University of São Paulo
"Luiz de Queiroz" College of Agriculture

Determination of empirical parameters for root water uptake models

Marcos Alex dos Santos

Thesis presented to obtain the degree of Doctor of Science. Area: Agricultural Systems Engineering

Piracicaba
2015

Marcos Alex dos Santos
Agronomist

Determination of empirical parameters for root water uptake models

Advisor:
Prof. Dr. **QUIRIJN DE JONG VAN LIER**

Thesis presented to obtain the degree of Doctor of Science. Area: Agricultural Systems Engineering

Piracicaba
2015

Dados Internacionais de Catalogação na Publicação
DIVISÃO DE BIBLIOTECA - DIBD/ESALQ/USP

Santos, Marcos Alex dos
Determination of empirical parameters for root water uptake models / Marcos Alex dos Santos. - - Piracicaba, 2015.
71 p. : il.

Tese (Doutorado) - - Escola Superior de Agricultura "Luiz de Queiroz".

1. Transpiração 2. Optimização 3. Modelagem 4. Solo 5. Parâmetros I. Título

CDD 631.432
S237d

Aos meus queridos pais, Miguel José dos Santos e Vilma Gonzaga dos Santos, pela educação, força, amor e carinho,

Ao meu irmão Melquisedeque, que, juntamente com meus pais, contribui intensamente para minha formação;

Ao meu irmão Mercel, companheiro de vida acadêmica,

À minha querida irmã Camila,

DEDICO

ACKNOWLEDGEMENT

A Deus, por ter me dado força e coragem nos momentos difíceis.

Ao meu orientador Quirijn de Jong van Lier, pelo apoio, amizade, conhecimentos adquiridos e, sobretudo, pela paciência e compreensão;

À Escola Superior de Agricultura "Luiz de Queiroz" (ESALQ/USP) e ao Programa de Pós-graduação em Engenharia de Sistemas Agrícolas, pela oportunidade e apoio;

Aos funcionários de Departamento de Engenharia de Biossistemas da ESALQ, em especial Angela Derigi Silva, Davilmar Aparecida Colevatti, Luiz Fernando Novello, Francisco Bernardo Dias;

Aos professores do departamento de Engenharia de Biossistemas, em especial aos professores Sérgio de Oliveira Moraes, Paulo Leonel Libardi e Jarbas Honório de Miranda e Sérgio Nascimento Duarte pelos ensinamentos;

Aos meus professores e orientadores de graduação da UFAL, em especial: José Leonaldo de Souza, Gustavo Bastos Lyra, Iêdo Teodoro e Guilherme Bastos Lyra, pela amizade, incentivo e contribuições em minha formação;

Ao Conselho Nacional de Desenvolvimento Científico e Tecnológico (CNPq) pela concessão da bolsa de doutorado e à Coordenação de Aperfeiçoamento de Pessoal de Nível Superior (CAPES) pela concessão das bolsas de estágio *sandwich* e doutorado;

Aos amigos e funcionários do FISOL/CENA-USP pelos bons momentos: Andre F. Bezerra, Everton Alves, Lívia Previatello, Ana Luiza, Thalita Oliveira, Thaís Rodrigues, Victor Meriguetti, Hanoi Medina, Robson Arthur, João Eduardo Pilotto;

Aos amigos da república "Ubueiro" Carlos Antonio Costa do Nascimento, Connan Ayade Salvador e Eduardo Zavaski pelo incentivo, conhecimentos e conselhos. Também sou grato pela generosidade, compreensão e boa convivência.

Aos amigos de república Sales Fernandes, Aloisio Coelho e José Bruno Malaquias pela boa convivência e bons momentos;

Aos Amigos e companheiros de ESALQ pelos momentos agradáveis durante esses anos, em especial: Luciano Roberto da Silveira, Francisco Dirceu Duarte Arraes, Angelica Durigon, Roque Pinho, Helon de Freitas, Marcelo Dias Oliveira, Fernando Henrique, Verena Beníco, Ismael Meurer, Laiane Nascimento, Cezar Rebouças, Isaac Ponciano, Marinaldo Ferreira Pinto, Alexsandro Almeida, Leticia de Abreu Faria (Eva), Wagner Wolff, Marcos Araújo;

Aos amigos e criadores da TEXSALQ (template em TEX puro usado na confecção desta tese —https://github.com/lrsilveira/texsalq), Luciano e Andre, pelo fantástico trabalho e ajustes na reta final;

A todos os meus familiares, em especial meus tios pelo apoio e incentivo. Não me arrisco a listar nomes, pois seria injusto esquecer de alguém;

Àqueles de minha cidade natal, Coruripe-AL, que me deram apoio e incentivo desde meu período de graduação, em especial a Joaquim Beltrão Siqueira e Dalva Edith Reis Beltrão;

À cooperativa pindorama, em especial a Klécio José dos Santos, Alda Júlia Santos e Marinalva pelo apoio e incentivo desde o início de minha carreira.

From the Netherlands, I would like to Thank:

To Professor Jos C. van Dam, who kindly received at Wageningen University, for his friendly orientation. Furthermore, I am very grateful for receiving me at his place and for the short bike rides and walkings over Wageningen.

To the Department of Environmental Sciences of Wageningen University and Research Centre for all the support during my stay.

To my friends over there who made my stay even more agreeable, especially to: Renée van der Salm , Susan van der Salm, Nadia Jones, Sha, Xiaomei Yang, Lucrezia Caon, Severine, Akalu Teshome, Innocent Nyakudya, Sija Stofberg, Célia Bento, Bruno Freire, Ammar Adham, Karrar Al-Timimy, Demie Moore, Isaurinda Baptista, Lingtong Gai, Bastian Hornung, Francesco Bimbo.

The future belongs to those who
believe in the beauty of their dreams.

Eleanor Roosevelt

CONTENTS

RESUMO

Determinação de parâmetros empíricos para modelos de extração de água do solo

Embora modelos físicos de extração de água do solo sejam importantes para analisar detalhes mecanísticos do sistema, seus parâmetros hidráulicos não são facilmente disponíveis, e assim são menos utilizados em situações práticas. Entretanto, modelos empíricos são facilmente aplicados devido a sua simplicidade e baixo requerimento de dados, porém seus parâmetros empíricos e habilidade em descrever a dinâmica da extração de água do solo precisa ser mais investigada. O uso combinado de modelos empíricos e físicos pode ser útil nesse contexto. O objetivo geral deste trabalho é testar se os parâmetros de modelos empíricos de extração de água do solo podem ser determinados através de simulações feitas como um modelo físico de extração de água do solo. Fez-se uma revisão sobre os principais modelos empíricos usados em modelos hidrológicos, assim como algumas alternativas foram apresentadas. Alguns desses modelos foram analisados para diferentes cenários de tipo de solo, demanda atmosférica e densidade de comprimento de raiz R. A análise foi feita otimizando-se os parâmetros empíricos dos modelos a fim de obter o melhor ajuste com o modelo físico. Em seguida, fez-me uma análise mais detalhada sobre o desempenho de um modelo empírico sugerido nas analises anteriores, como o objetivo de fornecer os valores de seus parâmetros empíricos para diferentes cenários de tipo de solo, R, profundidade do sistema radicular e transpiração potencial. Analisou-se também a variação desses parâmetros empíricos em função da condutividade hidráulica da raiz. Os resultados mostraram que (i) o modelo empírico de Feddes, que é largamente utilizado, só apresenta bom desempenho em cenários de baixo R — ou seja, para cenários com baixa compensação de extração de água do solo— e, para cenários de médio a alto R, o modelo não é capaz de representar adequadamente o dinâmica de extração de água do solo simulada pelo modelo físico; (ii) O modelo de Jarvis só apresenta desempenho adequado em cenários de baixo R e, para alto R, o modelo não é capaz de representar adequadamente a distribuição de extração simulada pelo modelo físico; (iii) inserindo-se a função de redução proposta no presente trabalho no modelo de Jarvis, ou seja o modelo JMm, proporciona melhores estimativas da distribuição de extração de água do solo; (iv) Os modelos propostos apresentam o melhor desempenho em descrever as predições feitas pelo modelo físico; (v) os parâmetros dos modelos empíricos podem ser obtidos em um único experimento de secagem do solo, definindo-se a função objetivo em função da extração de água do solo; (vi) Os parâmetros empíricos do modelo proposto variam em função dos cenários avaliados.

Palavras-chave: Transpiração; Optimização; Modelagem; Solo; Parâmetros

ABSTRACT

Determination of empirical parameters for root water uptake models

Physical root water uptake models can provide more insight into the mechanism, but their physical plant hydraulic parameters are hardly-ever available, making them less attractive in practical applications. Conversely, empirical root water uptake modes are more readily used because of their simplicity and lower data requirements, but their empirical parameters and ability in describing the dynamics of root water uptake need further investigation. Combining physical and empirical models might be an effective way to address these issues. In this thesis, it is tested the feasibility of deriving parameters for empirical root water uptake models by using predictions performed by an enhanced mechanistic root water uptake model. It is also reviewed the major root water uptake models that have been used together with larger eco-hydrological models and some alternatives are also presented. All these models are analyzed for different scenarios concerning soil type, atmospheric demand and root length density. Evaluation was performed by optimizing their empirical parameters so that the best fitting with the physical model is achieved. At last, further analyzes are performed for an empirical model pointed at the previous analyzes, and the empirical parameters for this model are provided for different scenarios regarding soil type, root length density R, rooting depth and potential transpiration T_p as well as for three levels of radial root hydraulic conductivity. It is shown that (i) the largely-used Feddes empirical root water uptake model performs well only under circumstances of low R — that is for the scenarios of low root water uptake “compensation”— and from medium to hight R, the model can not mimic properly the root uptake dynamics as predicted by the physical model; (ii) the Jarvis model provides good predictions only for low and medium R scenarios and for high R the model can not mimic the uptake patterns predicted by the physical model; Using the proposed reduction function in Jarvis model, that is the JMm model, helps to improve water uptake predictions; (iii) the proposed models are capable of predicting similar root water uptake patterns by the physical model and the statistical indices point them as the best alternatives to mimic root water uptake predictions by the physical model; (iv) the parameters of empirical models can be retrieved in a single experiment of soil drying-out by defining the objective function in terms of root water uptake; (v) the empirical parameters provided by the proposed model varies with the scenarios as well as its overall performance.

Keywords: Transpiration; Optimization; Modeling; Soil; Parameters

1 INTRODUCTION

With the increasingly world population and the triggering climate changes, thorough and efficient crop and water management in order to increase crop yield while minimizing water use and the impact on the environment is one of the major ongoing world challenging. A powerful and effective way to address theses issues is by the use of simulation models, which usually integrate the current knowledge of the involved processes. However, in order to achieve suitable model accuracy, a thorough understanding on the soil-plant-atmosphere interactions is of paramount importance as well as good the quality of the model input parameters.

The tension-cohesion theory is widely accepted to describe the ascent of water in plants. According to it, water is passively extracted from the soil by the roots and flows through the plant up to the leaf. The driving force is the water potential gradient originated at the mesophyll tissue where transpiration takes place due to stomata opening to intake CO_2, required for photosynthesis. Mechanistic modeling of this process for the entire system relies on the detailed description of the hydraulic resistances. The soil-to-root pathway has been well described whereas the descriptions within the plant has lagged behind and is a major shortcoming in applying mechanistic models.

Root water uptake provides a key linkage between the two environments exploited by plants: the soil and atmosphere — which is abstracted in eq. (2.1): on the left side it is included the atmospheric factors affecting plant transpiration and on the right side the soil conditions affecting water flow from soil to roots. Thereby, modeling of many soil and atmospheric related processes depend on soil root water uptake computation. Larger hydrological models, crop growth models land surface schemes include some parametrization of root water uptake. Mechanistic root water uptake models can provide more into insight the mechanism, as for instance the relation between plant transpiration and soil hydraulic conditions, which is crucial for crop water management and hydrological studies. However, mechanistic models are not easily applied because they require plant hydraulic parameters, which are scarce. Conversely, empirical root water uptake models usually base their estimations on the empirical relations between plant transpiration and soil hydraulic conditions. Because of their simplicity, these models are preferably more used and incorporated in larger models. Nevertheless, their empirical parameters and their ability in describing the dynamics of root water uptake need further investigation.

Combining physical and empirical models might be an effective way to address these issues.

In this thesis it is tested the feasibility of deriving parameters for empirical root water uptake models by using predictions performed by an enhanced mechanistic root water uptake model. In Chapter 2, the major root water uptake models that have been used together with larger eco-hydrological models are critically reviewed and a new proposal is also presented. All these models are analyzed for different scenarios concerning soil type, atmospheric demand and root length density. Evaluation was performed by optimizing their empirical parameter so that the best fitting with the physical model is achieved. This work led to indicate a suitable empirical model to which parametrization should be performed. Following up the results provided in Chapter 2, Chapter 3 further evaluates and provides empirical parameter values for a model indicated in Chapter 2.

2 SELECTION AND PARAMETERIZATION OF SIMPLE EMPIRICAL CONCEPTS FOR ROOT WATER UPTAKE MODELING

Abstract

Physical root water uptake models are important to give insight into the process, but their physical plant hydraulic parameters are hardly-ever available, making them less attractive in practical applications. Empirical models are more readily used because of their simplicity and lower data requirements. The general purpose of this study is to evaluate the capability of some empirical models to mimic the dynamics of water uptake distribution under varying environmental conditions performed in numerical experiments with a detailed physical model. A review of some empirical models that have been used as sub-models in ecohydrological models is also presented and suggest some alternative empirical models. The parameters of the empirical models are determined by inverse modeling of simulated depth-dependent root water uptake so that it becomes clear to which extent the empirical models can mimic the dynamic patterns of root water uptake. The several scenarios also allowed to give more insight into the behavior of the physical model, specially under wet soil conditions and high potential transpiration. The largely-used Feddes empirical root water uptake model performs well only under circumstances of low root length density R, that is for the scenarios of low root water uptake "compensation". From medium to hight R, the model can not mimic properly the root uptake dynamics as predicted by the physical model. The Jarvis model provides good predictions only for low and medium R scenarios. For high R, the model can not mimic the uptake patterns predicted by the physical model. Using our proposed reduction, that is the JMm model, helps to improve water uptake predictions. The proposed models are capable of predicting similar root water uptake patterns by the physical model. The statistical indices point them as the best alternatives to mimic root water uptake predictions by the physical model.

Keywords: Transpiration; Modeling; Optimization; Soil

2.1 Introduction

Determining the relation between plant transpiration and soil hydraulic conditions and how plants distribute water uptake over depth is a challenging subject. Its study is motivated by the importance of transpiration on global climate and crop growth (CHAHINE, 1992) as well as by the role root water uptake plays in soil water distribution (YU et al., 2007). The common modeling 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 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; VAN NOORDWIJK, 1987; HEINEN, 2001; RAATS, 2007; DE JONG VAN LIER et al., 2008; DE JONG VAN LIER et al., 2013).

In many one- and two-dimensional problems macroscopic root water uptake is modeled 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); Feddes, Kowalik and Zaradny (1978); Lai and Katul (2000); Li, De Jong and Boisvert (2001); Vrugt et al. (2001); Li et al. (2006)). Most of these models are derived from the Feddes, Kowalik and Zaradny (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; BLAKE; FARRELL, 1975; GREEN; CLOTHIER, 1995; GREEN; CLOTHIER, 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 the mechanism of root water uptake as a non-local process affected by non-uniform soil water distribution (JAVAUX et al., 2013). Accordingly, the 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 levels 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; LI et al., 2006; LAI; KATUL, 2000). These models have been incorporated into larger soil water flow models and tested at site-specific environments that promoted better estimates of model outcomes such as soil water content and plant transpiration (ex. Braud, Varado and Olioso (2005); Yadav, Mathur and Siebel (2009); Dong et al. (2010)). Comparisons with physically-based models (JARVIS, 2011; DE WILLIGEN et al., 2012) implicitly accounting for compensation have also stressed that models that do not account for compensation (like Feddes, Kowalik and Zaradny (1978)) are less accurate with respect to plant transpiration and soil water content estimates.

Recently, De Jong van Lier et al. (2013) developed an enhanced mechanistic model for predicting water potentials along the soil-root-leaf pathway, which allows prediction of water uptake and plant transpiration. This model was successfully incorporated into the eco-hydrological model SWAP (VAN DAM et al., 2008) by employing a piece-wise function between leaf pressure head and relative transpiration, which reduced the number of empirical parameters compared to other relations (ex. Fisher, Charles-Edwards and Ludlow (1981)). Besides soil hydraulic parameters and root geometry parameters, this new model requires information about root radial hydraulic conductivity, xylem axial conductance and a limiting leaf water potential, data that are often lacking, making it less attractive to be used in common field applications.

Empirical models are more readily used because of their relative simplicity and lower data requirements. On the other hand, their empirical parameters are not physically defined and their limitations in describing the mechanism of processes under varying environmental conditions are usually not well-established. Indeed, threshold values for the Feddes, Kowalik and Zaradny (1978) transpiration reduction function are provided in literature (TAYLOR; ASHCROFT, 1972; DOORENBOS; KASSAM, 1986) for some crops regarding some levels of transpiration demand. Nevertheless, experimental (DENMEAD; SHAW, 1962; ZUR et al., 1982) and theoretical (GARDNER, 1960; DE JONG VAN LIER; METSELAAR; VAN DAM, 2006) studies indicate that this parameter does not vary solely with crop type and atmospheric demand, but also with root system parameters and soil hydraulic properties. Moreover, parameters reported in literature usually refer to the fraction of available soil water that keeps plant transpiration at potential level, which does not in essence correspond to the parameter definition of these empirical models. Therefore, more precisely defined values for crops accounting for more environmental factors are necessary in order to apply these models in wider 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 water uptake distribution under varying environmental conditions performed in numerical experiments with a detailed physical model (DE JONG VAN LIER et al., 2013). The detailed physical model accounts for resistances from the soil to plant leaf. We first review some empirical models that have been used as sub-models in ecohydrological models and suggest some alternative empirical models. The parameters of the empirical models are determined by inverse modeling of simulated depth-dependent root water uptake. In this way it becomes clear to which extent the empirical models can mimic the dynamic patterns of root water uptake.

2.2 Theory

Root water uptake and plant transpiration are directly linked through the continuity principle for water flow in the soil-plant-atmosphere pathway:

$$T_a = \int_{z_m} S(z)dz \tag{2.1}$$

where T_a (L) is the plant transpiration and S ($L^3L^3T^{-1}$) is the root water uptake, dependent on plant properties and soil hydraulic conditions, a function of soil depth z (L), and z_m (L) the maximum rooting depth. Eq. (2.1) 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; KLEPPER, 1978).

In a macroscopic modeling approach, root water uptake is calculated as a sink term S in the Richards equation, which for the vertical coordinate is given by:

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z}\left[K(\theta)\Big(\frac{\partial h}{\partial z} + 1\Big)\right] - S \tag{2.2}$$

where θ (L^3 L^{-3}) is the soil water content, h (L) the soil water pressure head, K (L T^{-1}) the soil hydraulic conductivity, t (T) the time and z (L) the vertical coordinate (positive upward). To apply eq. (2.2), an expression for S is needed. Physical expressions in analogy to Ohm's law have been suggested (see the review of Molz (1981) for some examples) as well as expressions derived by upscaling microscopic models (DE WILLIGEN; VAN NOORDWIJK, 1987; FEDDES; RAATS, 2004; DE JONG VAN LIER et al., 2008; DE JONG VAN LIER et al., 2013). Alternatively, simple empirical models requiring less information on 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; FEDDES; KOWALIK; ZARADNY, 1978), which can be formulated as:

$$S(z) = S_p(z)\alpha(h[z]) \tag{2.3}$$

where $\alpha(h)$ is the root water uptake reduction function, defined by Feddes, Kowalik and Zaradny (1978) as a piece-wise linear function of h (Fig. 2.1). According to this approach, a reduction in S due to $\alpha(h[z]) < 0$ directly implies a transpiration reduction, making $\alpha(h)$ to be called a transpiration reduction function. S_p is the potential root water uptake, which is determined by partitioning potential transpiration T_p along depth. Several ways to estimate S_p have been proposed (PRASAD, 1988; LI; DE JONG; BOISVERT, 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^3L^{-3}):

$$S_p(z) = \frac{R(z)}{\displaystyle\int_{z_m} R(z)dz} T_p = \beta(z)T_p \tag{2.4}$$

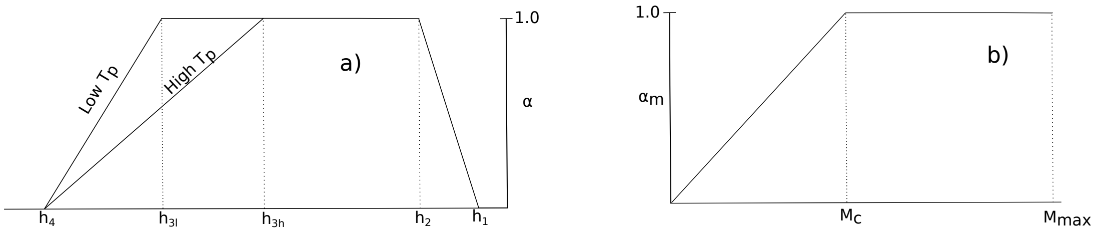

Figure 2.1 - a) Feddes, Kowalik and Zaradny (1978) root water uptake reduction function. h_2 and h_3 are the threshold parameters for reduction in root water uptake due to oxygen deficit and water deficit, respectively. The subscripts l and h stands for low and high potential transpiration T_p. h_1 and h_4 are the soil pressure head values below and above which root water uptake is zero due to oxygen and water deficit, respectively. b) Root water uptake reduction function α_m as a function of matric flux potential M; M_c is the critical value of M from which the uptake is reduced and M_{max} is the maximum value of M, dependent on soil type

where β (L^{-1}) is the normalized root length density.

Different functions to calculate α have been suggested, normally considering α a function of θ (ex. Lai and Katul (2000); Jarvis (1989)) or h (ex. Feddes, Kowalik and Zaradny (1978)) or a combination of both (LI et al., 2006). Using h seems to be more feasible because of its relation to soil water energy and the fact that obtained parameter of such a function would be more likely to be applicable to different soils. Some reduction functions use effective saturation. Parameter values for these functions can be used for any kind of soil by means of the soil water retention curve. These types of reduction functions are generally associated to reservoir models for soil water balance. Regarding the shape of the reduction curve, they can be smooth non-linear 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 water uptake (or plant transpiration) is reduced due to soil moisture 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 α is linearly related nor to soil water content neither to pressure head either. A linear relation to the matric flux potential M, a composite soil hydraulic function defined in eq. (2.5), is physically more plausible.

$$M = \int_{h_w}^{h} K(h)\, dh \tag{2.5}$$

where h_w is the soil pressure head at wilting point. Experimental confirmation was found by Casaroli, De Jong Van Lier and Dourado Neto (2010). Therefore, a more suitable expression for α would be a piece-wise linear function of M (Fig. 2.1). Root water uptake can then be calculated by the Feddes model (eq. (2.3)) by replacing its reduction function by the alternative illustrated in Fig. 2.1.

2.2.1 Physically based root water uptake model

By upscaling earlier findings (DE JONG VAN LIER; METSELAAR; VAN DAM, 2006; METSELAAR; 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:

$$S(z) = \rho(z)(M(z) - M_0) \tag{2.6}$$

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

$$\rho(z) = \frac{4}{r_0^2 - a^2 r_m^2(z) + 2[r_m^2(z) + r_0^2]\ln[a r_m(z)/r_0]} \tag{2.7}$$

where $r_m (= \sqrt{1/\pi R})$ (L) is the rhizosphere radius — defined as the half distance between neighboring roots— and a the relative distance from r_0 to r_m where water content equals bulk 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 plant leaf), assuming no water changes within the plant tissue and by coupling eq. (2.6) for water flow within the rhizosphere, they derived the following expression relating water potentials and T_a:

$$h_0(z) = h_l + \varphi(M_s(z) - M_0(z)) + \frac{T_a}{L_l} \tag{2.8}$$

where L_l (T^{-1}) is the overall conductance over the root-to-leaf pathway and h_l (L) the leaf pressure head. Notice that S can be calculated by eq. (2.6) upon solving eq. (2.8). φ (T L^{-1}) is defined as:

$$\varphi(z) = \frac{\rho r_m^2(z) \ln \frac{r_0}{r_x}}{2K_{root}} \tag{2.9}$$

where K_{root} (L T^{-1}) is the radial root tissue conductivity (from root surface to root xylem) and r_x (L) the xylem radius. T_a is a function of h_l, which was defined piece-wisely by imposing a limiting value h_w on h_l:

$$T_r = \begin{cases} 1 & : h_l > h_w \\ 0 \leq T_r \leq 1 & : h_l = h_w \\ 0 & : h_l < h_w \end{cases} \tag{2.10}$$

where T_r $(= T_a/T_p)$ is the relative plant transpiration. Plant water stress, a condition for which $T_a < T_p$, is defined at the plant level (TARDIEU, 1996) and onsets when $h_l = h_w$. Because T_a and h_l are unknowns, eq. (2.8) and (2.10) can not be solved analytically, but an efficient numerical algorithm is described in De Jong van Lier et al. (2013).

Fig. 2.2 helps understanding how water uptake is distributed over depth. h_l can be regarded as a plant level measure of water deficit stress over the whole root zone: as soil gets drier, h_l is reduced, which increases the driving force for water uptake (see water uptake for the several values of h_l in Fig. 2.2). As soil pressure head h_s decreases, high uptakes are only achieved by lower h_l. For a certain h_l value, water uptake is substantially reduced as h_s decreases. If h_l is not reduced as h_s gets lower, S becomes negative (negative S is not shown in Fig. 2.2, but it is part of an extension of each curve) and water will flow from root to soil. This may happen in a case when some parts of the root zone are wetter and uptake from these parts satisfies transpiration demand, and h_l is not reduced.

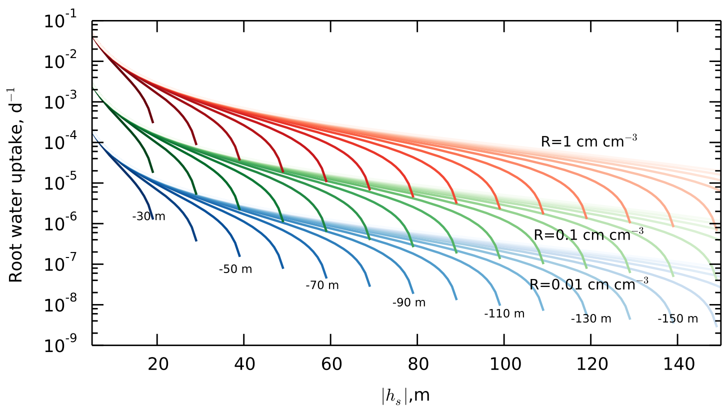

Figure 2.2 - Root water uptake as a function of soil pressure head h for three values of root length density (0.01, 0.1 and 1.0 cm cm^{-3}) and leaf pressure head values ranging from -30 to -200 m by -10 m interval shown by colors gradient (lighter colors indicate lower values and some values are also indicated in the plot). These results were obtained by the analytical solution of eq. (2.8) 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^{-1} and the soil and plat hydraulic parameters were taken from De Jong van Lier et al. (2013)

Fig. 2.2 also shows that root water uptake is sensitive to both R and h_s, and that it can be locally balanced by the amount of roots and soil water content. Under homogeneous soil water distribution, water uptake is partitioned proportional to R. For non-homogeneous conditions, water uptake for lower R can be the same as for higher R depending on the stress level (indicated by h_l) and the h_s (see Fig .2.2). This is in agreement with experimental results reported by several authors (ARYA; BLAKE; FARRELL, 1975; ARYA et al., 1975; GREEN; CLOTHIER, 1995; VERMA et al., 2014) who found less densely-rooted but wetter parts of the root zone to be corresponding to a significant part of uptake when more densely-rooted parts of the soil are drier, allowing the plant to maintain transpiration at potential rates. Due to empirical model concepts that only use R for distributing uptake over depth (for non-stressed conditions), these results have been interpreted as due to a mechanism labeled “compensation” by which uptake is “increased” from wetter layers to compensate the “reduction” in the drier layers (JARVIS, 1989; SIMUNEK; HOPMANS, 2009). Clearly, this compensation concept is based on a reference uptake distribution (i.e. the one provided by R distribution) and is only important in empirical models. In physical models, discriminating compensation becomes less important since in such models it is an implicit part of the root water uptake mechanism.

In order to account for root water uptake pattern changes due to heterogeneous soil water distribution, i.e. compensation, several empirical models have been developed over the years. These models follow the general framework of the Feddes, Kowalik and Zaradny (1978) equation given by eq. (2.3)). Below we review these and present a new empirical alternative.

2.2.2 Empirical root water uptake models accounting for compensation

2.2.2.1 The Jarvis (1989) model

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

$$\omega = \int_{z_m} \alpha(z)\beta(z)dz. \tag{2.11}$$

where, differently from Feddes, Kowalik and Zaradny (1978), α was defined as a function of the effective saturation. In principle, any definition of α is applicable in eq. (2.11), and in this paper we will refer to the Feddes, Kowalik and Zaradny (1978) reduction function unless mentioned. Whereas Feddes, Kowalik and Zaradny (1978) assume the root water uptake reduction directly to reflect in plant transpiration reduction, the Jarvis (1989) approach employs a so-called “whole-plant stress function” given by:

$$\frac{T_a}{T_p} = \min\left\{1, \frac{\omega}{\omega_c}\right\} \tag{2.12}$$

where ω_c is a threshold value of ω for the transpiration reduction. Substituting eq. (2.3) and (2.4) into eq. (2.1) (the continuity principle) and combining to eq. (2.12), results in:

$$S(z) = S_p\alpha(z)\alpha_2, \text{ where } \alpha_2 = \frac{1}{\max\left\{\omega, \omega_c\right\}} \tag{2.13}$$

where α_2 is called the compensation factor of root water uptake, distinct from the Feddes model (eq. (2.3)) and which can be derived by defining T_a by eq. (2.12). In the Jarvis (1989) model, α accounts for local reduction of root water uptake and transpiration reduction is computed by eq. (2.12). When $\omega = 1$, there is no water uptake 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 water uptake over the whole root zone by the factor α_2. When $\omega < \omega_c$, the uptake is still increased by the factor α_2 but the potential transpiration rate can not be met. The threshold value ω_c places a limit on the plant's ability to deal with soil water stress. When ω_c tends to zero, eq. (2.12) tends to 1, and the plant can fully compensate uptake and transpire at the potential rate provided that at least somewhere in the root zone $\alpha > 0$.

An analogy to stomata functioning is described by eq. (2.12) (JARVIS, 1989; JARVIS, 2011), putting this model in a more physical context. However, operational and physical limitations of this model have been raised (SKAGGS et al., 2006; JAVAUX et al., 2013). A new parameter (ω_c) is introduced, which should be determined by inverse modeling and is dependent on atmospheric demand, rooting properties (usually related to root length density) and soil type. Another difficulty is the conceptual limitation raised by Skaggs et al. (2006). In a clear example they showed that the model does not mimic properly compensation and it affronts the definition of α, which can be noticed by analyzing eq. (2.13): root water uptake is reduced by α, but increased by the factor $1/\max[\omega, \omega_c]$, making the meaning of α unclear. Another limitation is the of linking compensation to plant stress, making it to fail in predicting compensation under wet condition with a heterogeneous soil pressure head distribution (JAVAUX et al., 2013).

Using the linear piece-wise Feddes reduction for α, care must be taken in setting up and interpreting the threshold parameters of this function. The Feddes, Kowalik and Zaradny (1978) model does not account for compensation, and the threshold pressure head value below which root water uptake 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. In the Jarvis models, 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 Jarvis (1989) model is higher than the equivalent in the Feddes model. In that sense, h_3 for the Jarvis (1989) model is hard to determine experimentally. Inverse modeling by optimizing outcomes of soil water flow models with measured values of field experiments is an option.

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

The Jarvis (1989) model was shown to be "numerically" identical to De Jong van Lier et al. (2008) physical model, but only under limiting hydraulic conditions (JARVIS, 2010; JARVIS, 2011). We briefly review this similarity and its implications on the empirical concept of the Jarvis (1989) model.

De Jong Van Lier, Metselaar and Van Dam (2006) derived eq. (2.6) for describing root water uptake. Plant transpiration is obtained by integrating eq. (2.6) over z_m as defined in eq. (2.1), leaving two unknowns: M_0 and T_a. In order to solve for these, De Jong van Lier et al. (2008) defined T_a as a piecewise function as follows:

$$\frac{T_a}{T_p} = \min\left\{1, \frac{\mathrm{T_{p_{max}}}}{\mathrm{T_p}}\right\} \tag{2.14}$$

where $T_{p_{\max}}$ (L T^{-1}) is the maximum possible transpiration rate attained when $M_0 = 0$, given by:

$$T_{p_{\max}} = \int_{z_m} \rho(z) M(z)\, dz. \tag{2.15}$$

From eq. (2.14) when $T_{p_{\max}} < T_p$, drought stress occurs and $T_a = T_{p_{\max}}$. In this situation, pressure head at the root surface reaches $h_w \rightarrow M_0 = 0$ and $S(z)$ becomes:

$$S(z) = \rho(z) M(z). \tag{2.16}$$

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

$$M_0 = \frac{\int_{z_m} \rho(z) M(z) dz \; - T_p}{\int_{z_m} \rho(z) dz} \tag{2.17}$$

Jarvis (2011) observed the similarities between eq. (2.14) and (2.12) of the models. Notice also the algebraic similarity between ω (eq. (2.11)) and $T_{p_{\max}}$ (eq. (2.15)). Thus, Jarvis (2010) showed that both models provide the same results for the stressed phase if α and $\beta(z)$ are defined as follows:

$$\alpha = \frac{M}{M_{max}} \tag{2.18}$$

$$\beta = \frac{\rho(z)}{\displaystyle\int_{z_m} \rho(z) dz} \tag{2.19}$$

where M_{max} is the maximum value of M(i.e., at $h = 0$). By substituting eq. (2.18) and (2.19) into eq. (2.15) and comparing eq. (2.12) with eq. (2.14), ω_c is found to be equal to:

$$\omega_c = \frac{T_p}{M_{max} \int_{z_m} \rho(z)\, dz} \tag{2.20}$$

Substitution of eq. (2.18) to (2.20) into eq. (2.12) and (2.11) results in eq. (2.16) of De Jong van Lier et al. (2008) model for stressed condition. Consequently, both models provide the same numerical results. For unstressed condition, the same substitution results in:

$$S(z) = \rho(z)M(z)\frac{T_p}{T_{p_{max}}} = \frac{\rho(z)M(z)}{\int_{z_m} \rho(z)M(z)\, dz} T_p \tag{2.21}$$

Eq. (2.21) is different from eq. (2.6) and the models can not be correlated for these conditions. The Jarvis (1989) model predicts root water uptake by a weighting factor between ρ and M throughout rooting depth. This comparison shows that the only shared similarity between Jarvis (1989) and De Jong van Lier et al. (2008) model is the way of defining plant transpiration. Jarvis (1989) applied the concept of transpiration to the empirical Feddes, Kowalik and Zaradny (1978) model, whereas De Jong van Lier et al. (2008) applied it to an upscaled single-root expression for water uptake. Defining α and β by eq. (2.18) and (2.19), respectively, allowed to correlate both models only for stressed conditions. These definitions and the resulting model will be further analyzed.

2.2.2.3 The Li, De Jong and Boisvert (2001) model

Li, De Jong and Boisvert (2001) proposed to distribute potential transpiration over the root zone by a weighted stress index ζ, being a function of both root distribution and soil water availability:

$$\zeta(z) = \frac{\alpha(z)R(z)^{\lambda}}{\int_{z_m} \alpha(z)R(z)^{\lambda} dz} \tag{2.22}$$

where α (-) and R (L L^{-3}) were previously defined and the exponent λ is an empirical factor that defines the shape of root water distribution over depth. The smaller λ, the more water is taken up in deeper soil layers. Thus, S_p is given by:

$$S_p = \zeta(z)T_p \tag{2.23}$$

and root water uptake is calculated by substituting eq. (2.23) into (2.3), following the Feddes approach.

Defining S_p 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. (2.22). However, the choice of α to represent soil water availability in eq. (2.22) does not mimic properly the compensation mechanism. Compensation takes place before transpiration reduction. Using α in eq. (2.22) means that compensation will only take place after the onset of transpiration reduction when α in one or more layers is less than unity. The λ parameter may also be interpreted as to accounts for compensation under non-stressed condition. Compensation, however, and shape of root water uptake distribution constantly changes as soil dries. A constant λ can not account for that.

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

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

$$\zeta(z) = \frac{\mathit{\Gamma}(z)R(z)}{\displaystyle\int_{z_m} \mathit{\Gamma}(z)R(z)dz} \tag{2.24}$$

where $\mathit{\Gamma}$ is a soil hydraulic function to account for water availability. Molz and Remson (1970) used soil water diffusivity D ($\mathrm{L^2T^{-1}}$), and Selim and Iskandar (1978) used soil hydraulic conductivity K ($\mathrm{LT^{-1}}$) for $\mathit{\Gamma}$ in eq. (2.24). Root water uptake is then calculated by substituting eq. (2.24) into eq. (2.23) and then into eq. (2.3) following the Feddes approach.

These models may better represent root water uptake and compensation than the Li, De Jong and Boisvert (2001) model. The compensation is implicitly accounted for by means of $\mathit{\Gamma}$ in ζ. In drier soil layers, $\mathit{\Gamma}$ is reduced, whereas in wetter soil layers $\mathit{\Gamma}$ is increased, thus increasing root water uptake in these layers before the onset of transpiration reduction. Heinen (2014) compared different types of $\mathit{\Gamma}$ in eq. (2.24) 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 $\mathit{\Gamma}$ provides very different patterns of root water uptake, but did not indicate a preference for a specific one.

2.2.3.4 Proposed empirical model

In describing soil water availability, matric flux potential M may be a better choice than K or D, since it integrates K and h together (or D and θ). The exponent λ can also provide flexibility on distribution of T_P over depth as was shown by Li, De Jong and Boisvert (2001). Therefore, we propose a new weighted stress index, defined as:

$$\zeta(z) = \frac{R^{\lambda} M(h)}{\displaystyle\int_{z_m} R^{\lambda} M(h) dz} \tag{2.25}$$

2.3 Material and Methods

Table 2.1 summarizes the empirical root water uptake (RWU) models evaluated in this study. They all follow the basic Feddes model (eq. (2.3)), diverging only on how RWU is partitioned over rooting depth or how α is defined. In each model, except in Jarvis (2010), we made a simple modification by changing the Feddes reduction function for the proposed reduction function (Fig. 2.1), and these modified versions were also evaluated. The threshold values of Feddes, Kowalik and Zaradny (1978) reduction function for anoxic conditions (h_1 and h_2) were set to zero. The value parameter h_4 was set to -150 m. The other parameters of the models were obtained by optimization as described in Section 2.3.2.

Table 2.1 - Summary of empirical models used. α_f and α_p are the Feddes, Kowalik and Zaradny (1978) (Fig. 2.1) and proposed reduction functions (Fig. 2.1), S_p (eq. 4) is the potential root water uptake, ω (eq. 11) and ω_c are the weighted stress index and threshold value in Jarvis (1989) model and ζ_m (eq. 25) is the weighted stress index in the proposed models

Model	Acronym	Equation
Feddes, Kowalik and Zaradny (1978) model	FM	$S(z) = S_p\alpha_f$
Modified Feddes, Kowalik and Zaradny (1978) model	FMm	$S(z) = S_p\alpha_p$
Jarvis (1989) model	JM	$S(z) = S_p\frac{\alpha_f}{\max\{\omega,\omega_c\}}$
Modified Jarvis (1989) model	JMm	$S(z) = S_p\frac{\alpha_p}{\max\{\omega,\omega_c\}}$
Jarvis (2010) model	JMII	Eq. (2.11) to (2.13) with parameters given by eq. (2.18) to (2.20)
proposed model I	PM	$S(z) = \zeta_m T_p \alpha_f$
proposed model II	PMm	$S(z) = \zeta_m T_p \alpha_p$

All these models were embedded as sub-models into the ecohydrological model SWAP (VAN DAM et al., 2008) in order to solve eq. (2.2) and to apply it for all kind of soil water flow conditions. Different scenarios of root length density, atmospheric demand and soil type (described in Section 2.3.1) were set up in order to analyze the behavior and sensitivity of the models. Simulation results of SWAP in combination with each of the

RWU models were compared to the SWAP predictions when combined to the physical RWU model developed by De Jong van Lier et al. (2013). Differences in predictions are caused by the respective RWU model and will be referred to as such.

The values of the De Jong van Lier et al. (2013) model parameters used in the simulations are listed in Table 2.2. The value of K_{root} and L_l is within the range reported by De Jong van Lier et al. (2013).

Table 2.2 - 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}	$3.5 \cdot 10^{-8}$	m d^{-1}
L_l	$1 \cdot 10^{-6}$	d^{-1}
h_w	-200	m

2.3.1 Simulation scenarios

2.3.1.1 Drying-out simulation

Boundary conditions for these simulations were no rain/irrigation and a constant atmospheric demand over time. The simulation continued until simulated plant transpiration by the physical RWU model approached zero. Soil evaporation was set to zero making the soil to dry out only due to root water uptake or drainage at the bottom. Free drainage (unit hydraulic gradient) at the maximum rooting depth was the bottom boundary condition. The soil was initially in 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: 1 and 5 mm d^{-1}. We also considered three types of soil and three levels of root length density, described in the next paragraphs.

Soil type

Soil date for three top soils from the Dutch Staring series Wösten et al. (1999) were used. The physical properties of these soils, described by the Mualem-van Genuchten functions (MUALEM, 1976; VAN GENUCHTEN, 1980) for the $K - \theta - h$ relations, are listed in Table 2.3. These soils are identified in this text as clay, loam and sand (Table 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^{-3}, respectively. For all cases, we

Table 2.3 - Mualem-van Genuchten parameters for three soils of the Dutch Staring series Wösten et al. (1999) used in simulations. θ_s and θ_r are the saturated and residual water content, respectively; K_s is saturated hydraulic conductivity and α, λ and n are fitting parameters

Staring soil ID	Textural class	θ_r	θ_r	K_s	α	λ	n
		m m^{-3}	m m^{-3}	m d^{-1}	m^{-1}	-	-
B3	Sand	0.02	0.46	0.1542	1.44	-0.215	1.534
B11	Clay	0.01	0.59	0.0453	1.95	-5.901	1.109
B13	Loam	0.01	0.42	0.1298	0.84	-1.497	1.441

set the maximum rooting depth z_{max} equal to 0.5 m. Root length density over depth z was described by the exponential function:

$$R(z_r) = R_0(1 - z_r)\exp^{-bz_r} \tag{2.26}$$

where R_0 (L L^{-3}) 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. (2.26) 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 $\bar{R}$ is usually reported in the literature. Assuming R of such a crop given by eq. (2.26), it can be shown that:

$$\int_0^1 R_0(1 - z_r)\exp^{-bz_r}\ dz_r = \bar{R} \tag{2.27}$$

Solving eq. (2.27) for R_0 and substituting into eq. (2.26) gives:

$$R(z_r) = \frac{b^2\bar{R}}{b + \exp^{-b} - 1}(1 - z_r)\exp^{-bz_r} \qquad (b > 0) \tag{2.28}$$

Fig. 2.3 shows $R(z_r)$ calculated from eq. (2.28) for different values of b and $\bar{R} = 1$ cm cm^{-3}. As b approaches to zero, eq. (2.28) tends to be linear, however it is not defined for $b = 0$. In our simulations b was set equal to 2.0.

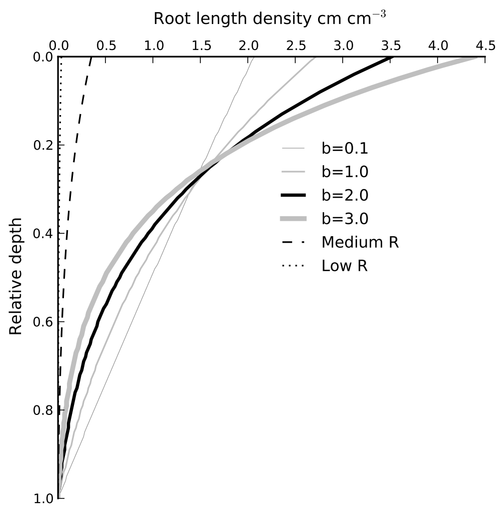

Figure 2.3 - Root length density distribution over depth calculated by eq. (2.28) for several values of b and $R_L = 1.0$ cm cm^{-3} and for low and medium R with $b = 2$

2.3.2 Optimization

The parameters of the empirical root water uptake models were estimated by solving the following constrained optimization problem:

$$\begin{aligned} &\text{minimize} \quad \Phi(\mathbf{p}) = \sum_{\mathrm{i=1}}^{\mathrm{n}} \sum_{\mathrm{j=1}}^{\mathrm{m}} [\mathrm{S}^{*}_{\mathrm{i,j}} - \mathrm{S}_{\mathrm{i,j}}(\mathbf{p})]^2 \\ &\text{subject to} \quad \mathbf{p} \in \Omega \end{aligned} \tag{2.29}$$

where $\Phi(\mathbf{p})$ is the objective function to be optimized, $S^{*}_{i,j}$ is the RWU simulated by SWAP model together with the De Jong van Lier et al. (2013) model at time i and depth j and $S_{i,j}(\mathbf{p})$ is the corresponding RWU predicted by SWAP in combination with one of the empirical models shown Table 2.1. $\mathbf{p}$ is the model parameter vector to be optimized, constrained in the domain Ω. Both $\mathbf{p}$ and Ω vary depending on the empirical RWU model used. Table 2.4 shows the parameters of each empirical RWU model that were optimized and their respective constraints Ω. m and n are the number of soil layers and days of the simulation, respectively. The Jarvis (2010) model has no empirical parameters and therefore requires no optimization.

Table 2.4 - Parameters of the root water uptake models estimated by optimization and their respective constraints Ω

Model	Parameter	Ω	Unit
FM	h_3	$-150 < h_3 < 0$	m
FMm	M_c	$0 < M_c < M_{max}$ †	$m^2\ d^{-1}$
JM	h_3	$-150 < h_3 < 0$	m
	ω_c	$0 < \omega_c \leq 1$	-
JMm	M_c	$0 < M_c < M_{max}$ †	$m^2\ d^{-1}$
	ω_c	$0 < \omega_c \leq 1$	-
PEM	h_3	$-150 < h_3 < 0$	m
	l_m	$0 < l_m \leq 1$	-
PEMm	M_c	$0 < M_c < M_{max}$ †	$m^2\ d^{-1}$
	l_m	$0 < l_m \leq 1$	-

Eq. (2.29) was solved by using the PEST (Parameter ESTimation) tool (DOHERTY; BREBBER; WHYTE, 2005) coupled to our versions of SWAP. PEST is a non-linear parameter estimation program that solves eq. (2.29) 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 $\mathbf{p}$ and assessed the ability of PEST to retrieving $\mathbf{p}$. These reference runs served to set up properly PEST for our case. For high non-linear problems as the one in eq. (2.29) GLM depends on the initial values of **b**. We used five sets of initial values for **p** in order to guarantee that GLM found the global minimum and also to check the uniqueness of the solution.

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

2.3.3 Growing season simulation

The models were evaluated by simulating a whole year growing season experiment with real weather data (KNMI Royal Dutch Meteorological Institute, www.knmi.nl) from De Bilt weather station — the Netherlands — 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. (2.28) ($b = 2.0$) down to 50 cm. We also performed simulations for the same three types of soils and root length densities, but 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; PEREIRA; RAES,). Potential evapotranspiration ET_p is obtained by multiplying ET_0 by a crop factor set to 1. ET_p was partitioned into potential evaporation E_p and T_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^{-1} and was linearly interpolated for levels of T_p in between. For $T_p > 5$ mm d^{-1} or $T_p < 1$ mm d^{-1}, the values estimated for these corresponding T_p levels 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 staring with the final pressure heads of the previous simulation until convergence.

2.4 Results

2.4.1 Drying-out simulation

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

In this section, we first focus on the behavior of the De Jong van Lier et al. (2013) model in predicting RWU for the evaluated scenarios in the drying-out experiment. Fig. 2.4 shows the water uptake patterns for the case of the clay soil, 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 of roots in deeper layers is not sufficient to supply high water uptake rates. When the upper layers become drier, transpiration reduction is immediate. 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 at potential rates for more time (see Fig. 2.4). Accordingly, the plant exploits the whole root zone and little water is left when transpiration reduction onsets, causing a sudden drop in transpiration curve. Regarding T_p, the RWU patterns are very similar for both evaluated rates, differing only on time scale: for high T_p the onset of transpiration reduction and the shift in RWU front occur earlier. The patterns for sand and loam soil (not shown here) show very similar features.

The leaf pressure head h_l over time shown in Fig. 2.4 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 and thus maintaining water uptake corresponding to the potential demands. As a consequence, uptake in wetter layers become more important. Transpiration reduction only onsets when h_l reaches the limiting leaf pressure head h_w ($= -200$ m), after significant changes in the RWU patterns, characterized by increased uptake in deeper layers.

For the high T_p–low R scenarios, transpiration reduction onsets 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 attend the

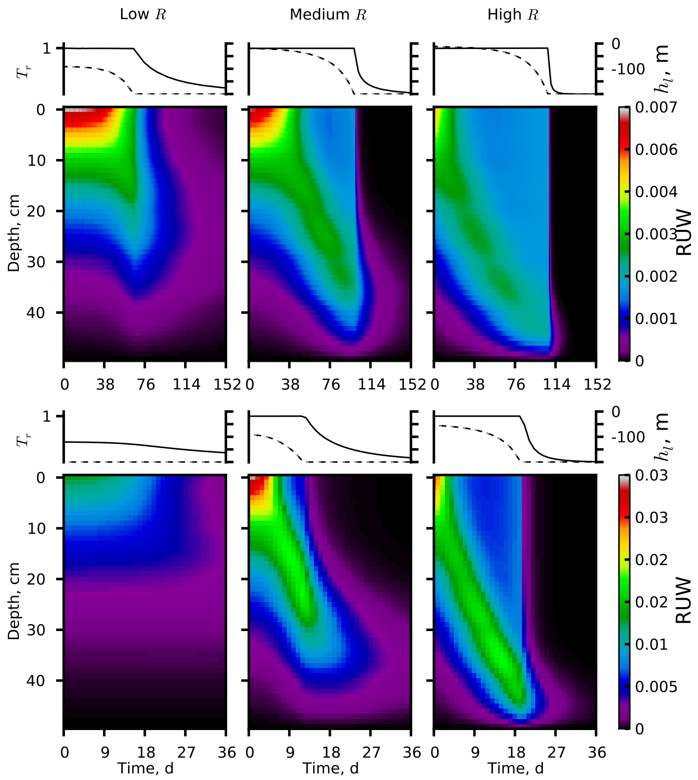

Figure 2.4 - Time-depth root water uptake (RWU) pattern, leaf pressure head (h_l, dashed line) and relative transpiration (T_r, continuous line) simulated by SWAP model together with the De Jong van Lier et al. (2013) model for clay soil, two levels of potential transpiration: 1 and 5mm d^{-1} (first 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)

atmospheric demand can not be supported by such a root system with a low R and hydraulic parameters given in Table 2.2. Higher atmospheric demand (here represented by T_p) increases the reduction of h_l caused by the hydraulic resistance to water flow within the plant, and the transpiration rate (so as water uptake) is a function of h_l. The physical model assumes a parsimonious relationship (eq.(2.10)) between transpiration and h_l: transpiration rate is only reduced when h_l reaches a limiting value h_w, 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 only root system properties and plant hydraulic parameters (Table 2.2). Fig 2.5 shows $T_{p,max}$ as a function of K_{root} for some values of L_l with constant soil pressure head over root zone equals to -1 m for the low R in the sandy soil. It can be seen that K_{root} is limiting the plant transpiration and that L_l becomes important only for higher K_{root}. The potential transpiration can be achieved by

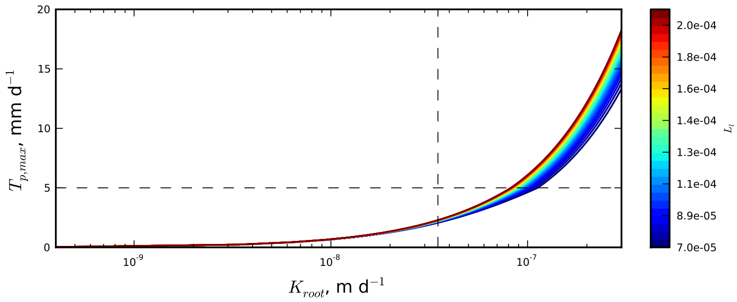

Figure 2.5 - Maximum possible transpiration $T_{p,max}$ as a function of root hydraulic conductivity K_{root} for some values of the overall conductance over the root-to-leaf pathway L_l computed by De Jong van Lier et al. (2013) model for low root length density and constant soil pressure head over depth equals to -1 m for sandy soil. The dashed vertical line highlights the value of $K_{root} = 3.5\ 10^{-8}$ m d^{-1} that was used in our simulations. Horizontal dashed line highlights the value of potential transpiration

raising K_{root} up to about 10 $^{-7}$ m d^{-1}. This can also be achieved by decreasing h_w (not shown in Fig. 2.5).

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 plant with a low R may not be able to realize high potential transpiration. Furthermore, plant 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 very complex and depends on other several environmental factors such as air temperature, solar radiation and CO_2 concentration. Thus, 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, Perrier and Leuning (2003) model.

2.4.1.2 Root water uptake pattern predicted by the empirical models

In this section, we evaluate the empirical RWU models (the models and their abbreviations are listed in Table 2.1) based on the comparison of RWU patterns and transpiration reduction over time with the respective predictions from De Jong van Lier et al. (2013) model (VLM). All the empirical model predictions are performed with their optimized parameters shown in Table 2.5 (which are discussed in Section 2.4.1.4), 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. 2.6 and 2.7 for low and high T_p , respectively.

Both versions of Feddes model (FM and FMm) predicted enhanced water uptake from the upper soil layers. When the 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 α_f and α_m are less than 1), the predicted RWU patterns by the models become different (Fig. 2.6 and 2.7).

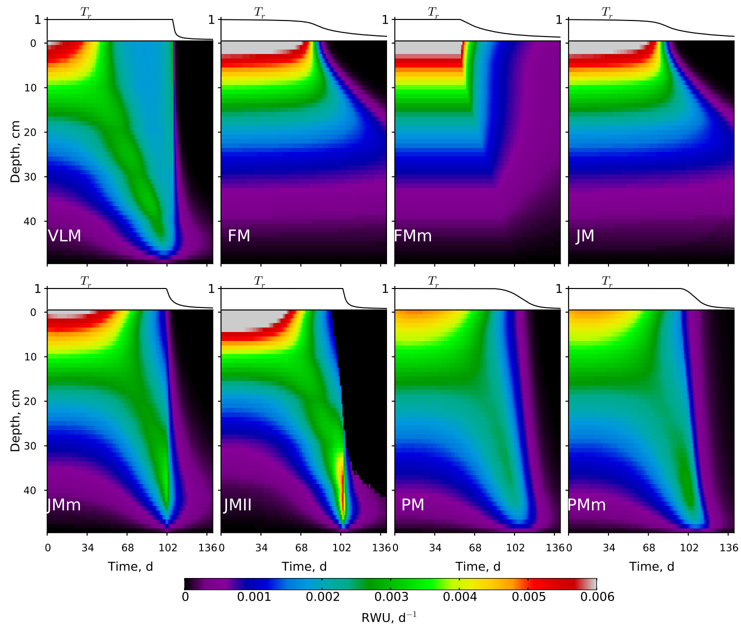

Figure 2.6 - Time-depth root water uptake (RWU) pattern and relative transpiration (T_r) simulated by SWAP model together with De Jong van Lier et al. (2013) sink and the others empirical models for sandy soil texture, high root length density and $T_p = 1$ mm d^{-1}

After a period of reduced water uptake, the length of which depends on R, T_p and h_3, water uptake 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 2.8). α_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, Dourado Neto and Metselaar (2009). Thus, α_m is sharply reduced after $M > M_c$, causing substantial reduction in water uptake even when h is slightly below the threshold value. Therefore, water uptake proceeds at low rates for longer time. Conversely, due to the linear shape of α_f, water uptake predicted by FM remains higher for a longer time after $h < h_3$. Therefore, there is no abrupt change in RWU patterns, especially at low T_p as shown in

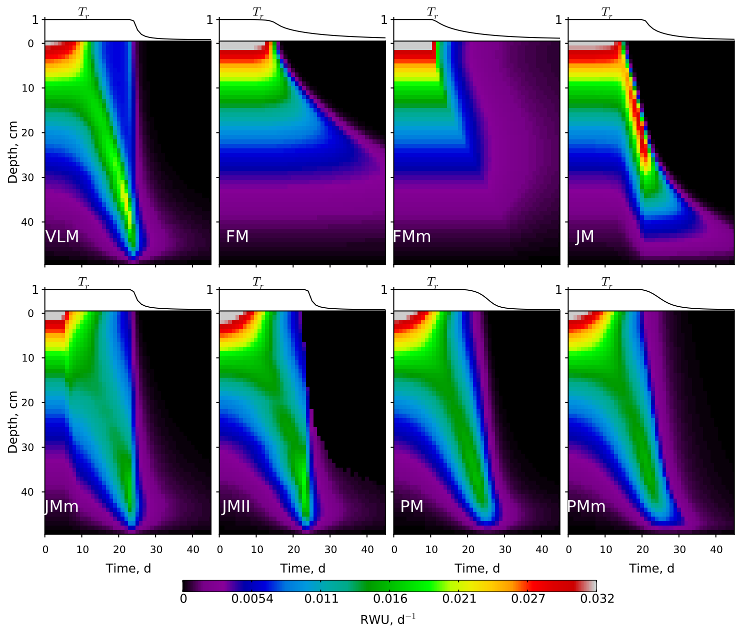

Figure 2.7 - Time-depth root water uptake (RWU) pattern and relative transpiration (T_r) simulated by SWAP model together with De Jong van Lier et al. (2013) sink and the others empirical models for sandy soil texture, high root length density and $T_p = 5$ mm d^{-1}

Fig 2.6. When h comes close to h_4, α_f is still relatively high and soil water depleted, making h to rapidly approach h_4. Another diverging feature between α_f and α_m, also shown in Fig 2.8, is that the shape of α_m varies with soil type (regardless the value of its threshold parameter M_c), whereas α_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 curve over time only slightly, but RWU patterns are strongly affected (Fig 2.6 and 2.7).

The RWU patterns predicted by JM and JMm models can be very different, as shown by Fig 2.6 for the high R–low T_p scenario. In fact, the JM model did not predict any compensation at all because the optimal ω_c was equal to unity (Table 2.5) — thus becoming identical to FM — and the optimal h_3 for JM and FM were similar. In these high R–low T_p scenarios with a high R in deep soil layers allowing water uptake at higher rates when surface soil layers becomes drier (as predicted by VLM), any attempt to reduce ω_c in order to JM predict compensation makes JM's RWU pattern to deviate even more from the VLM pattern. This is illustrated in Fig 2.6 and by the optimal h_3 and ω_c values shown in Table 2.5. The optimal h_3 for all soil types in this scenario was equal or close to zero to become as close as possible to the VLM uptake pattern. Decreasing h_3 or ω_c in order to compute compensation makes JM predict higher uptake from upper layers, increasing the discrepancy between the models. The optimal ω_c for all soil types was equal to 1 (in other words: meaning no compensation). Water uptake in the upper layers predicted by VLM is substantially reduced within a few days, whereas reducing ω_c in JM model to predict compensation causes also an increase of uptake in upper layers. The model, therefore, can not be calibrated for the high compensation scenarios evaluated here. Conversely, the JMm was able to reproduce considerably well VLM pattern for this scenario due to the shape of α_m as discussed above. As soon as $M > M_c$ at the upper layers, water uptake decreases at a higher rate, which is compensated by increasing uptake from the wetter, deeper layers. This agrees more closely to VLM predictions.

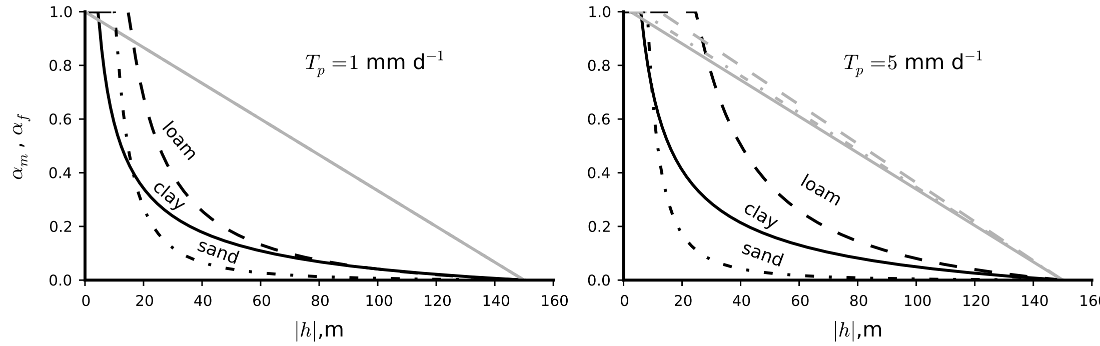

Figure 2.8 - The Feddes, Kowalik and Zaradny (1978) (α_f, gray lines) and proposed (α_m, black lines) water uptake reduction functions as a function of soil pressure head h using their respective optimized parameters for the scenario of high root length density, three types of soil and two potential transpiration levels

For high T_p (Fig 2.7), the JM model can predict compensation ($\omega_c < 1$), however its predicted water uptake pattern is very different from JMm and VLM. JM predicts a higher water uptake near the soil surface for a longer time than the other models that account for compensation. This makes soil water depletion to be more intense and water uptake 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 ω_c (= 0.19), which increases water uptake from the deeper layers where $h > h_4$. JMm behaved very differently with uptake over the first few days (when $M_s > M_c$) in accordance with R distribution. After $M < M_c$ at upper soil layers, uptake pattern starts to change gradually and uptake is increased at lower depths.

The proposed models (PM and PMm) are capable of predicting similar RWU patterns predicted by VLM. For the low T_p–high R scenario (Fig 2.6), water uptake is more uniformly distributed over depth than VLM model over the first days and uptake at upper layers is lower than that predicted by VLM model. For high T_p (Fig 2.7), they better represent root water uptake patterns. In general, there is not much difference of water uptake 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 modes appear to be less precise than the other modes that account for water uptake compensation.

JMII does not mimic well the RWU pattern 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 is compensated by a higher uptake from deeper layers. The model is very sensitive to either R or M. For the high R–high T_p scenarios JMII provides better uptake pattern predictions (Fig 2.7). However, the model does not perform well in the other scenarios of low and medium R (data not shown here), which will be discussed in Section 2.4.1.3.

2.4.1.3 Statistical indices

The performance of the empirical models is analyzed by the coefficient of determination r^2 and the model efficiency coefficient E (NASH; 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 2.4.1.1. The empirical models (except for JM and JMm by setting $\omega_c > 1$) are not able to reproduce these results, thus these scenarios are not taken into account on analyzing the performance of the models.

These statistical indices for the evaluated scenarios of each model are concisely shown by the boxplots in Fig. 2.9. The width of whiskers indicates how spread-out the statistical indices for each model performed in the evaluated scenarios are. 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, showed by the presence of an outlier and lower medium. JMm performed as good as the proposed models, and only in two scenarios it had bad performance as shown by the outliers in Fig. 2.9. The wider whiskers and presence of outliers of the others models confirm their poorer performances.

Among the models that account for water uptake compensation, JM 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 α_m to replace Feddes original reduction function

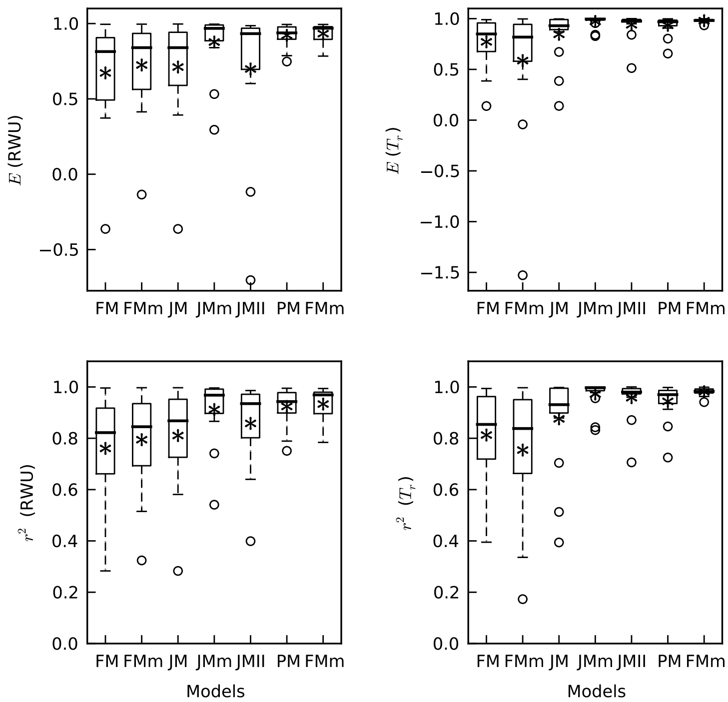

Figure 2.9 - Box plot of the statistical indices r^2 and E for the comparison of root water uptake (RWU) and actual transpiration (T_a) predicted by each empirical model with the De Jong van Lier et al. (2013) model predictions for the drying-out simulations for three levels of root length density and three types of soil and two potential transpiration levels. The symbols $*$ and $\circ$ represent the average and outliers, respectively

α_f in Jarvis (1989) model 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. 2.9 usually refer to this scenario.

On predicting transpiration all models accounting for compensation performed well, except JM. It can be noticed that JMII performed much better on predicting transpiration than RWU. The poorest performance also took place in the high R scenarios.

2.4.1.4 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 2.5. The threshold reduction transpiration parameters h_3 and M_c (for FM and FMm, respectively) stands for the soil hydraulic conditions from which the plant can not meet its potential transpiration rate. Conceptually, the more the amount of roots, the lower is the h_3 or M_c due to the larger root surface area for water uptake, i.e. the plant can extract water in drier soil conditions. Similarly, lower h_3 and M_c are expected

Table 2.5 - Optimal parameters of each empirical model for all scenarios in the drying-out experiment

			FM	FMm	JM		JMm		PM		PMm	
Soil	Tp	RD	h_3	M_c	h_3	ω_c	M_c	ω_c	h_3	l	M_c	l
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

for low T_p. This can also be deduced from Fig. 2.6 and 2.7 by means of the predictions of relative transpiration and water uptake by VLM.

The optimal h_3 and M_c values for FM and FMm, respectively, shown in Table 2.5 do not seem logical when interpreting their conceptual meaning: they increase as R or T_p increases, contradicting their conceptual relation to R and T_p levels. In drying-out scenarios, top soil layers become rapidly drier due to the higher initial uptake. As a result, uptake from these layers starts to decrease whereas water uptake in deeper, wetter layers increases. The higher the R, the more intense is this process as seen by the VLM predictions in Section 2.4.1.1. Because FM and FMm do not account for this, decreasing h_3 or M_c so as to search for conceptually meaningful values would make these models to predict higher water uptake at upper layers (in accordance with R distribution) for a longer time, increasing the discrepancy with VLM predictions. Therefore, their best fitted values are physically unpredictable due to the model assumptions.

In order to interpret the parameters in Table 2.5 for JM, first recall that α in JM stands for the local water uptake reduction owing to soil resistance. Thus, its h_3 parameter refers the local soil pressure at which water uptake starts to reduce. It may be argued that water uptake 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 JM accounts for compensation, water uptake 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. RUW predictions by VLM show that water uptake reduction from top layers starts at higher h_s

as R increases. Therefore, h_3 in JM should increase as R increases. The values of h_3 for JM shown in Table 2.5 agrees to this conceptual meaning. The JMm's M_c parameter can be interpreted likewise.

The JM's ω_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, ω_c should be less than for the medium and high R scenarios. The reason for $\omega_c = 1$ was discussed in Section 2.4.1.2. Conversely, ω_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 values for both models are very close. The optimal l values are low sensitive to soil types and more sensitive to R.

2.4.2 Growing season simulation

In this experiment we evaluated the models under real weather conditions of De Bilt — the Netherlands — during the relatively dry year 2006. We considered the same soil types and crop characteristics as the drying-out experiment. Thus, it was possible to use the calibrated parameters for each model for the corresponding soil type and root length density from the drying-out experiment. We did not evaluate the models for the low R scenario because the empirical models (except JM and JMm) can not be calibrated for high T_p (as discussed in Section 2.4.1.1) . This evaluation is also important to analyze whether calibration of an empirical model with a single drying-out experiment type results in consistent behavior in other circumstances.

Table 2.6 shows the accumulated actual transpiration simulated by SWAP using all the root water uptake models. Accumulated actual transpiration predicted by VLM for low R was much lower and approximately equal for the three soil types (40.45, 40.05 and 40.08 mm d^{-1} for clay, loam and sand soil, respectively). Indeed, the higher the R more the difference of accumulated transpiration between soil types. Most water is extracted from the clay soil, followed by sand and loam soil. Little difference of accumulated transpiration is found between medium and high R . However, for sandy soil the accumulated transpiration was lower for high R and practically identical for loam soil and slightly higher for high R in sand soil.

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

Table 2.6 - Accumulated actual transpiration predicted by the De Jong van Lier et al. (2013) and all the empirical models for three types of soil (clay, loam and sand) and two levels of root length density R (medium and high) for the growing season experiment

	Clay		Loam		Sand	
Model	Medium R	High R	Medium R	High R	Medium R	High R
VLM	46.33	46.51	43.63	43.61	45.53	44.81
PEMm	45.79	46.28	43.63	43.75	45.67	46.41
PEM	45.68	45.74	43.36	43.34	46.18	46.26
JMII	45.83	46.12	43.59	43.63	45.53	46.32
JMm	45.52	46.11	42.91	43.79	45.29	46.11
JM	45.72	45.10	43.36	43.12	46.00	45.89
FMm	42.66	40.11	42.69	40.81	43.23	41.70
FM	43.48	43.16	42.64	41.61	44.60	44.29

Overall, the highest underestimates occurred for high R. All the other models predict close values. Therefore, for total actual transpiration concerns any of the evaluated models accounting for compensation might be suitable provided it is well calibrated.

An overall analysis of the models performance is shown in Fig. 2.10. The best performances are obtained by the models that account for compensation. An improvement of JM by using the proposed reduction function can be observed. Among the models that account for compensation, JM had the worst performance. JMII also was poor in predicting root water uptake. Overall, the best performances were also obtained by the proposed models (PM and PMm) and by the modified Jarvis (1989) model (JMm). These results also assure that the strategy to calibrate empirical models in a single drying-out experiment is warranted.

2.5 Conclusions

Several simple root water uptake models have been developed over the years and here outline some of these models and also proposed other alternatives based on the these works. Some of these models were embedded as sub-models into the eco-hydrological SWAP (VAN DAM et al., 2008) and evaluation was based on the comparison of root water uptake predictions performed by the physical De Jong van Lier et al. (2013) model (also embedded into the SWAP model) for two numerical experiments for different scenarios of soil type, root length density and potential transpiration. The parameters of the empirical models were determined by inverse modeling of simulated root water uptake. The several scenarios allowed giving more insight into the behavior of the De Jong van Lier et al. (2013) model, especially under wet soil conditions and high potential transpiration. We found that for the low R–high T_p scenarios the physical model predicts plant transpiration reduction in wet soil conditions. For such cases, the maximum plant

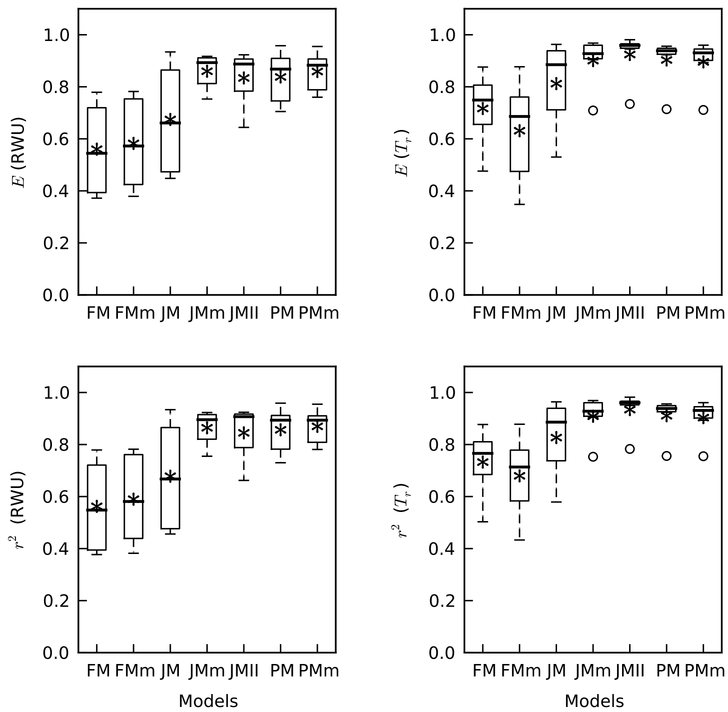

Figure 2.10 - Box plot of the statistical indices r^2 and E for the comparison of root water uptake (RWU) and actual transpiration (T_a) predicted by each empirical model with De Jong van Lier et al. (2013) model for the growing season experiment for two levels of root length density and three types of soil. The symbols $*$ and $\circ$ represent the average and outliers, respectively

transpiration rate is dependent on plant 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 largely-used Feddes, Kowalik and Zaradny (1978) empirical root water uptake model performs well only under circumstances of low root length density R, that is for the scenarios of low root water “compensation”. From medium to hight R, the model can not mimic properly the root uptake dynamics as predicted by the physical model, resulting in very poor predictions. Besides, the best h_3 values do not make sense when interpreting its conceptual meaning. Using our proposed root water uptake reduction function, that is the FM model, does not improve its performance either.

The Jarvis (1989) model provides good predictions only for low and medium R scenarios. For high R, the model can not mimic the uptake patterns predicted by the physical model. Using our proposed reduction, that is the JMm model, helps to improve water uptake predictions. Similarly, the JMII model dot not show good performance for high R–low T_p scenarios.

The proposed models are capable of predicting similar root water uptake patterns by the De Jong van Lier et al. (2013) model. The statistical indices point them as the best alternatives to mimic root water uptake predictions by the De Jong van Lier et al. (2013) model.

The simulations for a growing season experiment confirmed the overall model performance found in the first experiment and suggest that a single experiment of soil drying-out is sufficient to analyze the performance of root water uptake models and retrieve their empirical parameters by defining the objective function in terms of root water uptake.

References

ALLEN, R.G.; PEREIRA, L.S.; RAES, D. **Crop evapotranspiration**. Roma: FAO 1998. 297 p. (FAO Irrigation and drainage paper 56).

ARYA, L.M.; BLAKE, G.R.; ; FARRELL, D.A. A field study of soil water depletion patterns in presence of growing soybean roots: Iii. rooting characteristics and root extraction of soil water. **Soil Science Society of America Journal**, Madison, v. 39, n. 3, p. 437–444, 1975.

ARYA, L.M.; BLAKE, G.R.; FARRELL, D.A. A field study of soil water depletion patterns in presence of growing soybean roots: Ii. effect of plant growth on soil water pressure and water loss patterns. **Soil Science Society of America Journal**, Madison, v. 39, n. 3, p. 430–436, 1975.

BRAUD, I.; VARADO, N.; OLIOSO, A. Comparison of root water uptake modules using either the surface energy balance or potential transpiration. **Journal of Hydrology**, Amsterdam, v. 301, n. 1, p. 267–286, 2005.

BROOKS, R.H.; COREY, A.J. **Hydraulic properties of porous media**. Fort Collins: Colorodado State University, 1964. 27 p.

CASAROLI, D.; DE JONG VAN LIER, Q.; DOURADO NETO, D. Validation of a root water uptake model to estimate transpiration constraints. **Agricultural Water Management**, Amsterdam, v. 97, n. 9, p. 1382–1388, 2010.

CHAHINE, M.T. The hydrological cycle and its influence on climate. **Nature**, Londres, v. 359, n. 6394, p. 373–380, 1992.

COWAN, I.R. Transport of water in the soil-plant-atmosphere system. **Journal of Applied Ecology**, Malden, p. 221–239, 1965.

DE JONG VAN LIER, Q.; DOURADO NETO, D.; METSELAAR, K. Modeling of transpiration reduction in van genuchten–mualem type soils. **Water Resources Research**, Washington, v. 45, n. 2, p. W02422, 2009.

DE JONG VAN LIER, Q.; METSELAAR, K.; VAN DAM, J.C. Root water extraction and limiting soil hydraulic conditions estimated by numerical simulation. **Vadose Zone Journal**, Madison, v. 5, n. 4, p. 1264–1277, 2006.

DE JONG VAN LIER, Q.; VAN DAM, J.C.; METSELAAR, K.; DE JONG, R.; DUIJNISVELD, W.H.M. Macroscopic root water uptake distribution using a matric flux potential approach. **Vadose Zone Journal**, Madison, v. 7, n. 3, p. 1065–1078, 2008.

DE JONG VAN LIER, Q.; VAN DAN, J.C.; DURIGON, A.; SANTOS, M.A.; METSELAAR, K. Modeling water potentials and flows in the soil-plant system comparing hydraulic resistances and transpiration reduction functions. **Vadose Zone Journal**, Madison, v. 12, n. 3, 2013.

DENMEAD, O.T.; SHAW, R.H. Availability of soil water to plants as affected by soil moisture content and meteorological conditions. **Agronomy Journal**, Madison, v. 54, n. 5, p. 385–390, 1962.

DE WILLIGEN, P.; VAN DAM, J.C.; JAVAUX, M.; HEINEN, M. Root water uptake as simulated by three soil water flow models. **Vadose Zone Journal**, Madison, v. 11, n. 3, 2012.

DE WILLIGEN, P.; VAN NOORDWIJK, M. **Roots, plant production and nutrient use efficiency**. 182 p. Thesis (PhD) — Wageningen University, 1987.

DOHERTY, J.; BREBBER, L.; WHYTE, P. **PEST: Model-independent parameter estimation**. Corinda: Watermarker Numerical Computing, 2005. 336 p. (PEST Manual).

DONG, X.; PATTON, B.D.; NYREN, A.C.; NYREN, P.E.; PRUNTY, L.D. Quantifying root water extraction by rangeland plants through soil water modeling. **Plant and soil**, Dordrecht, v. 335, n. 1-2, p. 181–198, 2010.

DOORENBOS, J.; KASSAM, A. **Yield response to water.** Rome: FAO, 1986. 193 p. (FAO Irrigation Drainage Paper, 33).

FEDDES, R.; KOWALIK, P.; KOLINSKA-MALINKA, K.; ZARADNY, H. Simulation of field water uptake by plants using a soil water dependent root extraction function. **Journal of Hydrology**, Amsterdam, v. 31, n. 1, p. 13–26, 1976.

FEDDES, R.; KOWALIK, P.; ZARADNY, H. **Simulation of field water use and crop yield.** Wageningen: Pudoc, 1978. (Simulation Monograph Series).

FEDDES, R.A.; RAATS, P.A.C. Parameterizing the soil–water–plant root system. In: FEDDES, R.A.; ROOIJ, G.H.; VAN DAM, J.C. (Ed.). **Unsaturated-zone modeling: Progress, challenges, and applications**. Wageningen: Kluwer Academic Publ., 2004. chap. 4, p. 95–141.

FISHER, M.J.; CHARLES-EDWARDS, D.A.; LUDLOW, M.M. An analysis of the effects of repeated short-term soil water deficits on stomatal conductance to carbon dioxide and leaf photosynthesis by the legume macroptilium atropurpureum cv. siratro. **Functional Plant Biology**, Collingwood, v. 8, n. 3, p. 347–357, 1981.

GARDNER, W.R. Dynamic aspects of water availability to plants. **Soil Science**, Philadelphia, v. 89, n. 2, p. 63, 1960.

GREEN, S.; CLOTHIER, B. The root zone dynamics of water uptake by a mature apple tree. **Plant and Soil**, Dordrecht, v. 206, n. 1, p. 61–77, 1999.

GREEN, S.R.; CLOTHIER, B.E. Root water uptake by kiwifruit vines following partial wetting of the root zone. **Plant and soil**, Dordrecht, v. 173, n. 2, p. 317–328, 1995.

HEINEN, M. Fussim2: brief description of the simulation model and application to fertigation scenarios. **Agronomie**, Les Ulis, v. 21, n. 4, p. 285–296, 2001.

_____. Compensation in root water uptake models combined with three-dimensional root length density distribution. **Vadose Zone Journal**, Madison, v. 13, n. 2, 2014.

JARVIS, N. A simple empirical model of root water uptake. **Journal of Hydrology**, Amsterdam, v. 107, n. 1, p. 57–72, 1989.

_____. Comment on“macroscopic root water uptake distribution using a matric flux potential approach”. **Vadose Zone Journal**, Madison, v. 9, n. 2, p. 499–502, 2010.

_____. Simple physics-based models of compensatory plant water uptake: concepts and eco-hydrological consequences. **Hydrology and Earth System Sciences Discussions**, Gottingen, v. 8, n. 4, p. 6789–6831, 2011.

JAVAUX, M.; COUVREUR, V.; VANDERBORGHT, J.; VEREECKEN, H. Root water uptake: From three-dimensional biophysical processes to macroscopic modeling approaches. **Vadose Zone Journal**, Madison, v. 12, n. 4, 2013.

JAVAUX, M.; SCHRÖDER, T.; VANDERBORGHT, J.; VEREECKEN, H. Use of a three-dimensional detailed modeling approach for predicting root water uptake. **Vadose Zone Journal**, Madison, v. 7, n. 3, p. 1079–1088, 2008.

LAI, C.T.; KATUL, G. The dynamic role of root-water uptake in coupling potential to actual transpiration. **Advances in Water Resources**, Oxford, v. 23, n. 4, p. 427–439, 2000.

LI, K.Y.; DE JONG, R.; BOISVERT, J.B. An exponential root-water-uptake model with water stress compensation. **Journal of Hydrology**, Amsterdam, v. 252, n. 1, p. 189–204, 2001.

LI, K.Y.; DE JONG, R.; COE, M.T.; RAMANKUTTY, N. Root-water-uptake based upon a new water stress reduction and an asymptotic root distribution function. **Earth Interactions**, Boston, v. 10, n. 14, p. 1–22, 2006.

LI, Y.; FUCHS, M.; COHEN, S.; COHEN, Y.; WALLACH, R. Water uptake profile response of corn to soil moisture depletion. **Plant, Cell & Environment**, Malden, v. 25, n. 4, p. 491–500, 2002.

METSELAAR, K.; DE JONG VAN LIER, Q. The shape of the transpiration reduction function under plant water stress. **Vadose Zone Journal**, Madison, v. 6, n. 1, p. 124–139, 2007.

MOLZ, F.; REMSON, I. Extraction term models of soil moisture use by transpiring plants. **Water Resources Research**, Washington, v. 6, n. 5, p. 1346–1356, 1970.

MOLZ, F.J. Models of water transport in the soil-plant system. **Water Resources Research**, v. 17, n. 5, p. 1245–1260, 1981.

MUALEM, Y. A new model for predicting the hydraulic conductivity of unsaturated porous media. **Water resources research**, Washington, v. 12, n. 3, p. 513–522, 1976.

NASH, J.; SUTCLIFFE, J. River flow forecasting through conceptual models part i – a discussion of principles. **Journal of hydrology**, Amsterdam, v. 10, n. 3, p. 282–290, 1970.

PASSIOURA, J. Water transport in and to roots. **Annual Review of Plant Physiology and Plant Molecular Biology**, Palo Alto, v. 39, n. 1, p. 245–265, 1988.

PRASAD, R. A linear root water uptake model. **Journal of Hydrology**, Amsterdam, v. 99, n. 3-4, p. 297–306, 1988.

RAATS, P. Steady flows of water and salt in uniform soil profiles with plant roots. **Soil Science Society of America Journal**, Madison, v. 38, n. 5, p. 717–722, 1974.

RAATS, P.A.C. Uptake of water from soils by plant roots. **Transport in porous media**, Nova York, v. 68, n. 1, p. 5–28, 2007.

SANTOS, M.A.; DE JONG VAN LIER, Q.; VAN DAN, J.C.; BEZERRA, A.H.F. Selection and parametrization of simple empirical concepts for root water uptake modeling. **HESS**, 2015. No prelo.

SELIM, H.; ISKANDAR, I. Nitrogen behavior in land treatment of wastewater: A simplified model. In: **State of Knowledge in Land Treatment of Wastewater**. Hanover: Cold Regions Research and Engineering Laboratory, USA, 1978. v. 1, p. 171–179.

SIMUNEK, J.; HOPMANS, J.W. Modeling compensated root water and nutrient uptake. **Ecological modelling**, Amsterdam, v. 220, n. 4, p. 505–521, 2009.

SKAGGS, T.H.; Van Genuchten, M.T.; SHOUSE, P.J.; POSS, J.A. Macroscopic approaches to root water uptake as a function of water and salinity stress. **agricultural water management**, Amsterdam, v. 86, n. 1, p. 140–149, 2006.

TARDIEU, F. Drought perception by plants do cells of droughted plants experience water stress? **Plant growth regulation**, Dordrecht, v. 20, n. 2, p. 93–104, 1996.

TAYLOR, H.; KLEPPER, B. The role of rooting characteristics in the supply of water to plants. **Advances in Agronomy**, San Diego, v. 30, p. 99–128, 1978.

TAYLOR, S.; ASHCROFT, G. **Physical Edaphology.** San Francisco: WH Freeman and Company, 1972.

TUZET, A.; PERRIER, A.; LEUNING, R. A coupled model of stomatal conductance, photosynthesis and transpiration. **Plant, Cell & Environment**, Malden, v. 26, n. 7, p. 1097–1116, 2003.

VAN DAM, J.C.; GROENENDIJK, P.; HENDRIKS, R.F.A.; KROES, J.G. Advances of modeling water flow in variably saturated soils with swap. **Vadose Zone Journal**, Madison, v. 7, n. 2, p. 640–653, 2008.

VANDOORNE, B.; BEFF, L.; LUTTS, S.; JAVAUX, M. Root water uptake dynamics of var. under water-limited conditions. **Vadose Zone Journal**, Madison, v. 11, n. 3, 2012.

VAN GENUCHTEN, M.T. A closed-form equation for predicting the hydraulic conductivity of unsaturated soils. **Soil Science Society of America Journal**, Madison, v. 44, n. 5, p. 892–898, 1980.

VERMA, P.; LOHEIDE, S.P.; EAMUS, D.; DALY, E. Root water compensation sustains transpiration rates in an australian woodland. **Advances in Water Resources**, Oxford, v. 74, p. 91–101, 2014.

VRUGT, J.; WIJK, M.v.; HOPMANS, J.W.; ŠIMUNEK, J. One-, two-, and three-dimensional root water uptake functions for transient modeling. **Water Resources Research**, Washington, v. 37, n. 10, p. 2457–2470, 2001.

WÖSTEN, J.; LILLY, A.; NEMES, A.; BAS, C. L. Development and use of a database of hydraulic properties of european soils. **Geoderma**, Amsterdam, v. 90, n. 3, p. 169–185, 1999.

YADAV, B.K.; MATHUR, S.; SIEBEL, M.A. Soil moisture dynamics modeling considering the root compensation mechanism for water uptake by plants. **Journal of Hydrologic Engineering**, Reston, v. 14, n. 9, p. 913–922, 2009.

YU, G.R.; ZHUANG, J.; NAKAYAMA, K.; JIN, Y. Root water uptake and profile soil water as affected by vertical root distribution. **Plant Ecology**, Dordrecht, v. 189, n. 1, p. 15–30, 2007.

ZUR, B.; JONES, J.; BOOTE, K.; HAMMOND, L. Total resistance to water flow in field soybeans: Ii. limiting soil moisture. **Agronomy Journal**, Madison, v. 74, n. 1, p. 99–105, 1982.

3 PROVIDING PARAMETER VALUES FOR AN EMPIRICAL ROOT WATER UPTAKE MODEL

Abstract

Simple empirical macroscopic root water uptake models rely on calibration of their parameters. The objective of this paper is to provide the parameters of an empirical root water uptake model based on predictions performed by a physical model considering transpiration reduction due to soil water depletion. Both models were incorporated into the eco-hydrological model and optimizations were performed using the PEST tool. The parameters (h_3 and l) are provided for several crop characteristics, soil type and atmospheric demand. The sensitivity of plant hydraulic parameters on the calibrated optimal empirical parameters and model accuracy is also evaluated. The results show the empirical model can suitably mimic the dynamics of root water uptake predicted by the physical but its performance depends on the scenario, performing worse for high root length density and low potential transpiration. The empirical parameters are also provided for three levels of radial root hydraulic conductivity, but it is suggested to take the values for the medium level when no information about root hydraulic conductivity is available. Sensitivity of root water uptake to model parameters varies with the scenarios and l is largely more sensitive h_3 parameter. For some cases, the model is totally insensitive to h_3 as the proper l is used. As h_3 values for the three levels of root length density and rooting depth do not show great discrepancy, any calibrated value for these parameters can be used. The empirical parameter values provided here are not definitive. Calibration with experimental results is necessary to support the values.

Keywords: Transpiration reduction function, Optimization, Limiting soil pressure head, Root length density

3.1 Introduction

Almost all water taken up from the soil by the roots is transpired to the atmosphere. On global scale, this has an important impact on the climate as evidences show plants play a major role in driving precipitation inland from the ocean (MAKARIEVA; GORSHKOV, 2007). On a smaller scale, several processes are also dependent on the amount of water taken up from the soil by the roots, that is, root water uptake. Among these processes is plant transpiration related to soil hydraulic conditions, having a direct effect on plant growth and yield (ASSENG et al., 1998; VAN DEN BERG; DRIESSEN, 2002) and the movement of salts, nutrients and pesticides in the soil (GARDENAS et al., 2006). Thereby, root water uptake is built-in as a sub-process in many larger models such as crop growth, land surface scheme and hydrological models.

Root water uptake modeling is usually grouped into two approaches referred to as the microscopic (or mesoscopic) and macroscopic approach. The microscopic approach derives from the landmark work of Gardner (1960) in which soil water flow toward a root single root is described by the Richards equation for cylindrical coordinates with proper boundary conditions (GARDNER, 1960; PASSIOURA, 1988, DE JONG VAN LIER; METSELAAR; VAM DAM, 2006). The macroscopic approach is used in many soil water simulation models and it is based on the addition of a source-sink term S in the Richards equation to account for root water uptake:

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z}\left[K(\theta)\left(\frac{\partial h}{\partial z} + 1\right)\right] - S \tag{3.1}$$

where θ (L^3 L^{-3}) is the soil water content, h (L) the soil water pressure head, K (L T^{-1}) the soil hydraulic conductivity, t (T) the time and z (L) the vertical coordinate (positive upward).

In general, simple empirical models for root water uptake — also called as transpiration reduction functions — are incorporated in hydrological models to account for S in eq. (3.1). For instance, the largely-used eco-hydrolical model SWAP (KROES et al., 2008) employs the Feddes, Kowalik and Zaradny (1978) reduction function and the HYDRUS model (SIMUNEK; VAN GENUCHTEN; SEJNA, 2005) uses the Van Genuchten (1987) reduction function and alternatively the Jarvis (1989) model that includes the so-called "compensation" mechanism (JARVIS, 2011; JAVAUX et al., 2013; Santos et al., 2015). These two reduction functions have been applied in many field experiments (ex. Markewitz et al. (2010); Li, De Jong, Boisvert (2001)) and usually, except for the Feddes, Kowalik and Zaradny (1978) reduction function, show suitable performance when comparing the soil water content or plant transpiration predicted by a soil water flow model in which the reduction function is built-in. The Feddes, Kowalik and Zaradny (1978) reduction function does not account for dynamic distribution of water uptake due to soil water depletion in the rooting zone profile, denominated root water uptake "compensation" (SANTOS et al., 2015). Consequently, many works (ex. Jarvis (1989); Li, De Jong and Boisvert (2001); Li et al. (2002)) focused on implementing this mechanism into the empirical Feddes, Kowalik and Zaradny (1978) model, which promoted improvements on the model predictions. However, it should be stressed that comparison based on soil water content might not properly allow for critical analysis of root water uptake models (DE JONG VAN LIER et al., 2013) and the sensitivity of root water uptake to soil water content depends on the soil type (HUPET et al., 2003). For instance, Santos et al. (2015) recently showed that Jarvis (1989) model does not mimic well root water uptake predictions from the physically-based de Jong van Lier et al. (2013) model, especially in the scenarios where compensation occurs.

One of the major shortcomings in applying transpiration reduction functions is the need for calibration of their empirical parameters that vary according to crop type, soil type and atmospheric demand. An old and not revised compilation is provided by Taylor and Ashcroft (1972) for the Feddes, Kowalik and Zaradny (1978) reduction function. However, several studies show it can not properly mimic root water uptake dynamics even after calibrating their empirical parameters (LI et al., 2002; DE WILLIGEN et al., 2012; SANTOS et al., 2015). Santos et al. (2015) assessed different empirical root water uptake models by comparing with predictions from the de Jong van Lier et al. (2013) physical model for different scenarios and found that their proposed models showed the best performance. To apply these models, their empirical parameters must be found for wide range of crops, soil type and climate conditions and an further analysis about the influence of de Jong van Lier et al. (2013) model hydraulic parameters on the calibrated parameters is required. Concerning crops, the root length density and rooting depth are the main crop parameters affecting root water uptake. These parameters show considerable variation within crops as can be seen from the compilation made by De Willigen and van Noordwijk (1987) (Fig. 3.1). Therefore, it is more appropriate to provide the empirical parameters related to these crop characteristics.

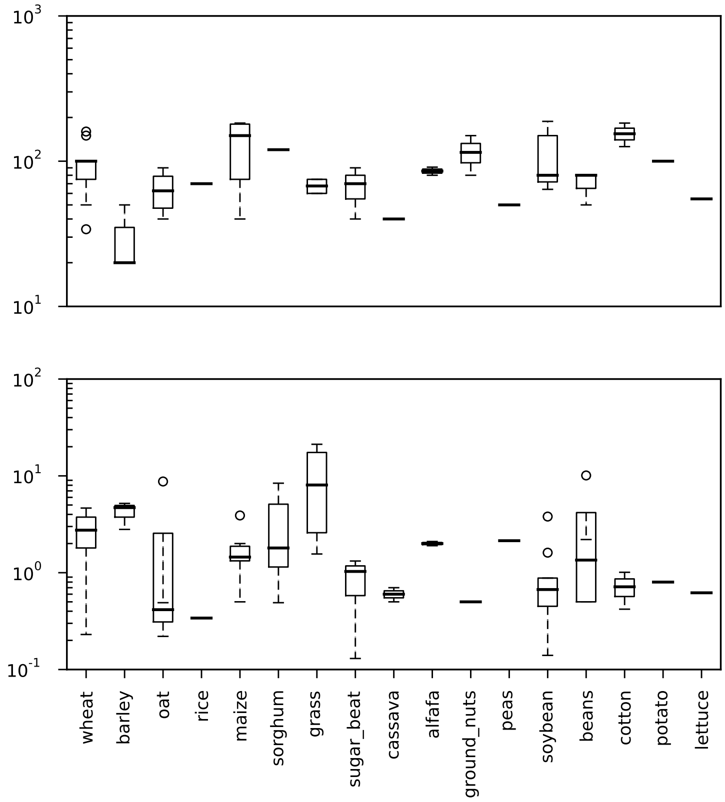

Figure 3.1 - Rooting depth (m, at the top) and root length density (cm cm^{-3}, at the bottom) for some crops reported by De Willigen and van Noordwijk (1987)

As a follow up from Santos et al. (2015) who assessed some empirical root water models, the objective of this paper is to provide suitable values for the empirical models suggested by Santos et al. (2015) for several crop characteristics, soil type and atmospheric demand by comparing with root water uptake predictions performed by the de Jong van Lier et al. (2013) physical model. We also investigated the influence of plant hydraulic parameters on the calibrated optimal empirical parameters and model accuracy. Both models were incorporated into the eco-hydrological model and optimizations were performed by the PEST model (DOHERTY; BREBBER; WHYTE, 2005).

3.2 Methodology

We determined the empirical parameter values of the Santos et al. (2015) root water uptake (RWU) model. This model is based on the general empirical concept of partitioning potential transpiration T_p over depth multiplied by a coefficient accounting for transpiration reduction due to limiting hydraulic conditions as follows:

$$S(z) = S_p \alpha(z) \tag{3.2}$$

where S_p ($L^3\ L^{-2}\ T^{-1}$) is the potential RWU, α is the transpiration reduction function and z (L) is the soil depth. Based on other attempts (MOLZ; REMSON, 1970; SELIM; ISKANDAR, 1978; LI; DE JONG; BOISVERT, 2001), Santos et al. (2015) proposed the following expression for S_p:

$$S_p(z) = \frac{R^\lambda M(h)}{\displaystyle\int_{z_m} R^\lambda M(h) dz} T_p \tag{3.3}$$

where R is the root length density ($L\ L^{-3}$), λ is an empirical parameter, z_m is the rooting depth, h is the soil pressure head (L) and M is the soil matric flux potential ($L^2\ T^{-1}$), defined as:

$$M = \int_{h_w}^{h} K(h)\, dh \tag{3.4}$$

where h_w is h at wilting point. In eq (3.2) and (3.3), Santos et al. (2015) found that using the Feddes, Kowalik and Zaradny (1978) (Fig. 3.2) and his proposed reduction function provides similar model accuracy after calibrating the empirical parameters. Thus, in this

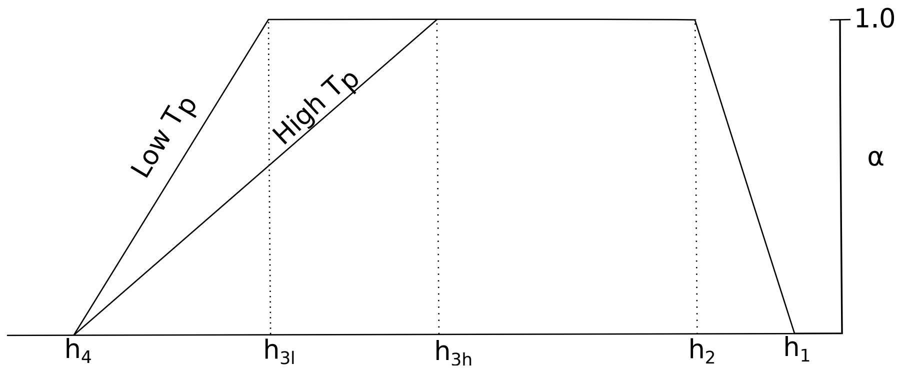

Figure 3.2 - The Feddes, Kowalik and Zaradny (1978) root water uptake reduction function. h_2 and h_3 are the threshold parameters for reduction in root water uptake due to oxygen deficit and water deficit, respectively. The subscripts l and h stands for low and high potential transpiration T_p. h_1 and h_4 are the soil pressure head values below and above which root water uptake is zero due to oxygen and water deficit, respectively

work we chose to use eq. (3.3) in combination with the Feddes, Kowalik and Zaradny (1978) reduction function.

This aims only the transpiration reduction due to dry soil conditions. Thus, the threshold parameters of the Feddes, Kowalik and Zaradny (1978) reduction function for anoxic conditions (h_1 and h_2 shown in Fig. 2.1) were not considered and set to zero. For h_4 the usual value of -150 m was used. Thus, only the l and h_3 remains to be determined.

The empirical parameters were obtained by inverse modeling by comparing RWU predicted by the physical model developed by de Jong van Lier et al. (2013) as described below. Both the Santos et al. (2015) (eq. (3.2) to (2.5)) and the de Jong van Lier et al. (2013) models were incorporated as sub-models into the larger eco-hydrological model SWAP (VAN DAM et al., 2008) in order to apply the sub-models to varying soil water and boundary conditions. Simulations were performed for different scenarios of crop characteristics, soil type and atmospheric demand as described below. Sensitivity of the physical model parameters on the empirical parameters was also evaluated.

3.2.1 The physical model

The physical model developed by de Jong van Lier et al. (2013) was used to provide RWU data to determine the parameters of the Santos et al. (2015) empirical model. We refer to de Jong van Lier et al. (2013) and Santos et al. (2015) for full model description and provided only short overview. In this model, RWU is computed by estimating the pressure at root surface h_0 as function of leaf pressure head and bulk soil hydraulic conditions:

$$h_0(z) = h_l + \varphi(M_s(z) - M_0(z)) + \frac{T_a}{L_l} \qquad (3.5)$$

where L_l (T^{-1}) is the overall conductance over the root-to-leaf pathway, h_l (L) the leaf pressure head and M_s and M_0 are the bulk soil matric flux potential and M at the root surface and φ (T L^{-1}) is defined as:

$$\varphi(z) = \frac{\rho r_m^2(z) \ln \frac{r_0}{r_x}}{2K_{root}} \tag{3.6}$$

where K_{root} (L T^{-1}) is the radial root tissue conductivity (from root surface to root xylem) and r_x (L) the xylem radius. Plant transpiration is a function of h_l, which was defined piece-wisely by imposing a limiting value h_w on h_l. Plant transpiration and RWU distribution are determined by the soil hydraulic conditions and by plant hydraulic parameters.

3.2.2 Numerical experiment

Santos et al. (2015) showed that an experiment of soil drying-out with no rain/irrigation is sufficient to retrieve the parameters by inverse modeling. We set up a similar experiment with initial soil water content corresponding to a pressure head of -1 m at the soil surface to -0.9 m at the bottom (1.2 m depth). The simulation continued until simulated plant transpiration by the de Jong van Lier et al. (2013) RWU model approached zero. Soil evaporation was set to zero making the soil to dry out only due to RWU or drainage at the bottom. Free drainage (unit hydraulic gradient) at 1.2 m depth was the bottom boundary condition. We performed simulations for two levels of atmospheric demand given by potential transpiration T_p: 1 and 5 mm d^{-1}.

3.2.2.1 Scenarios

Root length density and rooting depth

Root length density as well as maximum rooting depth varies considerably for each crop as shown in Fig. 3.1. Thus, instead of determining the parameter for a specific crop, we provided the parameter values for some levels root length density and rooting depth. For root length density, three levels were used: 0.01, 0.1 and 1 cm cm^{-3}, defined hereafter as low, medium and high root length density, respectively. For the maximum rooting depth, we used 0.3, 0.5 and 1 m.

The variation of root length density over depth was assumed exponential, given by (SANTOS et al., 2015):

$$R(z_r) = \frac{b^2 \bar{R}}{b + \exp^{-b} - 1}(1 - z_r) \exp^{-b z_r} \qquad (b > 0) \tag{3.7}$$

where $\bar{R}$ is the average R value and b an empirical parameter set to 2.0.

Soil type

Data for three top soils from the Dutch Staring series (WOSTEN et al., 1999) were used. The physical properties of these soils, described by the Mualem-van Genuchten functions (MUALEM, 1976; VAN GENUCHTEN, 1980) for the $K-\theta-h$ relations, are listed in Table 3.1. These soils are identified in this text as clay, loam and sand (Table 3.1).

Table 3.1 - Mualem-van Genuchten parameters for three soils of the Dutch Staring series (WOSTEN et al., 1999) used in simulations. θ_s and θ_r are the saturated and residual water content, respectively; K_s is saturated hydraulic conductivity and α, λ and n are fitting parameters

Staring soil ID	Textural class	θ_r	θ_r	K_s	α	λ	n
		m m^{-3}	m m^{-3}	m d^{-1}	m^{-1}	-	-
B3	Sand	0.02	0.46	0.1542	1.44	-0.215	1.534
B11	Clay	0.01	0.59	0.0453	1.95	-5.901	1.109
B13	Loam	0.01	0.42	0.1298	0.84	-1.497	1.441

The physical model parameters

The plant hydraulic parameters in the de Jon van Lier et al. (2013) model affect the way RWU is distributed over depth as well as the transpiration the onset of transpiration reduction. In order to account for this, the simulations were performed for three levels of radial root hydraulic conductivity (K_{root}): $1 \cdot 10^{-9}$, $1 \cdot 10^{-8}$ and $1 \cdot 10^{-7}$ m d^{-1}. All other parameters and a summary of the scenarios are listed in Table 3.2.

Table 3.2 - Parameters and simulation scenarios

Description	Symbol	Scenario	Value	Unit
Scenarios				
Potential transpiration	T_p	low	1.0	mm d^{-1}
		high	5.0	mm d^{-1}
Root lenght density	R	low	0.01	cm cm^{-3}
		medium	0.1	cm cm^{-3}
		high	1.0	cm cm^{-3}
Rooting depth	Z_m	low	0.3	m
		medium	0.5	m
		high	1.0	m
Soil type		clay	Table 3.1	
		loam	Table 3.1	
		sand	Table 3.1	
Radial root hydraulic conductivity	K_{root}	low	$1 \cdot 10^{-9}$	m d^{-1}
		medium	$1 \cdot 10^{-8}$	m d^{-1}
		high	$1 \cdot 10^{-8}$	m d^{-1}
Parameters				
Xylem root radius	r_x		0.2	mm
Root radius	r_0		0.5	mm
Overall conductance over the root-to-leaf pathway	L_l		$1 \cdot 10^{-6}$	d^{-1}
Leal pressure head	h_w		-200	m

3.2.3 Optimization

The parameters of the empirical RWU models were estimated by minimizing the following objective function defined in terms of RWU:

$$\begin{aligned} &\text{minimize} \quad \mathit{\Phi}(\mathbf{p}) = \sum_{\mathrm{i=1}}^{\mathrm{n}} \sum_{\mathrm{j=1}}^{\mathrm{m}} [\mathrm{S}^*_{\mathrm{i,j}} - \mathrm{S}_{\mathrm{i,j}}(\mathbf{p})]^2 \\ &\text{subject to} \qquad\qquad \mathbf{p} \in \mathit{\Omega} \end{aligned} \tag{3.8}$$

where $S^*_{i,j}$ is the RWU simulated by SWAP model together with the de Jong van Lier et al. (2013) model at time i and depth j and $S_{i,j}(\mathbf{p})$ is the corresponding RWU predicted by SWAP in combination with the Santos et al. (2015) empirical model. $\mathbf{p}$ is the h_3 and l parameter set to be optimized. The constraining limits were $0 < h_3 <= h_4$ and $0 < l <= 3$, respectively. m is the number of soil layers and n the number of days of the simulation. The optimal parameter set was determined by solving eq. (3.8) using the PEST tool (Parameter ESTimation) (DOHERTY; BREBBER; WHYTE, 2005).The PEST tool was coupled to the SWAP model and optimization was performed for each scenario. As the success of PEST in converging to the best values depends on the initial parameter set values, we repeated optimizations for six random sets of values. This also served to check the uniqueness of the solution . The set resulting in the lowest $\mathit{\Phi}$ was chosen. Upon setting PEST, we performed reference runs of SWAP with the Santos et al. (2015) empirical model using random values of $\mathbf{p}$ and tested the ability of PEST for retrieving $\mathbf{p}$.

3.3 Results

3.3.1 Selection of the scenarios

In the de Jon van Lier et al. (2013) model (here referred to as *the physical model*), a maximum possible transpiration allowed by the plant $T_{p,max}$ occurs when $h_l = h_w$ and soil hydraulic resistance is negligible (SANTOS et al., 2015). The $T_{p,max}$ depends on the plant hydraulic properties and on the root system geometry, represented in the physical model by the distribution over depth of the root length density. $T_{p,max}$ also depends on T_p and when $T_{p,max} < T_p$, the plant transpiration is solely determined by plant hydraulic properties and atmospheric demand. A limiting potential transpiration $T_{p,lim}$ can be defined as the maximum value of T_p for which $T_{p,max}$ equals T_p. This is used herein to identify constraining conditions and scenarios whose $T_{p,max} < T_{p,lim}$. For instance, in the scenario of low K_{root} and low R, the $T_{p,lim}$ is lower than the low T_p value. The optimizations were not performed for such conditions.

Fig. 3.3 shows the dependence of $T_{p,lim}$ on K_{root} and L_l for the three levels of root length density R and rooting depth z_m. It shows that K_{root} and the root length density are the most effective parameters in attaining high transpiration rates. A Deeper rooting system also increases $T_{p,lim}$, but it is less effective. For low K_{root}, $T_{p,lim}$ is lower than the low T_p level even for high R and the deepest z_m, whereas for high R, considerably high $T_{p,lim}$ values are attained even at low K_{root}.

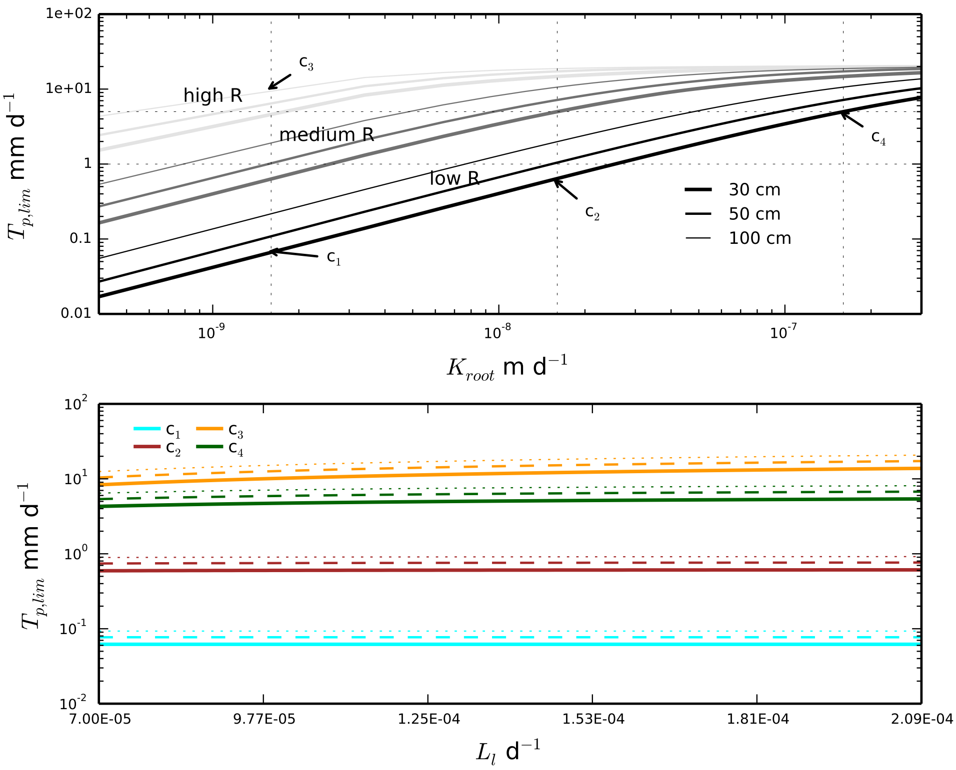

Figure 3.3 - (Top) Limiting potential transpiration $T_{p,lim}$ as a function of radial root hydraulic conductivity K_{root} for the three levels of root length density R and maximum rooting depth (z_m) for wet soil conditions in the loam soil; the other plant hydraulic parameters are given in Table 3.2. (Bottom) $T_{p,lim}$ as a function of the root-to-leaf conductance for the selected curves of the top figure for three values of the limiting leaf water potential h_w (-20000,-25000 and -30000 — continuous, dashed and dotted lines, respectively)

The dashed lines in Fig. 3.3 highlight the K_{root} and T_p values used in the scenarios for the optimizations. The optimizations were not performed in the scenarios whose $T_{p,lim}$ was lower than the low T_p level (1 mm d^{-1}). This mostly happened for the low K_{root}, as seen in Fig. 3.3, where the $T_{p,lim}$ was lower than the low T_p for all scenarios of R and z_m.

The dependence of $T_{p,lim}$ on L_l and h_l is also shown in Fig. 3.3. $T_{p,lim}$ is insensitive to these parameters, irrespectively of the transpiration rate.

3.3.2 Model performance

An overall analysis on the performance of the empirical model is shown in boxplots of the statistical indices (root mean square error – RMSE–, coefficient of determination –r^2– and the Nash-Sutcliffe coefficient of efficiency –E (LEGATES; MCCABE JR, 1999))— Fig. 3.4, calculated by comparing RWU predictions made by the physical model for each scenario. The RMSE (d^{-1}) provides an overall measure of the absolute error in terms of RWU units, whereas the r^2 and E are relative measures related to the precision and accuracy of the model, respectively. RMSE is biased by the water flux values and thus it is higher for the high T_p scenarios.

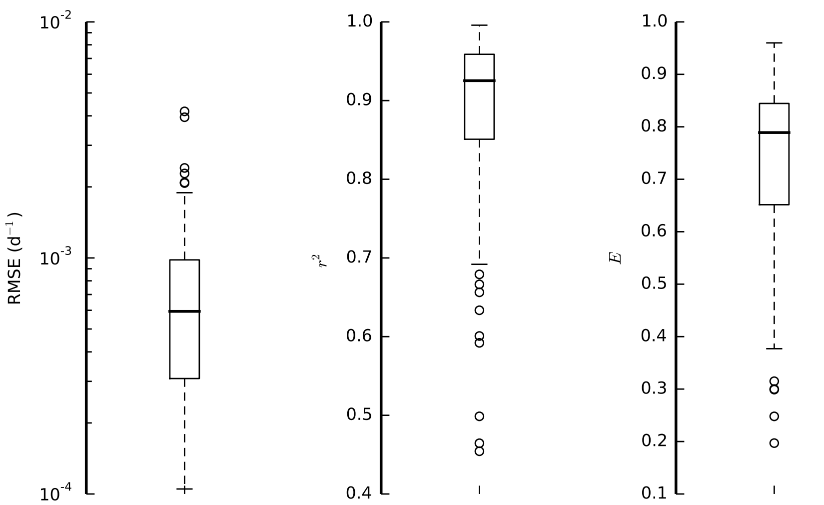

Figure 3.4 - Box-plot of the statistical indices for the de Jon van Lier et al. (2015) model in predicting root water uptake using the optimal parameters for the evaluated scenarios

The boxplots from Fig. 3.4 shows a considerable range in the performance of the model. For some scenarios, RWU predicted by the empirical model is in close agreement with the physical model predictions, whereas for other cases the empirical model does not fit well. The outliers in Fig. 3.4 represent the values out of the overall model performance, corresponding to the scenarios where the model performs worse. Regarding RMSE, these scenarios correspond mostly to scenarios of low z_m and high T_p. As RMSE is biased by water flux values, these outliers are mostly due to higher RWU per soil layer occurring at high T_p and lower z_m scenarios.

The relative statistical indices r^2 and E are better indicators of the scenarios outlying model performance (Table 3.3). With few exceptions, most of the scenarios are of high K_{root}, medium–to–high R and low T_p. The lower model performance for higher R is already expected (SANTOS et al., 2015). For such conditions, RWU front moves

Table 3.3 - Scenarios at which the models have low performance, corresponded to the outliers shown in Fig. 3.4. The superscripts label some scenarios further discussed in the paper

Scenarios					Statistical indices	
K_{root}	soil type	R	z_m	T_p	r^2	E
high	clay	medium	high	low	0.45	0.12
high	clay	high	low	low	0.50	0.37
high	clay	high	medium	low	0.37	0.10
high^{S_1}	clay	high	high	low	0.02	-1.54
high	loam	medium	high	low	0.65	0.40
high	loam	high	low	low	0.17	-0.21
high^{S_2}	loam	high	medium	low	0.04	-0.69
high	loam	high	high	low	0.00	-1.57
high	loam	high	high	high	0.68	0.58
high	sand	high	medium	low	0.47	0.27
high	sand	high	high	low	0.05	-1.05
medium	clay	high	high	low	0.37	-0.02
medium	loam	high	high	low	0.63	0.37

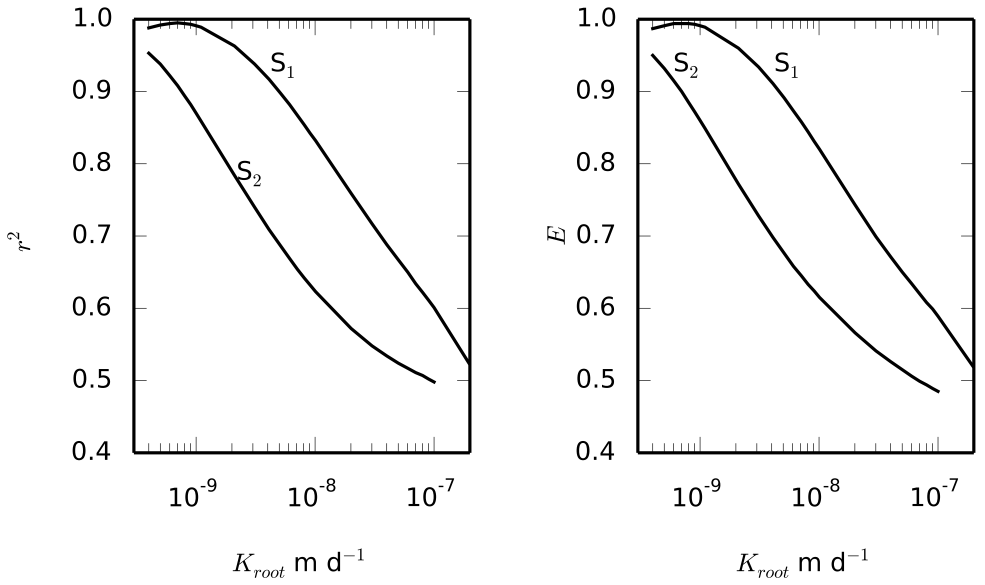

Figure 3.5 - Statistical indices calculated by comparing root water uptake predicted by the Santos et al. (2015) model using the optimal parameters with predictions by the de Jong van Lier et al. (2013) model for several K_{root} in the scenarios S_1 and S_2 (see Table 3.3)

gradually downward as the soil water in the upper layers is depleted. Fig. 3.5 shows that model performance also decreases considerably as K_{root} increases. This indicates that K_{root} also has an important effect on RWU distribution.

Fig. 3.6 and 3.7 show the effect of K_{root} on the dynamics of RWU distribution. Similarly as the amount of roots (SANTOS et al., 2015), the increase of K_{root} enhances the water uptake in sparsely-rooted but wetter parts of the root zone as the upper and more densely root zones become drier. Although the Santos et al. (2015) model was

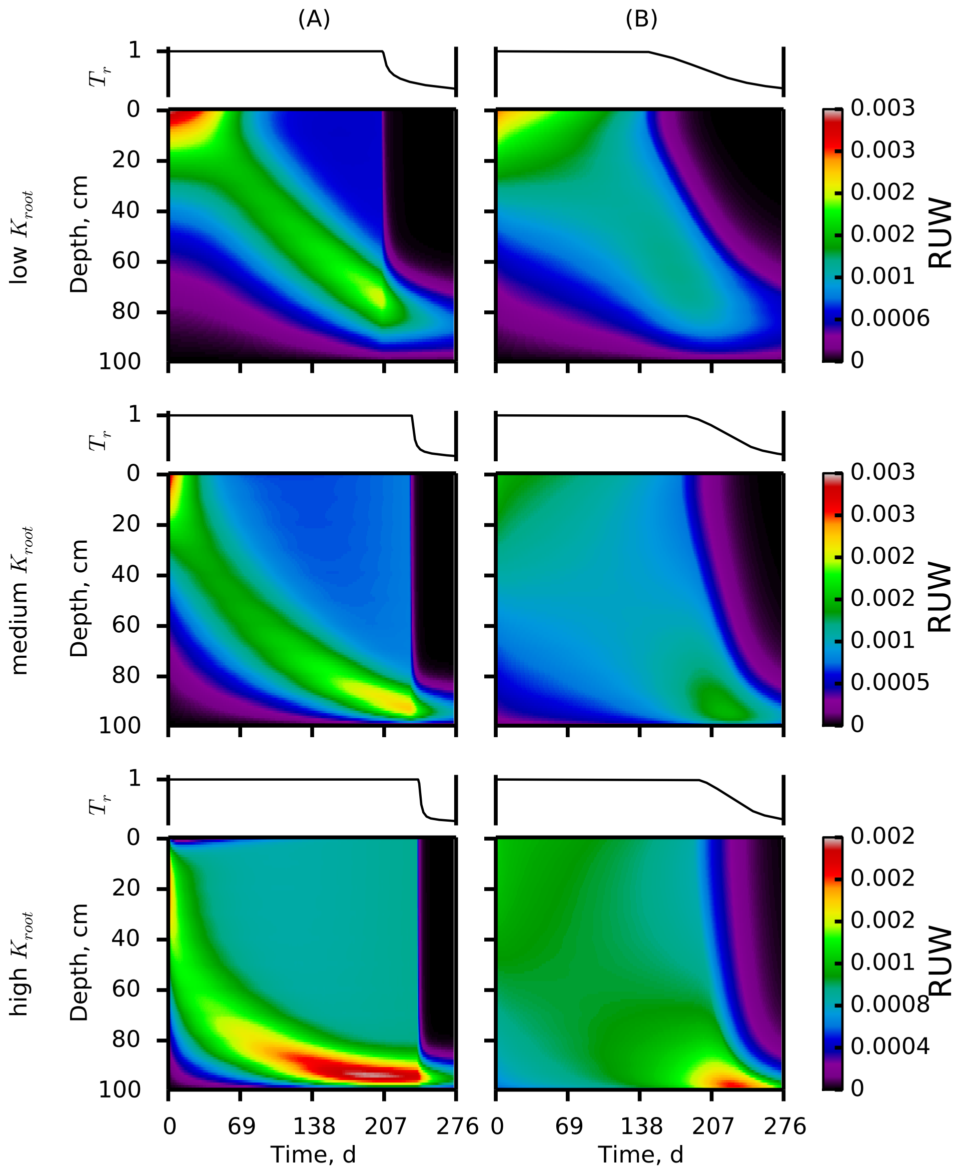

Figure 3.6 - Time-depth root water uptake (RWU) distribution and relative transpiration for the scenario high R–high z_m–low T_p–clay soil for the three levels of K_{root} simulated by the de Jong van Lier et al. (2013) physical model (A) and the counterpart simulated by the Santos et al. (2015) empirical models (B) using its optimal parameters

proposed to improve RWU predictions for such conditions, it becomes less accurate as this process is enhanced when both R and K_{root} are higher.

3.3.3 Optimal parameters

In Fig. 3.8 an overall overview of the distribution of the optimal empirical parameter values of the Santos et al. (2015) model along their domain is given for the evaluated scenarios. In this figure, the relative scaled error for each optimal value in RWU is indicated by the size of the symbols. It can be noticed that the soil type affects

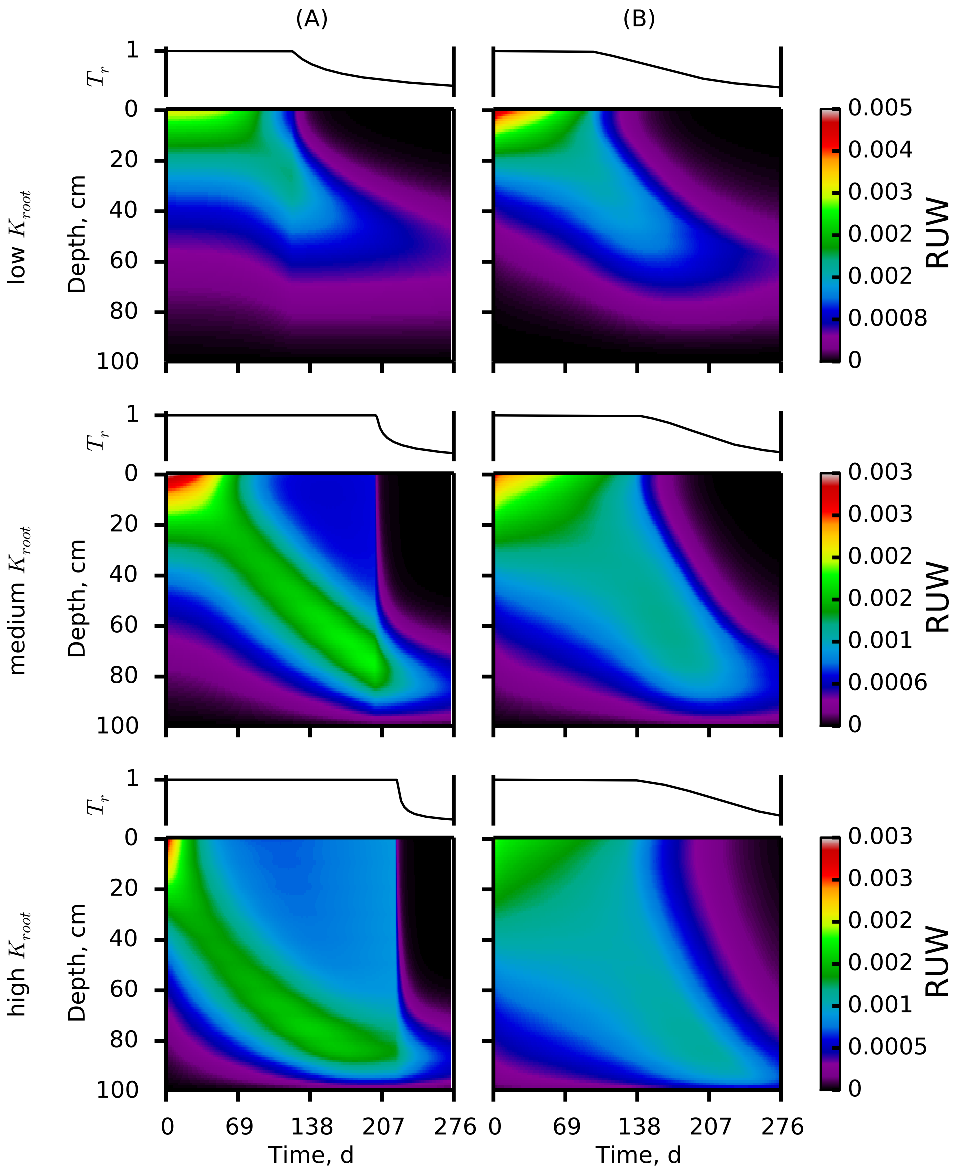

Figure 3.7 - Time-depth root water uptake (RWU) distribution and relative transpiration for the scenario medium R–high z_m–low T_p–clay soil for the three levels of K_{root} simulated by the de Jong van Lier et al. (2013) physical model (A) and the counterpart simulated by the Santos et al. (2015) empirical model (B) using their optimal parameters

considerably the optimal parameters. The l values for loam soil are all smaller than 1.5 and the h_3 values are mostly more negative than -100 m. Larger l values are mainly obtained for the sand soil, where the h_3 values are mostly close to zero.

The effect of plant parameters and T_p on the optimal parameter values can also be found in Fig. 3.8. The rooting depth, shown by different symbols with the same color, has a small effect on the optimal values. In contrast, the root length density R affects considerably the optimal values. An example is shown in Fig. 3.8 by connecting three points corresponding to the three levels of R for the same other conditions. The K_{root}

has also considerable effect on the optimal values. The dependence of these parameters on the optimal parameter values is further analyzed by the values listed in Table 3.4 and in following analyzes.

Regarding the relative error in Fig. 3.8, it can be seen that large errors appear in the three soil types, indicating that the model performance is less dependent on the soil type. Although considerable large errors occur for 30 and 50 cm depth, the largest errors are located for 100 cm depth and from medium to high R scenarios.

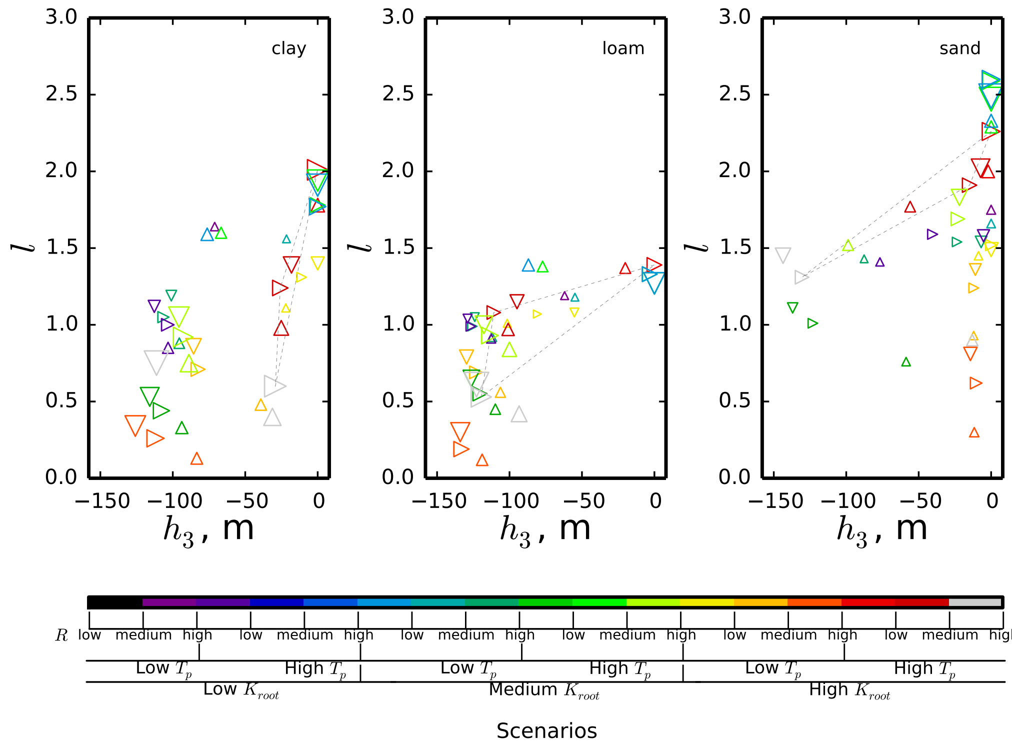

Figure 3.8 - Optimal parameter values for the Santos et al. (2015) model for the evaluated scenarios indicated by the colors. The size of the symbols are scaled according to the error in root water uptake predictions compared to the de Jong van Lier et al. (2013) model

3.3.4 Variation of the empirical parameters

Table 3.4 lists the optimal empirical parameters of Santos et al. (2015) model for the evaluated scenarios. As discussed in Section 3.3.1, in some scenarios $T_{p,max}$ is lower than T_p and optimizations were not performed for those scenarios.

It can be noticed that both h_3 and l parameters show variation to all scenarios and some patterns can be noticed as described in the following. Increasing the parameters z_m, R and K_{root} allows for enhancement of RWU in the wetter, less densely-rooted (deeper) soil layers as the upper, more densely-rooted layers become drier as root water uptake progresses (Fig. 3.7 and 3.6). Except for some cases regarding z_m, l decreases as these

Table 3.4 - Optimal parameter values of the Santos et al. (2015) empirical model for all scenarios evaluated. The highlighted medium K_{root} values are indicated to be used when no information about K_{root} is available

			Low T_p						High T_p					
			Low K_{root}		Medium K_{root}		High K_{root}		Low K_{root}		Medium K_{root}		High K_{root}	
soil	R	z_m	h_3	l	h_3	l	h_3	l	h_3	l	h_3	l	h_3	l
clay	0.01	30	–	–	–	–	0.0	1.4	–	–	–	–	0.0†	2.1†
		50	–	–	–	–	-11.1	1.3	–	–	–	–	0.0	2.0
		100	–	–	**-21.5**	**1.6**	-22.0	1.1	–	–	**-21.3‡**	**1.6‡**	0.0	1.8
	0.10	30	–	–	**-101.0**	**1.2**	-85.7	0.9	–	–	**0.0**	**1.9**	-18.1	1.4
		50	–	–	**-108.4**	**1.1**	-82.6	0.7	–	–	**0.0**	**1.8**	-25.8	1.2
		100	-71.1	1.6	**-95.5**	**0.9**	-39.2	0.5	-70.7‡	1.6‡	**-66.7**	**1.6**	-25.1	1.0
	1.00	30	-112.8	1.1	**-115.9**	**0.5**	-125.9	0.3	0.0	1.9	**-95.8**	**1.0**	-111.2	0.7
		50	-103.5	1.0	**-107.8**	**0.4**	-111.9	0.3	0.0	1.8	**-92.9**	**0.9**	-29.2	0.6
		100	-103.3	0.8	**-93.8**	**0.3**	-83.4	0.1	-76.3	1.6	**-88.9**	**0.8**	-31.2	0.4
loam	0.01	30	–	–	–	–	-55.2	1.1	–	–	–	–	0.0†	1.3†
		50	–	–	–	–	-80.8	1.1	–	–	–	–	0.0	1.4
		100	–	–	**-54.9**	**1.2**	-101.6	1.0	–	–	**-54.7‡**	**1.2‡**	-20.1	1.4
	0.10	30	–	–	**-124.0**	**1.0**	-129.7	0.8	–	–	**0.0**	**1.3**	-94.8	1.1
		50	–	–	**-125.7**	**1.0**	-123.2	0.7	–	–	**-3.2**	**1.3**	-110.9	1.1
		100	-62.0	1.2	**-112.0**	**0.9**	-106.3	0.6	-62.1‡	1.2‡	**-77.2**	**1.4**	-101.0	1.0
	1.00	30	-128.9	1.0	**-126.3**	**0.6**	-134.0	0.3	0.0	1.3	**-117.7**	**1.0**	-122.8	0.6
		50	-126.7	1.0	**-120.4**	**0.5**	-133.2	0.2	-3.2	1.3	**-113.5**	**0.9**	-119.4	0.5
		100	-112.7	0.9	**-109.8**	**0.5**	-118.9	0.1	-87.0	1.4	**-100.1**	**0.8**	-93.4	0.4
sand	0.01	30	–	–	–	–	0.0	1.5	–	–	–	–	0.0†	2.0†
		50	–	–	–	–	0.0	1.5	–	–	–	–	0.0	2.3
		100	–	–	**0.0**	**1.7**	-8.7	1.5	–	–	**0.0†**	**1.7‡**	-2.1	2.0
	0.10	30	–	–	**-6.9**	**1.5**	-10.9	1.4	–	–	**0.0**	**2.5**	-7.3	2.0
		50	–	–	**-23.5**	**1.5**	-12.0	1.2	–	–	**0.0**	**2.6**	-14.9	1.9
		100	0.0	1.8	**-87.7**	**1.4**	-12.1	0.9	0.0‡	1.8‡	**0.0**	**2.3**	-55.9	1.8
	1.00	30	-5.3	1.6	**-137.0**	**1.1**	-14.3	0.8	0.0	2.5	**-21.9**	**1.8**	-143.6	1.4
		50	-40.4	1.6	**-123.0**	**1.0**	-10.3	0.6	0.0	2.6	**-23.0**	**1.7**	-130.5	1.3
		100	-76.8	1.4	**-58.7**	**0.8**	-11.6	0.3	0.0	2.3	**-98.7**	**1.5**	-13.0	0.9

‡ High T_p equals to 1.7 mm d^{-1}
† High T_p equals to 4.3 mm d^{-1}

parameters get higher, indicating how l shapes the RWU distribution over depth by favoring RWU in deeper and wetter layers as it decreases. The h_3 parameter is defined as the soil pressure value below which water uptake is reduced from the defined potential uptake S_p (eq. (3.3)), reflecting directly in transpiration reduction. According to its definition, some logical meanings can be drawn regarding the relation between h_3 and root parameters (R and z_m) and atmospheric demand as previously discussed by Santos et al. (2015). For instance, for higher R and z_m, lower h_3 is expected because more roots will be available to extract water and the roots will exploit the soil in deeper wetter layers. This logical mechanism may hold true, but the changes in the RWU distribution by increasing R or z_m during the soil drying-out process should also taken into account. Increasing R or z_m makes RWU more uniformly distributed over depth and uptake in deeper layers increases more rapidly, followed by reduction of RWU in the upper soil layers as the soil dries out. This leads to a more depth-uniform soil water depletion over time. Consequently, the onset of transpiration reduction might occur at higher pressure head (more negative h_3) when compared to lower R and z_m.

Apart from the aforementioned crop-specific parameters, Table 3.4 also shows that both l and h_3 are affected by the soil type and T_p. The h_3 and l values are generally higher for sand soil. Less negative h_3 and higher l values are also found for high T_p. The high T_p increases the uptake per layer and the soil water is more rapidly depleted, leading to high h_3.

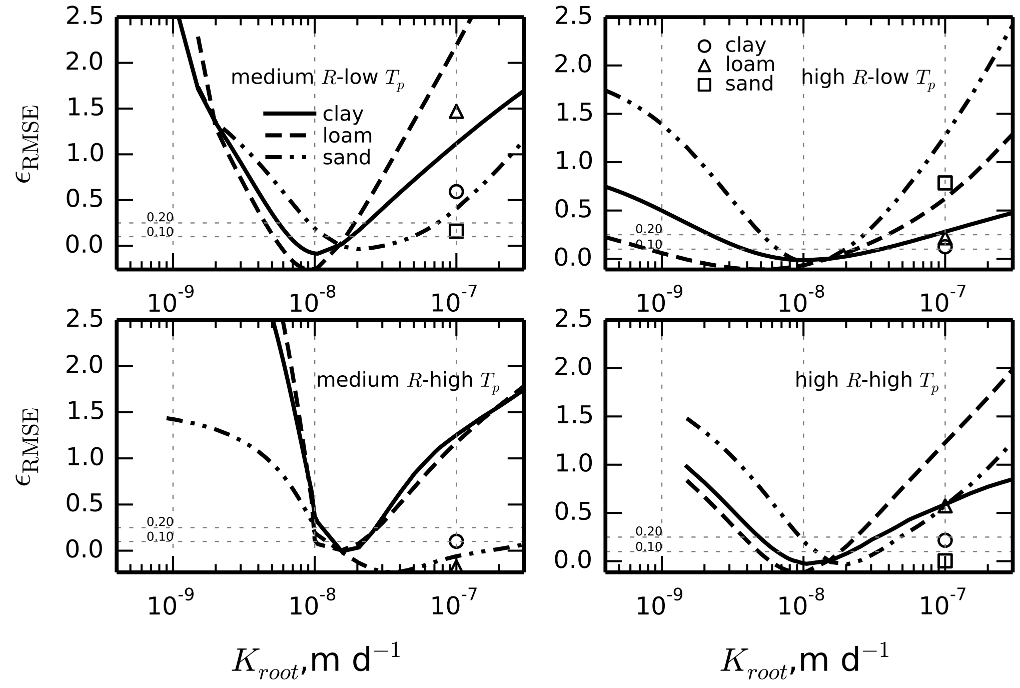

Figure 3.9 - Relative RMSE ϵ_{RMSE} (eq. (3.9)) as a function of root hydraulic conductivity K_{root} for the two levels of potential transpiration T_p and two levels of root length density R and the three soil types for the medium rooting depth z_m. Vertical lines indicate the three levels of K_{root} and horizontal lines ϵ_{RMSE} equals to 0.2 and 0.1. The symbols correspond to the ϵ_{RMSE} using the optimal parameters from the high K_{root} for each soil type

Special attention should be given to the dependence of the empirical parameters h_3 and l on K_{root} as information about K_{root} is scarce. Table 3.4 shows that considerable changes in l and h_3 occur when K_{root} increases from medium to high. The role of K_{root} played on the optimal parameters is further evidenced when computing the relative RMSE (ϵ_{RMSE}, Fig. 3.9) between RWU predicted by the Santos et al. (2015) model using the optimal h_3 and l values for the medium K_{root} given in Table 3.4 and RWU predicted by the physical model for any K_{root} value, defined as:

$$\epsilon_{\mathrm{RMSE}} = \frac{\mathrm{RMSE_i} - \mathrm{RMSE_{opt}}}{\mathrm{RMSE_{opt}}} \tag{3.9}$$

where $\mathrm{RMSE_{opt}}$ is the RMSE between RWU predicted by the Santos et al. (2015) model using the optimal h_3 and l values for the medium K_{root} and RWU predicted by the physical model setting K_{root} to the medium value and $\mathrm{RMSE_i}$ is the RMSE between RWU predicted by the Santos et al. (2015) model by using the same h_3 and l values and

RWU predicted the physical model for any K_{root} value. Changing K_{root} from medium to high can cause considerable discrepancy between the optimal parameters, but the ϵ_{RMSE} below 0.20 (Fig. 3.9) for a suitable range of K_{root} ($\epsilon_{\mathrm{RMSE}} < 0.1$ for a shorter range) around the medium value indicates that empirical parameters in Table 3.4 can be taken for the medium K_{root} assuming that K_{root} does not vary much from this value. The ϵ_{RMSE} also depends on the scenario evaluated — especially on soil type— and in some cases using the optimal value for medium K_{root} may give suitable model accuracy for a wider range of K_{root}. For such cases, using the optimal values for the medium K_{root} can result in similar model accuracy as using the optimal values for the right K_{root} (Fig. 3.9).

Analyzing the values in Table 3.4 shows that h_3 values for variation of some scenarios. Among the crop parameters in Table 3.4, z_m is the one that causes less variation in h_3. For comparison, the h_3 values compiled by Taylor and Ashcroft (1972) are also close for some group of crops. Conversely, the l parameter shows more variation. This suggests the RWU is more sensitive to the l parameter. Analogous to eq. (3.9), the following relative RMSE is defined:

$$\varepsilon_{\mathrm{RMSE}} = \frac{\mathrm{RMSE_i} - \mathrm{RMSE_{opt}}}{\mathrm{RMSE_{opt}}} \tag{3.10}$$

where $\mathrm{RMSE_{opt}}$ is the RMSE between RWU predicted by the Santos et al. (2015) model using the optimal parameter set for a given scenario and RWU predicted the physical model for the corresponding scenario, and $\mathrm{RMSE_i}$ is the RMSE between RWU predicted by the Santos et al. (2015) model using any empirical parameter set and RWU predicted the physical model for the corresponding scenario. Fig. 3.10 illustrates $\varepsilon_{\mathrm{RMSE}}$ for some scenarios and reassures that RWU is much more sensitive to l than h_3 and this sensitivity depends on the scenario. In numbers, for the clay soil scenario shown in Fig. 3.10 the optimal h_3 equals -108.4 m and $\varepsilon_{\mathrm{RMSE}} < 0.01$ for h_3 ranging from -130 to -90 m. For the sand soil, this range is even larger, including the entire h_3 range allowed, and in loam soil it is smaller. Any value within this range can be used without causing problems in the model accuracy and causes practically no changes in the RWU distribution (plots not shown). Looking at Table 3.4, the h_3 value for any z_m can be used equally for the scenarios evaluated in Fig. 3.10. This leads to conclude that there is no need to interpolate h_3 to match the parameters in Table 3.4 and more attention must be given to the l parameter, instead.

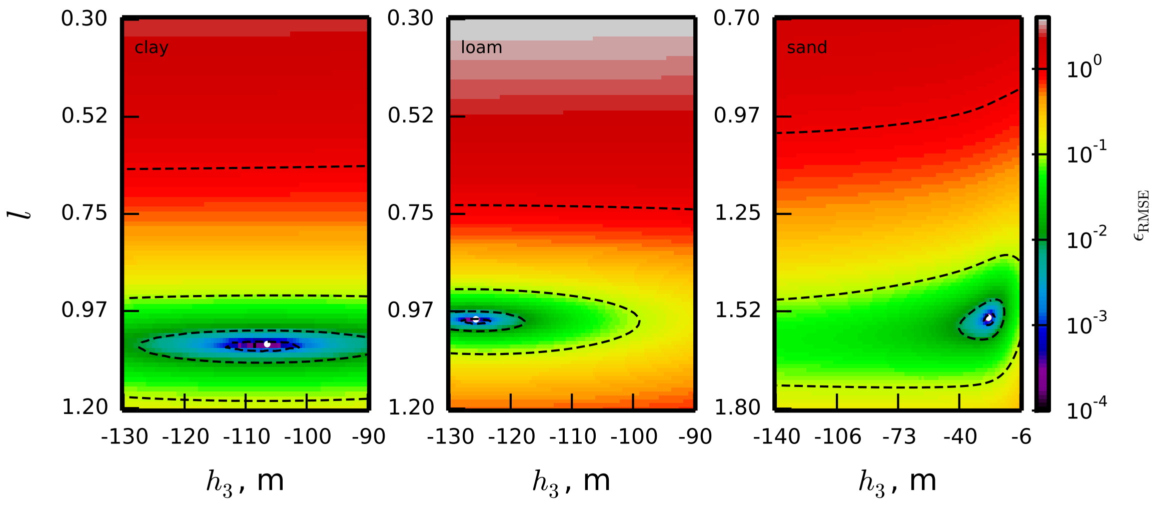

Figure 3.10 - Relative RMSE ($\varepsilon_{\text{RMSE}}$, eq. (3.10)) for the scenario of medium K_{root}–medium R–medium z_m–low T_p for the three soil types. The white point represents the optimal parameter set

3.4 Conclusion

The use of simple empirical root water uptake models requires calibration of respective empirical parameters. The widely used Feddes. Kowalik and Zaradny (1978) model does not properly predict root water uptake, especially as total root length density increases (SANTOS et al., 2015). In this study, we further evaluated and provided the values for the empirical parameters of the Santos et al. (2015) model comparing it to predictions performed by the de Jong van Lier et al. (2013) physical model.

The Santos et al. (2015) empirical model can suitably mimic the dynamics of root water uptake predicted by the de Jong van Lier et al. (2013) physical model for the several scenarios evaluated. For scenarios of high root length density and low potential transpiration the model performance decreased.

The empirical parameters h_3 and l are provided for different scenarios of root length density, rooting depth, soil type and potential transpiration. The values are also listed for three levels of radial root hydraulic conductivity, but it is suggested to use the values for the medium level when no information about root hydraulic properties is available.

The sensitivity of predicted root water uptake on the empirical parameters depends on the scenario but it is much more sensitive to parameter l than to h_3. For some cases, any h_3 value can be used without altering the model accuracy as long as correct l is used. As h_3 values for the three levels of root length density and rooting depth do not show great discrepancy, any calibrated value for these parameters can be used.

References

ASSENG, S.; RITCHIE, J.; SMUCKER, A.J.M.; ROBERTSON, M.J. Root growth and water uptake during water deficit and recovering in wheat.**Plant and soil**, Dordrecht, v. 201, n. 2, p. 265-273, 1998.

DE JONG VAN LIER, Q.; METSELAAR, K.; VAN DAM, J.C. Root water extraction and limiting soil hydraulic conditions estimated by numerical simulation, **Vadose Zone Journal**, Madison, v. 5, n.4, p. 1264–1277, 2006.

DE JONG VAN LIER, Q.; VAN DAM, J.C.; DURIGON, A.; SANTOS, M.A.; METSELAAR, K. Modeling water potentials and flows in the soil-plant system comparing hydraulic resistances and transpiration reduction functions. **Vadose Zone Journal**, Madison, v. 12, n. 3, 2013.

DE WLLIGEN, P.; VAN DAM, J.C.; JAVAUX, M.; HEINEN, M. Root water uptake as simulated by three soil water flow models. **Vadose Zone Journal**, Madison, v. 11, n. 3, 2012.

DE WILLIGEN, P.; VAN NOORDWIJK, M. **Roots, plant production and nutrient use efficiency**. 182 p. Tesis (PhD) — Wageningen University, 1987.

DOHERTY, J.; BREBBER, L.; WHYTE, P. **PEST: Model-independent parameter estimation**. Corinda: Watermarker Numerical Computing, 2005, 336 p (PEST Manual).

FEDDES, R.; KOWALIK, P.; ZARADNY. **Simulation of field water use and crop yield**. Wageningen: Pudoc, 1978. (Simulation Monograph Thesis).

GARDENAS, A.I.; SIMUNEK, J.; JARVIS, N.; VAN GENUCHTEN, M.T. Two-dimensional modelling of preferential water flow and pesticide transport from a tile-drained field. **Journal of Hydrology**, Amsterdam, v. 329, n. 3, p. 647–660, 2006.

GARDNER, W.R. Dynamic aspects of water availability to plants. **Soil Science**, Philadelphia, v.89, n. 2, p. 63, 1960.

HUPET, F.; LAMBOT, S.; FEDDES, R.A.; VAN DAM, J.C.; VANCLOOSTER, M. Estimation of root water uptake parameters by inverse modeling with soil water content data. **Water Resources Research**, Washington, v. 30, n. 11, 2003.

JARVIS, N. A simple empirical model of root water uptake. **Journal of Hydrology**, Amsterdam, v. 107, n. 1, p. 57–72, 1989.

_______. Simple physics-based models of compensatory plant water uptake: concepts and eco-hydrological consequences. **Hydrology and Earth System Sciences Discussions**, Gottingen, v. 8. n. 4, p. 6789–6831, 2011.

JAVAUX, M.; COUVREUR, V.; VANDERBORGHT, J.; VEREECKEN, H. Root water uptake: from three-dimensional biophysical processes to macroscopic modeling approaches. **Vadose Zone Journal**, Madison, v. 12, n. 4, p. 1–16, 2013.

KROES, J,G.; VAN DAM, J. C.; GROENENDIJK, P.; HENDRIKS, R.F.A.; JACOBS, C.M.J. **SWAP version 3.2. Theory description and user manual**. Wageningen: Alterra, 2008, 262p. (Alterra Report, 1649).

LEGATES, D. R.; MCCABE JR, G.J. Evaluating the use of goodness-of-fit measures in hydrologic and hydroclimatic model validation. **Water Resources Research**, Washington, v. 23, n. 1, p. 233–241. 1999.

LI, K.Y.; DE JONG, R.; BOISVERT, J.B. An exponential root-water-uptake model with water stress compensation. **Journal of Hydrology**, Amsterdam, v. 252, n. 1, p. 189–204, 2001.

LI, Y.; FUCHS, M.; COHEN, S.; COHEN, Y.; WALLACH, R. Water uptake profile response of corn to soil moisture depletion. **Plant, Cell & Environment**, Malden, v. 25, n. 4, p. 491–500, 2002.

MAKARIEVA, A.M.; GORSHKOV, V.G. Biotic pump of atmospheric moisture as driver of the hydrological cycle on land. **Hydrology and Earth System Sciences**, Gottingen, v. 11, n. 21, p. 1013–1033, 2007.

MARKEWITZ, D.; DEVINE, S.; DAVIDSON, E.A.; BRANDO, P.; NEPSTAD, D.C. Soil moisture depletion under simulated drought in the Amazon: impacts on deep root uptake. **New Phytologist**, Malden, v. 187, n. 3. p. 592–607, 2010.

MOLZ, F.J.; REMSON, I. Extraction term models of soil moisture use by transpiring plants. **Water Resources Research**, Washingtonm v. 6, n. 5, p. p. 1346–1356, 1970.

MUALEM, Y. A new model for predicting the hydraulic conductivity of unsaturated porous media. **Water resources research**, Washington, v. 12, n. 3, p. 513–522, 1976.

PASSIOURA, J.B. Water transport in and to roots. **Annual Review of Plant Physiology and Plant Molecular Biology**, Palo Alto, v. 39, n. 1, p. 245–265, 1988.

SANTOS, M. A.; DE JONG VAN LIER, Q.; VAN DAN, J.C.; BEZERRA, A.H.F. Selection and parametrization of simple empirical concepts for root water uptake modeling, **Hydrology Earth System Science**, Gottingen, 2015. In press.

SELIM, H.M.; ISKANDAR, I.K. Nitrogen behavior in land treatment of wastewater: A simplified model. In: **State of Knowledge in Land Treatment of Wastewater**. Hanover: Cold Regions Research and Engineering Laboratory, USA, v. 1, p. 171–179, 1978.

SIMUNEK, J. VAN GENUCHTEN, M.T.; SEJNA, M. **The HYDRUS-ET Software Package for Simulating the One-Dimentional Movement of Water, Heat and Multiple Solutes in Variably-Saturated Media. Version 3.0**, Riverside: University of California, 205 302 p. (HYDRUS soft. Ser. 1).

TAYLOR, S.A.; ASHCROFT, G.L. **Physical Edaphology**. San Francisco: WH Freeman and Company, 1972.

VAN DAM, J C.; GROENENDIJK, P.; hENDRIKS, R.F.A.; KROES, J.G. Advances of modeling water flow in variably saturated soils with SWAP. **Vadose Zone Journal**, Madison, v. 7. n. 2, p. 640–653, 2008.

VAN DEN BERG, M; DRIESSEN, P.M. Water uptake in crop growth models for land use systems analysis: I. A review of approaches and their pedigrees. **Agriculture, ecosystems & environment**, v. 92, n. 1, p. 21–36, 2002.

VAN GENUCHTEN, M. T. A closed-form equation for predicting the hydraulic conductivity of unsaturated soils. **Soil Science Society of America Journal**, Madison, v. 44, n. 5, p. 892–898, 1980.

_______. **A numerical model for water and solute movement in and below the root zone**. Florida: United States Department of Agriculture Agricultural Research Service US Salinity Laboratory, 1987.

WÖSTEN, J.H.M.; LILLY, A.; NEMES, A.; LE BAS, C. Development and use of a database of hydraulic properties of European soils. **Geoderma**, Amsterdam, v. 90, n. 3, p. 169–185, 1999.