing a single drying-out experiment to calibrate an empirical model is successful.

The selection of the best models based on AICalso indicates According to the AIC, PM, PMm and JMm as the best models are best in predicting RWU. Regarding  $T_r$  predictions, Fig. 13 shows considerably high statistical indices (E and  $r^2$ ) for all models that account for "compensation". However, the AIC, which penalizes the models with more parameters, indicates that JMII was the "best" model for most of the scenarios.

In general, the proposed models as well as JMm showed better performance than the other empirical models. It should be noted, however, that these models are based on M, making them closer to the physical De Jong van Lier et al. (2013) model. In this regard, it is important to separately compare JMf and JMm and PM and PMm. The only difference between JMf and JMm is the  $\alpha$  reduction, which resulted in considerable improvements as already discussed. In the proposed models, M is included in  $S_p(z)$  to distribute  $T_p$  over depth. In PMm,  $\alpha_m$  is used instead of the Feddes reduction function (used by PM). These simple modifications were sufficient to make these empirical models mimic the predictions made by the more complex physical model when fitted.

#### 5 Conclusions

Several simple RWU models have been developed over the years and here we outlined some of these models and also proposed alternatives. Some of these models were embedded as sub-models into the eco-hydrological model SWAP (Van Dam et al., 2008) and their evaluation was based on the comparison with RWU predictions performed by the physical De Jong van Lier et al. (2013) model (also embedded into the SWAP model) for two numerical experiments with several scenarios of soil type, root length density and potential transpiration rates. The parameters of the empirical models were determined by inverse modelling of simulated RWU. The simulated scenarios also allowed insight into the behaviour of the De Jong van Lier et al. (2013) model, especially under wet soil conditions and high potential transpiration. We found that for the In such scenarios and with a low R-high  $T_p$  scenarios, the De Jong van Lier et al. (2013) model predicts crop transpiration reduction reduction rate is becomes dependent on crop hydraulic parameters, especially the radial root hydraulic conductivity. More insight into these results may be obtained by coupling the De Jong van

Lier et al. (2013) physical model with stomatal conductance models. Regarding the performance of the empirical models we conclude:

- The widely-used Feddes et al. (1978) empirical RWU model performs well only only performs well under circumstances of low root length density R, that is for the scenarios of low in other words, when root water "compensation" is low. From medium to high R, the model cannot mimic properly the RWU dynamics as predicted by the De Jong van Lier et al. (2013) model, resulting in very poor predictions. Besides a poor performance. Moreover, the optimized  $h_3$  values are counterintuitive when interpreting their conceptual meaning. Using our Employing the proposed RWU reduction function (the FMm model) does not improve performance either with this respect.
- The JMf model provides good predictions only for low and medium R scenarios. For high R, the model cannot mimic the
   RWU patterns predicted by the De Jong van Lier et al. (2013) model. Using our proposed reduction function (the JMm model) the proposed JMm reduction function helps to improve RWU predictions. Similarly, the JMII model does not perform well for high R-low T<sub>p</sub> scenarios, as explained in Section 4.1.2.
  - The proposed models are <u>eapable of predicting able to predict</u> RWU patterns similar to those obtained by the De Jong van Lier et al. (2013) model. The statistical indices point them as the best alternatives to mimic RWU predictions by the De Jong van Lier et al. (2013) model.
  - Regarding the ability of the models in predicting plant transpiration, all models that accounts accounting for compensation have good performance. The AIC information indicates that JMII, which has no empirical parameters to be estimated, is the "best model". This model is also more suitable for blind predictions, as no empirical parameters need to be estimated.
- The simulations for a growing season experiment confirmed these findings, suggesting that a single an experiment of soil
   drying-out for two levels of potential transpiration, as designed in Section 3.2.1, is sufficient to analyse the performance of RWU models and retrieve their empirical parameters by defining the objective function in terms of RWU.

It should be noticed that the predictions from the De Jong van Lier et al. (2013) physical model do not represent a real system. However, they show to be consistent with the phenomena behaviour and have adequate sensitive to variables and system boundaries. In the usage of the empirical models, it is a common practice users to refer to the old parameters compilation made by Taylor and Ashcroft (1972), which does not account for the dependence of the parameters on soil type. Moreover, these parameters depend on type of transpiration reduction function, which is not clear in the Taylor and Ashcroft (1972) compilation but usually referred to as the Feddes model. The selected models based on the comparison with a detailed physical model, the proposed models and JMf, have one additional parameter, also dependent on soil type, root length densityand potential transpiration. Although the parameters for three soil types, root length density and potential transpiration are provided in this study, a more robust and complete calibration may be necessary, mainly because general values of plant hydraulic resistances were used. Due to the dependence of the empirical parameters on soil type and potential transpiration, parameterizing the selected empirical models for a specific crop might require more effort than when using the physical model whose parameters

can be determined independently. Using the physical model predictions, as in this study, seems a good strategy to calibrate the empirical models. Ultimately, the choice over empirical or physical model will be based on the desired complexity and understanding of the system, and on availability of parameter values.

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## List of tables

**Table 1.** Summary of empirical models used.  $\alpha_f$  and  $\alpha_m$  are the Feddes et al. (1978) (Fig. 1a) and proposed reduction functions (Fig. 1b),  $S_p$  (eq. 4) is the potential root water uptake,  $\omega$  (eq. 11) and  $\omega_c$  are the weighted stress index and threshold value in Jarvis (1989) model and  $\zeta_m$  (eq. 25) is the weighted stress index in the proposed models.

Model	Acronym	Equation
Feddes et al. (1978) model	FM	$S(z) = S_p \alpha_f$
Modified Feddes et al. (1978) model	FMm	$S(z) = S_p \alpha_m$
Jarvis (1989) model	JMf	$S(z) = S_P \frac{\alpha_f}{\max\{\omega, \omega_c\}}$
Modified Jarvis (1989) model	JMm	$S(z) = S_p \frac{\alpha_m}{\max\{\omega, \omega_c\}}$
Jarvis (2010) model	JMII	Eqs. 11 to 13 with parameters given by eqs. 18 to 20
proposed model I	PM	$S(z) = \zeta_m T_p \alpha_f$
proposed model II	PMm	$S(z) = \zeta_m T_p \alpha_m$

**Table 2.** Values of the parameters of De Jong van Lier et al. (2013) model used in the simulations.

Parameter	Value	Unit	
$r_0$	0.5	mm	
$r_x$	0.2	mm	
$K_{root}$	$3.5 \cdot 10^{-8}$	${\rm m}\ {\rm d}^{-1}$	
$L_l$	$1 \cdot 10^{-6}$	$\mathrm{d}^{-1}$	
$h_{ws}$	-150	m	
$h_{wl}$	-200	m	

**Table 3.** Mualem-van Genuchten parameters for three soils of the Dutch Staring series (Wösten et al., 1999) used in simulations.  $\theta_s$  and  $\theta_r$  are the saturated and residual water content, respectively;  $K_s$  is saturated hydraulic conductivity and  $\alpha$ ,  $\lambda$  and n are fitting parameters.

Staring soil ID	Textural	Reference	in	$\theta_r$	$\theta_r$	$K_s$	α	λ	$\overline{n}$
	class	this paper							
				${\rm m}{\rm m}^{-3}$	${\rm m}~{\rm m}^{-3}$	${\rm m}~{\rm d}^{-1}$	$\mathrm{m}^{-1}$	-	-
В3	Loamy	Sand		0.02	0.46	0.1542	1.44	-0.215	1.534
	sand								
B11	Heavy Clay	Clay		0.01	0.59	0.0453	1.95	-5.901	1.109
B13	Sand Loam	Loam		0.01	0.42	0.1298	0.84	-1.497	1.441

**Table 4.** Parameters of the root water uptake models estimated by optimization and their respective constraints  $\Omega$ .

Model	Parameter	Ω	Unit
FM	$h_3$	$-150 < h_3 < 0$	m
FMm	$M_c$	$0 < M_c < M_{max}$	$\mathrm{m}^2~\mathrm{d}^{-1}$
JMf	$h_3$	$-150 < h_3 < 0$	m
	$\omega_c$	$0 < \omega_c \le 1$	-
JMm	$M_c$	$0 < M_c < M_{max}$	$\mathrm{m}^2~\mathrm{d}^{-1}$
	$\omega_c$	$0 < \omega_c \le 1$	-
PM	$h_3$	$-150 < h_3 < 0$	m
	$l_m$	$0 < l_m \le 3$	-
PMm	$M_c$	$0 < M_c < M_{max}$	$\mathrm{m}^2~\mathrm{d}^{-1}$
	$l_m$	$0 < l_m \le 3$	-

Table 5. Optimal parameters of each empirical model for all scenarios in the drying-out experiment

			FM	FMm	JMf		JMn	JMm		PM		PMm	
Soil	Tp	R	$h_3$	$M_c$	$h_3$	$\omega_c$	$M_c$	$\omega_c$	$h_3$	$l_m$	$M_c$	$l_m$	
	${\rm mm}~{\rm d}^{-1}$	${\rm cm}{\rm cm}^{-3}$	cm	${\rm cm}^2{\rm d}^{-1}$	cm	-	${\rm cm}^2{\rm d}^{-1}$	-	cm	-	${\rm cm}^2{\rm d}^{-1}$	-	
clay	1	0.01	-1968.7	0.213	-284.5	0.711	0.366	0.494	-1615.7	1.322	0.227	1.290	
clay	1	0.10	-1211.0	0.329	-132.4	0.196	0.944	0.024	-7579.9	0.869	0.076	0.884	
clay	1	1.00	-1.7	0.950	-0.0	1.000	5.971	0.004	-10673.7	0.354	0.022	0.342	
loam	1	0.01	-7588.1	0.334	-5.0	0.457	22.483	0.016	-6927.6	1.086	0.408	1.084	
loam	1	0.10	-6085.6	0.487	-93.9	0.126	25.721	0.002	-11795.6	0.911	0.113	0.917	
loam	1	1.00	-17.0	5.014	-48.0	1.000	106.223	0.000	-10878.8	0.561	0.058	0.553	
sand	1	0.01	-1014.0	0.146	-291.6	0.942	0.288	0.436	-621.2	1.262	0.149	1.252	
sand	1	0.10	-1122.6	0.115	-113.6	0.407	1.925	0.005	-2351.3	1.179	0.024	1.159	
sand	1	1.00	-3.9	0.338	-0.0	1.000	25.887	0.000	-3158.0	0.717	0.005	0.706	
clay	5	0.10	-1397.7	0.334	-218.4	0.325	0.395	0.271	-5537.2	1.512	0.196	1.449	
clay	5	1.00	-260.6	0.792	-135.3	0.148	1.212	0.013	-6745.0	0.672	0.088	0.687	
loam	5	0.10	-5236.5	0.784	-0.0	0.277	2.306	0.100	-8322.9	1.165	0.488	1.157	
loam	5	1.00	-1249.5	2.563	-292.9	0.161	28.143	0.001	-8630.0	0.833	0.224	0.838	
sand	5	0.10	-918.0	0.190	-556.2	0.432	4.154	0.018	-1273.9	1.612	0.083	1.510	
sand	5	1.00	-582.3	0.533	-342.5	0.193	4.888	0.001	-3582.3	1.272	0.012	1.240	

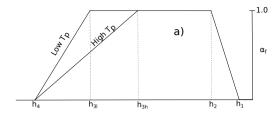
**Table 6.** Best models for the evaluated scenarios (root length density R, soil type and potential transpiration  $T_p$ ) based on Akaike's information criteria AIC through comparison of root water uptake (RWU) and relative transpiration ( $T_r$ ) predicted by De Jong van Lier et al. (2013) physical model in the drying-out experiment.

			Low $T_p$			High $T_p$	
	R	Clay	Loam	Sand	Clay	Loam	Sand
	Low	JMm	JMf	JMm	JMm	JMm	JMm
RWU	Medium	PMm	PMm	JMII	JMm	PM	PMm
	High	PMm	PMm	PM	PM	PMm	PM
	Low	JMm	JMm	JMm	JMm	JMm	JMm
$T_r$	Medium	JMm	JMm	JMII	JMm	PM	JMf
	High	PMm	PMm	PMm	JMII	JMm	JMm

**Table 7.** Best models for the evaluated scenarios (root length density R and soil type) based on Akaike's information criteria AIC through comparison of root water uptake (RWU) and relative transpiration ( $T_r$ ) predicted by De Jong van Lier et al. (2013) physical model in the growing season experiment.

	Cla	y	Loai	n	Sand		
	Medium R	High R	Medium R	High R	Medium R	High R	
RWU	JMm	PM	PM	PMm	JMm	JMm	
$T_r$	JMII	JMII	JMf	JMm	JMII	JMII	

## List of figures



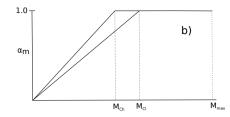


Figure 1. a) Feddes et al. (1978) root water uptake reduction function.  $h_2$  and  $h_3$  are the threshold parameters for reduction in root water uptake due to oxygen deficit and water deficit, respectively. The subscripts l and h stands for low and high potential transpiration  $T_p$ .  $h_1$  and  $h_4$  are the soil pressure head values above and below which root water uptake is zero due to oxygen and water deficit, respectively. b) Root water uptake reduction function  $\alpha_m$  as a function of matric flux potential M;  $M_{ch}$  and  $M_{cl}$  are the critical values of M for high and low  $T_p$ , respectively, from which the uptake is reduced and  $M_{max}$  is the maximum value of M, dependent on soil type.

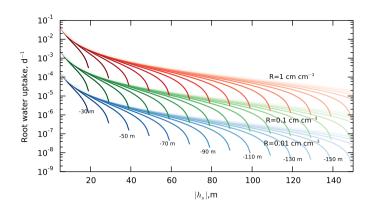


Figure 2. Root water uptake S—(RWU) as a function of soil pressure head  $h_s$  for three values of root length density (0.01, 0.1 and 1.0 cm cm<sup>-3</sup>) and leaf pressure head values ranging from -30 to -200 m by -10 m interval shown by colors gradient (lighter colors indicate lower values and some values are also indicated in the plot). These results were obtained by the analytical solution of eq. 8 given by De Jong van Lier et al. (2013) for a special case of Brooks and Corey (1964) soil. Plant transpiration was set to 1 mm d<sup>-1</sup>, rooting depth to 0.5 m, and the soil and plant hydraulic parameters were taken from De Jong van Lier et al. (2013).

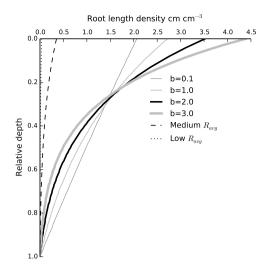
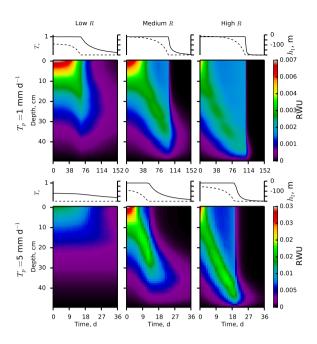


Figure 3. Root length density distribution over depth calculated by eq. 30 for several values of b and  $R_{avg} = 1.0$  cm cm<sup>-3</sup> and for low and medium  $R_{avg}$  with b = 2.



**Figure 4.** Time-depth root water uptake (RWU,  $d^{-1}$ ) pattern, leaf pressure head ( $h_l$ , dashed line) and relative transpiration ( $T_r$ , continuous line) simulated by SWAP model together with the De Jong van Lier et al. (2013) model for clay soil, two levels of potential transpiration  $T_p$ : 1 and 5 mm  $d^{-1}$  (first and second line of plots, respectively) and three levels of root length density R: low, medium and high (indicated at the top of the figure).

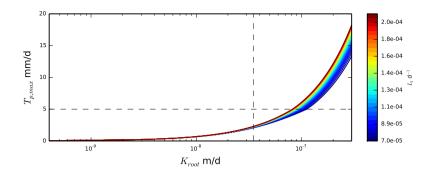


Figure 5. Maximum possible transpiration  $T_{p,max}$  as a function of root hydraulic conductivity  $K_{root}$  for some values of the overall conductance over the root-to-leaf pathway  $L_l$  computed by De Jong van Lier et al. (2013) model for rooting depth of 0.5 m, low root length density and constant soil pressure head over depth equals to -1 m for sandy soil. The dashed vertical line highlights the value of  $K_{root} = 3.5 \ 10^{-8} \ \mathrm{m} \ \mathrm{d}^{-1}$  that was used in our simulations. Horizontal dashed line highlights the value of potential transpiration.

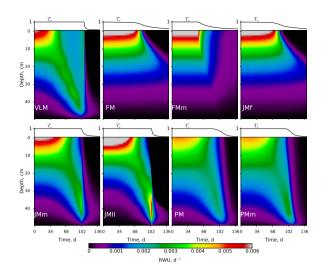


Figure 6. Time-depth root water uptake (RWU) pattern and relative transpiration  $(T_r)$  simulated by SWAP model together with De Jong van Lier et al. (2013) sink and the others empirical models for sand soil texture, high root length density and  $T_p = 1 \text{ mm d}^{-1}$ .

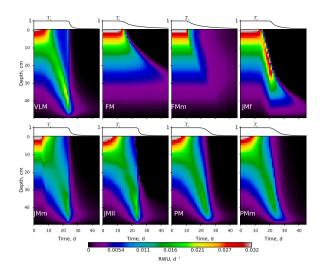


Figure 7. Time-depth root water uptake (RWU) pattern and relative transpiration  $(T_r)$  simulated by SWAP model together with De Jong van Lier et al. (2013) sink and the others empirical models for sandy soil texture, high root length density and  $T_p = 5 \text{ mm d}^{-1}$ .

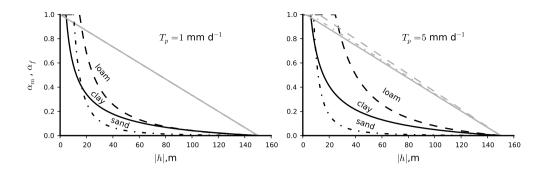


Figure 8. Feddes et al. (1978) ( $\alpha_f$ , gray lines) and proposed ( $\alpha_m$ , black lines) water uptake reduction functions as a function of soil pressure head h using their respective optimized parameters for the scenario of high root length density, three types of soil and two potential transpiration levels.

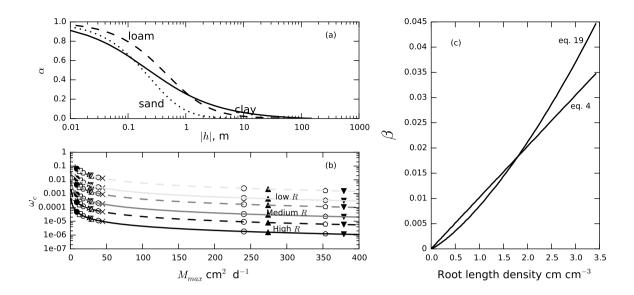


Figure 9. (a)  $\alpha$  of JMII model (eq. 18) as function of soil pressure head  $h_s$ , (b)  $\omega_c$  parameter (eq. 20) for different soil types (the three soil types used in the simulations and more soils from Wösten et al. (1999)), expressed by  $M_{max}$  and (c) the normalized root length density  $\beta$  computed by the eqs. 4 (JMf) and 19 (JMII) as function of root length density R, with R over depth given by eq. 30 with  $R_{avg}$  and  $\theta$  equal to 1.0 cm cm<sup>-3</sup> and 2, respectively.

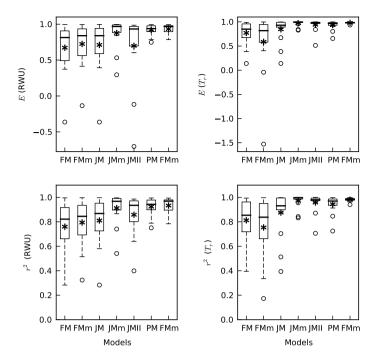


Figure 10. Box plot of the coefficient of determination  $r^2$  and model efficiency coefficient E for the comparison of root water uptake (RWU) and actual transpiration ( $T_a$ ) predicted by each empirical model with the De Jong van Lier et al. (2013) model predictions for the drying-out simulations for three levels of root length density and three types of soil and two potential transpiration levels. The symbols \* and  $\circ$  represent the average and outliers, respectively.

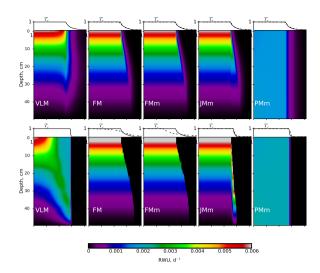


Figure 11. Time-depth root water uptake (RWU) pattern and relative transpiration  $(T_r)$  simulated by SWAP model together with De Jong van Lier et al. (2013) sink and some empirical models when optimization was performed with  $T_r$  instead of RWU for loam soil texture, low (first line of plots) and high (second line of plots) root length density and  $T_p = 1 \text{ mm d}^{-1}$ . The dashed lines indicate  $T_r$  when the models were optimized with RWU.

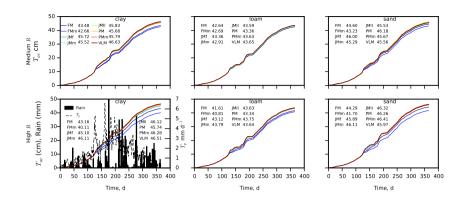


Figure 12. Time course of actual cumulative plant transpiration  $T_{ac}$  predicted by the De Jong van Lier et al. (2013) and all the empirical models for the three types of soil (clay, loam and sand) and two levels of root length density (medium and high), rain and potential transpiration  $T_p$  for the growing season experiment. The total  $T_{ac}$  values predicted by each model for the whole period are shown in the plot aside the model names.

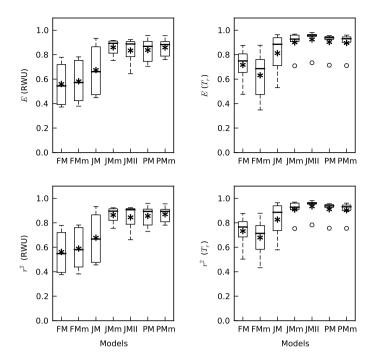


Figure 13. Box plot of the coefficient of determination  $r^2$  and model efficiency coefficient E for the comparison of root water uptake (RWU) and actual transpiration ( $T_a$ ) predicted by each empirical model with De Jong van Lier et al. (2013) model for the growing season experiment for two levels of root length density and three types of soil. The symbols \* and  $\circ$  represent the average and outliers, respectively.