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### Title

Implementation and Application of a Root Growth Module in HYDRUS

### Permalink

<https://escholarship.org/uc/item/9x31w9kx>

### Journal

Vadose Zone Journal, 17(1)

### ISSN

1539-1663

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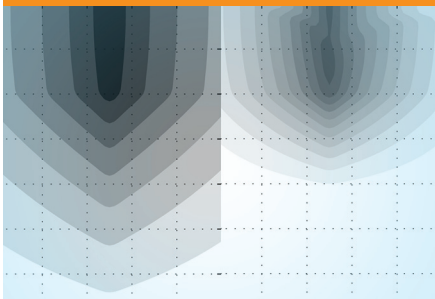
### Publication Date

2018

### DOI

10.2136/vzj2017.02.0040

Peer reviewed



#### Core Ideas

- A HYDRUS module was implemented to model root growth as a function of environmental stresses.
- Simulations were compared with experimental data for temperature stress effects on root growth.
- Temperature-dependent root growth parameters were fitted to experimental data using DREAM.
- A sensitivity analysis of model parameters revealed key parameters of the modeling approach.

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Received 6 Feb. 2017.  
Accepted 13 June 2017.

Citation: Hartmann, A., J. Šimůnek, M.K. Aidoo, S.J. Seidel, and N. Lazarovitch. 2018. Implementation and application of a root growth module in HYDRUS. *Vadose Zone J.* 17:170040. doi:10.2136/vzj2017.02.0040

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# Implementation and Application of a Root Growth Module in HYDRUS

Anne Hartmann,\* Jiří Šimůnek, Moses Kwame Aidoo, Sabine J. Seidel, and Naftali Lazarovitch

A root growth module was adapted and implemented into the HYDRUS software packages to model root growth as a function of different environmental stresses. The model assumes that various environmental factors, as well as soil hydraulic properties, can influence root development under suboptimal conditions. The implementation of growth and stress functions in the HYDRUS software opens the opportunity to derive parameters of these functions from laboratory or field experimental data using inverse modeling. One of the most important environmental factors influencing root growth is soil temperature. The effects of temperature in the root growth module was the first part of the newly developed HYDRUS add-on to be validated by comparing modeling results with measured rooting depths in an aeroponic experimental system with bell pepper (*Capsicum annuum* L.). The experiment was conducted at root zone temperatures of 7, 17, and 27°C. Inverse optimization was used to estimate a single set of parameters that was found to well reproduce measured time series of rooting depths for all temperature treatments. A sensitivity analysis showed that parameters such as the maximum rooting depth and cardinal temperatures had only a small impact on the model output and can thus be specified using values from the literature without significantly increasing prediction uncertainties. On the other hand, parameters that define the growth rate or the shape of the temperature stress function had a high influence. The root growth module that considers temperature stress only slightly increased the complexity of the standard HYDRUS models.

**Water uptake by root systems** can greatly affect water flow through the soil (Hao et al., 2005; Yu et al., 2007). The spatial pattern of root water uptake is determined by the spatial distribution of the root system, the knowledge of which is essential for predicting the spatial distribution of water contents and water fluxes in soils. The spatial distribution of roots and their growth are sensitive to various physical, chemical, and biological factors, as well as to soil hydraulic properties that influence the availability of water and oxygen for plants. It is thus important to describe root growth under the influence of various environmental factors to accurately simulate agricultural systems.

Various attempts have been made in the past to develop root growth models that account for the influence of various environmental factors such as temperature (Stone et al., 1983; Stone and Taylor, 1983; Williams et al., 1989; Jones et al., 1991; Kaspar and Bland, 1992; Bingham and Wu, 2011), aeration (Williams et al., 1989; Jones et al., 1991; Asseng et al., 1997), soil water availability (Jones et al., 1991; Clausnitzer and Hopmans, 1994; Somma et al., 1998; Tsutsumi et al., 2003; Leitner et al., 2010), and soil strength (Dexter, 1986; Williams et al., 1989; Jones et al., 1991; Grant, 1993; Asseng et al., 1997). Additional studies evaluating the impact of various environmental factors on root growth were listed by Wu et al. (2005). Existing models are either complex, three-dimensional root architecture models (Clausnitzer and Hopmans, 1994; Somma et al., 1998; Leitner et al., 2010; Bingham and Wu, 2011; Couvreur et al., 2012) or simpler root growth models that are implemented within more complex models such as EPIC (Williams et al., 1989) or CERES (Robertson et al., 1993). The model by Jones et al. (1991) considers the influence of various environmental factors on root growth in terms of the root length

per unit depth and as a result was found to be highly suitable for implementation into HYDRUS.

One of the most important environmental factors influencing root growth is soil temperature (Brouwer and de Wit, 1968; Aidoo et al., 2016). Extreme (both high and low) root zone temperatures may influence root growth and root development and affect both the fundamental functions of root nutrient and water uptake and tolerance of elemental deficiency and toxicity (Wu and Cheng, 2014). The ability of plants to absorb and accumulate both water and mineral nutrients from the soil is related to their capacity to develop an extensive root system (Taiz and Zeiger, 2002) to reach large parts of the soil profile (Garnett et al., 2009). In addition, it has been reported that salinity and mycorrhiza, coupled with extreme root zone temperatures, affect several morphological and anatomical changes such as a decrease in root biomass, the root specific surface area, the cortex width, and an altered xylem vessel density in different species (Valenzuela-Estrada et al., 2008; Rewald et al., 2012). These changes have been associated with extreme temperatures, freezing, and cold tolerance (Fowler et al., 1981). An overview of studies evaluating the impact of soil temperature on root growth for several crops such as maize (*Zea mays* L.), rapeseed (*Brassica napus* L.), wheat (*Triticum aestivum* L.), barley (*Hordeum vulgare* L.), rye (*Secale cereale* L.), oat (*Avena sativa* L.), and soybean [*Glycine max* (L.) Merr.] was provided by Kaspar and Bland (1992) and Smith et al. (2005). These studies have indicated that non-optimal root zone temperatures affect root growth and root development, resulting in a reduction in the rooting depth and the formation of smaller root systems. Especially with regard to climate change scenario analyses, there is a demand for improved modeling predictions of root growth under heat stress or heat stress combined with further environmental stresses (Seidel et al., 2016).

The HYDRUS software packages (Šimůnek et al., 2016) are widely used numerical models to simulate water flow and heat and solute transport in one-, two-, and three-dimensional, variably saturated porous media. The governing water flow equation that is solved by the HYDRUS models incorporates a macroscopic sink term to account for root water uptake (Feddes et al., 1978), which may be reduced from its positive values due to salinity and drought stresses. However, the macroscopic root water uptake model in the standard versions of HYDRUS (Šimůnek et al., 2008, 2016) does not consider the feedback of environmental conditions in the root zone on root growth, and root growth is fully defined using predefined input parameters (Šimůnek and Hopmans, 2009).

The objectives of this study thus were (i) to develop an add-on root growth module for the HYDRUS software packages (both HYDRUS-1D and HYDRUS-2D) to model root growth as a function of different environmental stresses such as temperature, aeration, and chemical soil conditions, and (ii) to use this newly developed add-on module to evaluate the effects of temperature on root growth using experimental data and to carry out a sensitivity

analysis. The study was conducted as follows. First, the modeling approach developed by Jones et al. (1991) was adapted and implemented into the HYDRUS software packages. The original modeling approach by Jones et al. (1991) is a layered root growth model that needs to be coupled to a crop growth model, which provides it with the daily allocation of dry matter to the root system, and that furthermore needs information about the soil profile characteristics influencing root growth. To overcome the need for input variables provided by a crop model, the modeling approach is instead combined with time-dependent root growth functions. Second, the capability of the newly developed root growth module to account for the effects of temperature on the vertical root penetration was evaluated using experimental data. The evaluation was performed using measured rooting depths with bell pepper in an aeroponic experimental system, which guarantees that the temperature-dependent root growth approach was evaluated using experimental root growth data generated only under the influence of temperature while limiting the effects of other factors. Third, a global sensitivity analysis using the Sobol' method (Sobol', 1993) was conducted to identify the key parameters of the root growth module and to indicate which parameters can be fitted using experimental data. The parameters to which the model is not sensitive cannot be estimated using experimental data and may be fixed using literature values. Finally, the global optimization algorithm DREAM (Vrugt, 2016) was used to fit the modeling results to the experimental data. The ability of the modeling approach to reproduce the data was evaluated using the sample standard deviation.

## Materials and Methods

We first describe the root growth model of Jones et al. (1991) and its implementation into the HYDRUS software packages. Then, we describe the aeroponic root growth experiment, which was used to validate the implemented root growth and temperature stress models. Finally, we describe the statistical approaches used to analyze the collected experimental data, such as the sensitivity analysis and parameter optimization.

### Modeling Root Growth as a Function of Environmental Stresses

#### Root Growth Model of Jones et al. (1991)

Jones et al. (1991) proposed a root growth model that simulates daily root growth in a layered soil as a function of different environmental conditions that are characterized by growth stress factors. Root growth and the development of root length density depend on environmental stress factors that range from 0 (no growth) to 1 (no stress). The model simulates (i) daily increases in the rooting depth, (ii) the length/weight ratio of new roots, (iii) root proliferation within different soil layers, and (iv) root senescence under the influence of various environmental factors. Jones et al. (1991) divided the stress factors into static and dynamic stress factors. Stress factors due to Al toxicity, Ca deficiency, and coarse fragments are considered to be static. Stress factors due to extreme

temperatures, soil strength, and poor aeration are considered to be dynamic.

To evaluate a potential daily increase in the rooting depth, Jones et al. (1991) proposed using either a function of the growth stage or a function of thermal time. Both functions require an additional input that should be provided by an output of a crop growth model. An actual increase in the rooting depth is then obtained by reducing the potential increase due to various stress factors (for more details, see the equations below).

The model also evaluates the depth-dependent root distribution within the soil profile based on the root length/mass ratio, which is used to describe a potential increase in root mass in a particular layer and which additionally depends on the root length density. To calculate an increase in the root mass in a soil layer, the model requires daily values of the dry matter allocation to the root system as an additional input, which has to be provided, in a way similar to the daily increases in rooting depth, by a crop growth model. The depth distribution of the root length density can also be influenced by root senescence, which is considered to be driven not only by time but also by low soil water contents or poor aeration (Jones et al., 1991).

### Implementation into HYDRUS

The HYDRUS programs numerically solve the Richards equation for saturated–unsaturated water flow and convection–dispersion type equations for heat and solute transport (Šimůnek et al., 2008, 2016). Extraction of water from the soil via the root system due to transpiration is expressed via a sink term in the Richards equation. The spatial variation in root length density needs to be specified to evaluate the spatial variation in the intensity of root water uptake.

The standard code of HYDRUS-1D offers the possibility of considering a time-dependent alteration of the root length density distribution. The time-dependent rooting depth can be either given as an input in a tabulated form or calculated using the Verhulst–Pearl logistic growth function. The time-dependent rooting depth is then used together with the Hoffman and van Genuchten (1983) function to calculate the spatial distribution of the root length density. The standard version of HYDRUS-1D does not consider the feedback between root growth and conditions in the soil; root growth is fully defined using input parameters (Šimůnek and Hopmans, 2009).

The standard code of HYDRUS-2D considers the root system to be static with time and does not allow for the dynamic development of the root system. To allow for the dynamic development of the root system and implementation of the Jones et al. (1991) root growth model, a two-dimensional, root length density distribution function (Vrugt et al., 2001a, 2001b) was combined with either the Verhulst–Pearl logistic growth function or a tabulated input of rooting depths (Hartmann and Šimůnek, 2015), in a similar

way to that in HYDRUS-1D. HYDRUS-2D can consider either a two-dimensional or radially symmetrical root length density distribution function and requires an additional parameter to describe the maximum horizontal or radial distance, respectively, of the root system.

The modeling approach proposed by Jones et al. (1991) was adapted and implemented into both HYDRUS software packages. To avoid the requirement to couple the root growth model with a crop growth model, the modeling approach of Jones et al. (1991) was slightly modified. In the newly developed root growth module, the development of the potential root system is still evaluated as in the standard HYDRUS models. The potential rooting depth, reached when the development of the root system would be independent of environmental conditions, is still evaluated using a time-dependent growth function. However, an actual rooting depth is evaluated from the potential rooting depth by taking into account various environmental stress factors, in a similar way to the approach of Jones et al. (1991). Similarly, an actual spatial pattern of the root length density distribution is evaluated based on the specified shape functions. Such functions represent the potential root length density distribution under optimal developmental conditions when no restrictions on root growth occur. Due to sub-optimal environmental conditions, the potential root distribution is altered to get an actual root distribution.

### Stress Factors

Stress factors  $S_x$  (dimensionless) influencing the vertical penetration of roots according to Jones et al. (1991) are listed in Table 1. Descriptions of the static stress factors accounting for the influence of Ca deficiency, Al toxicity, and excessive coarse fragments were provided by Jones et al. (1991) and Hartmann and Šimůnek (2015). Descriptions of the dynamic stress factors, which can vary with time and are thus of greater importance for a dynamic alteration of the root system development, are given below.

According to Jones et al. (1991), the bulk density, soil texture, and water content influence the soil strength and can thus represent a stress for root development. The soil strength stress factor  $S_{St}$  proposed by Jones et al. (1991) is calculated as

$$S_{St} = S_{BD} \sin\left(\frac{\pi}{2}\theta_f\right) \quad [1]$$

Table 1. Stress factors influencing root growth.

Parameter	Stress factor ( $S$ )
$S_T$	temperature stress
$S_{Ca}$	Ca deficiency
$S_{Al}$	Al toxicity
$S_{St}$	soil strength
$S_{Ae}$	aeration stress
$S_{CF}$	excessive coarse fragments

where the parameter  $\theta_f$  denotes the fractional water content and is calculated for each depth:

$$\begin{aligned} \theta_f &= 0 & \theta < \theta_L \\ \theta_f &= \frac{\theta - \theta_L}{\theta_U - \theta_L} & \theta_U \geq \theta \geq \theta_L \\ \theta_f &= 1 & \theta > \theta_U \end{aligned} \quad [2]$$

where  $\theta$  is the water content,  $\theta_L$  is the lower limit of the plant-extractable soil water (conventionally corresponding to the wilting point), and  $\theta_U$  is the drained upper limit of the soil water. In the HYDRUS implementation of this stress factor, corresponding pressure heads (instead of water contents) representing these limits have to be specified. These limiting pressure heads are then used to calculate corresponding water contents using the soil water retention curve.

The parameter  $S_{BD}$  in Eq. [1] is a factor accounting for the interacting effects of texture and bulk density of the moist soil. The factor is calculated as

$$\begin{aligned} S_{BD} &= 1 & BD < BD_O \\ S_{BD} &= \frac{BD_X - BD}{BD_X - BD_O} & BD_O \geq BD \geq BD_X \\ S_{BD} &= 0 & BD > BD_X \end{aligned} \quad [3]$$

The parameters  $BD$ ,  $BD_X$ , and  $BD_O$  denote the user-defined bulk density and the bulk densities above which root growth is first affected and completely inhibited. The parameters  $BD_X$  and  $BD_O$  are calculated using the user-defined percentage (w/w) of sand ( $WP_S$ ) of the considered soil:

$$\begin{aligned} BD_X &= 1.6 + 0.004 WP_S \\ BD_O &= 1.1 + 0.005 WP_S \end{aligned} \quad [4]$$

The aeration stress factor  $S_{Ac}$  considers the effect of poor aeration in highly saturated soils. The influence of this factor is calculated as

$$\begin{aligned} S_{Ac} &= S_{FT} + (1 - \theta_c) \frac{1 - S_{FT}}{1 - \theta_{cC}} & \theta_c \geq \theta_{cC} \\ S_{Ac} &= 1 & \theta_c < \theta_{cC} \end{aligned} \quad [5]$$

where  $\theta_c$  is the water-filled porosity, which is defined as the ratio of the actual water content and the saturated water content, and  $\theta_{cC}$  is the critical water-filled porosity above which the root system is affected by poor aeration. This value can be either defined by the user or calculated based on the approach given by Jones et al. (1991) from soil texture.

The parameter  $S_{FT}$  (0–1), which is crop type dependent, defines the fraction of normal root growth when the pore space is saturated. Its value has to be defined by the user. Setting  $S_{FT}$  equal to 1 implies that flooding has no effect on root growth. A value of 0 means that there is no growth in saturated soils.

An overview of several approaches to describe the influence of temperature on root growth rates using different mathematical expressions was provided by Yan and Hunt (1999) and Li et al. (2008). In our study, two functions were considered to account for the crop-specific dependence of root growth on temperature and to define the temperature stress factor. The approach of Yin et al. (1995) considers a flexible, bell-shaped, nonlinear function:

$$\begin{aligned} S_T(t, T) &= \left\{ \left[ \frac{T_c - T(t)}{T_c - T_{opt}} \right] \left[ \frac{T(t) - T_{min}}{T_{opt} - T_{min}} \right]^{(T_{opt} - T_{min}) / (T_c - T_{opt})} \right\}^{ct} \\ S_T(t, T) &= 0 & \text{for } T(t) < T_{min} \text{ and } T(t) > T_c \end{aligned} \quad [6]$$

where  $T$  is the temperature at the current time level,  $T_{min}$  is the minimum temperature when root growth starts,  $T_c$  and  $T_{opt}$  are the critical and optimum temperatures for root growth, respectively, and  $ct$  denotes the shape coefficient of the bell function. The second function is a sinusoidal stress function, which was described by Jones et al. (1991):

$$\begin{aligned} S_T(t, T) &= \sin \left[ \frac{\pi}{2} \frac{T(t) - T_{min}}{T_{opt} - T_{min}} \right] \\ S_T(t, T) &= 0 & \text{for } T(t) < T_{min} \\ S_T(t, T) &= 1 & \text{for } T(t) > T_{opt} \end{aligned} \quad [7]$$

where  $T$  is again temperature at the current time level, and  $T_{min}$  and  $T_{opt}$  are the minimum and optimum temperatures for root growth, respectively. HYDRUS users can select whether to use air temperature or temperature in the root zone in the temperature stress functions Eq. [6] and [7].

The difference in shapes between the two considered stress factor functions is displayed in Fig. 1. Both approaches use genotype-based parameters such as the minimum, optimum, and critical temperatures for root growth. These parameters, also referred

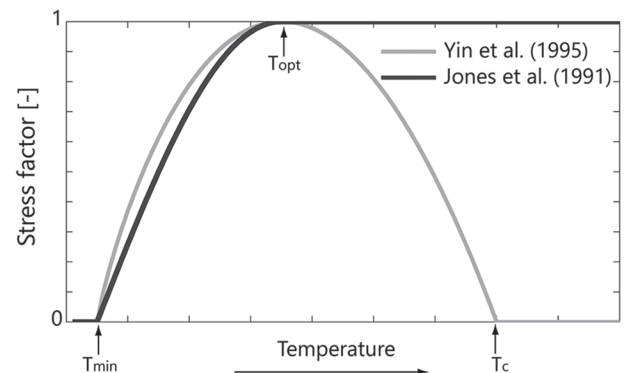


Fig. 1. Temperature stress functions according to Yin et al. (1995) and Jones et al. (1991). The positions of the cardinal temperatures—the minimum ( $T_{min}$ ), optimum ( $T_{opt}$ ), and critical ( $T_c$ ) temperatures for root growth—influence the skewness of the graphs.

to as *cardinal temperatures*, are crop specific and can be found in the literature for several crop types (e.g., Yan and Hunt, 1999). The equation by Yin et al. (1995) accounts for a reduction in root growth due to high temperatures. The equation of Jones et al. (1991) considers only a reduction in root growth due to low temperatures and assumes that root growth is not affected by temperatures above the optimum temperature.

It is possible to enable or disable the consideration of each individual stress factor when using the newly developed HYDRUS add-on module. Consequently, not all stress factors have to be considered simultaneously during simulations.

## Root Growth

Two approaches are implemented to calculate the actual rooting depth. In the first approach, the ordinary differential equation describing population growth is used to calculate the time-dependent development of the rooting depth:

$$\frac{dL_r}{dt} = rL_r \left( 1 - \frac{L_r}{L_m} \right) \quad [8]$$

where  $L_r$  [L] is the potential rooting depth when no stresses occur,  $L_m$  [L] is the maximum possible rooting depth,  $t$  is time [T], and  $r$  [T<sup>-1</sup>] is the growth rate. The actual rooting depth can be calculated by incorporating the stress factors directly into Eq. [8]:

$$\frac{dL_a}{dt} = rS(t)L_a \left( 1 - \frac{L_a}{L_m} \right) \quad [9]$$

where  $S(t)$  (dimensionless) represents environmental stresses and  $L_a$  [L] is the actual rooting depth subject to environmental stresses. By rearranging this equation and solving it using an explicit scheme,  $L_a$  can be computed at each time step:

$$L_a(t_i) = L_a(t_{i-1}) + r \min[S_1(t_i), S_2(t_i)] L_a(t_{i-1}) \times \left[ 1 - \frac{L_a(t_{i-1})}{L_m} \right] (t_i - t_{i-1}) \quad [10]$$

where  $S_1$  and  $S_2$  (dimensionless) are stress factors influencing the vertical penetration of roots according to Jones et al. (1991).

With this approach, previous reductions in root growth are taken directly into consideration when evaluating future root system development. Because the growth of the root system depends on the growth of the shoot, this approach implies that the root system is the limiting factor for the entire crop development. Thus, root and shoot growth are assumed to be synchronized, and previous reductions in root development will affect shoot development, which in turn affects future root growth.

Because a reduction in the root growth rate does not necessarily imply an equal reduction in the shoot growth rate, the second

approach accounts heuristically for the impact of various stresses on the reduction of root growth. This approach is based on using a time-dependent growth function to calculate the potential increase in the rooting depth at each time step. In this second approach, two time-dependent growth functions are considered to describe the potential increase in the rooting depth with time.

The first function is the Verhulst–Pearl logistic growth function, which is the analytical solution of Eq. [8], which has already been implemented in the standard HYDRUS-1D code and is now also available in the updated HYDRUS-2D code (Šimůnek et al., 2016):

$$L_r(t_i) = \left( \frac{L_o}{L_o + (L_m - L_o) \exp(-rt_i)} \right) L_m \quad [11]$$

where  $L_r$  [L] and  $L_o$  [L] are the potential and initial rooting depths, respectively,  $L_m$  [L] is the maximum possible rooting depth,  $r$  [T<sup>-1</sup>] is the growth rate, and  $t_i$  [T] is the time step. The second function to describe time-dependent root growth is a sinusoidal function proposed by Borg and Grimes (1986) based on analysis of 135 field observations of 48 crop species:

$$L_r(t_i) = L_m \left\{ 0.5 + 0.5 \sin \left[ 3.03 \left( \frac{t_i}{t_m} \right) - 1.47 \right] \right\} \quad [12]$$

where  $L_r$  and  $L_m$  are again the potential and the maximum possible rooting depths, respectively, and  $t_m$  [T] is the time when the maximum rooting depth is achieved.

The difference between rooting depths under unstressed conditions at two sequential points in time denotes a potential increase in the rooting depth:

$$d_p(t_i) = L_r(t_i) - L_r(t_{i-1}) \quad [13]$$

where  $d_p$  [L] is the potential increase in the rooting depth,  $L_r$  [L] is the potential rooting depth at a certain point in time calculated using a time-dependent root growth function, and  $t_i$  [T] is the time step. Thus,  $d_p$  denotes an increase in the rooting depth when zero influence by any environmental factor such as temperature is considered during the entire root growth period. The potential growth function thus assumes optimal conditions not only at a particular time but also prior to this time.

The actual increase in the rooting depth  $d_r$  [L] is calculated using the stress factors  $S_i$  (dimensionless):

$$d_r(t_i) = d_p(t_i) \min[S_1(t_i), S_2(t_i), S_0(t_{i-1})] \\ S_1 = \min(S_T, S_{Ca}, S_{Al}) \\ S_2 = \min(S_{St}, S_{Ac}, S_{CF})^{0.5} \\ S_0 = \frac{L_a(t_{i-1})}{L_r(t_{i-1})} \quad [14]$$

Integration of actual increases in rooting depths with time leads to the actual rooting depth  $L_a$ .

The approach of Jones et al. (1991) assumes that the environmental stresses  $S_{St}$ ,  $S_{Ac}$ , and  $S_{CF}$  have a lower influence on root growth due to possible compensation effects and that the most limiting stress factor determines the reduction in root growth. Other approaches can be found in the literature. For example, Somma et al. (1998) assumed that the potential increase in the rooting depth is multiplied by all stress factors accounting for the effects of soil strength, temperature, and nutrient concentration. Prasad et al. (2008) also discussed the influence of combined stresses. They pointed out that applying the minimum stress factor is a common procedure in many models but also stated that describing the interactions of different stress factors is still one of the greatest challenges in crop modeling. Because the combined effects of multiple stress factors are unknown, the approach proposed by Jones et al. (1991) was selected in this study.

The parameter  $S_0$  in Eq. [14] introduces an additional active stress factor into the calculation of the actual increase in the rooting depth that takes into account the influence of past reductions in growth. This factor is defined as the ratio of the actual rooting depth to the potential rooting depth at the previous time step. As a result, past reductions in root growth affect actual root growth. The same approach is used in HYDRUS-2D for both vertical and horizontal extents of the rooting system. While in HYDRUS-1D the stress factors are evaluated at the rooting depth, in the HYDRUS-2D model the stress factors reflect average conditions in the root zone.

We have implemented these two approaches because we believe that they their own advantages and disadvantages and thus can be complementary to HYDRUS users. For example, the former (theoretical) approach ultimately leads to the actual rooting depth reaching the maximum rooting depth as long as there is enough time for that. Note that growth continues as long as  $[(1 - L_a(t_{i-1})/L_m)]$  in Eq. [10] is positive. In this approach, future growth can thus fully compensate for past stresses. On the other hand, in the latter (heuristic) approach, earlier reductions in root growth have a permanent effect on future growth.

### Root Length Density Distribution

Five additional functions (Jones et al., 1991; Vrugt et al., 2001b; Hao et al., 2005) describing the spatial distribution of the root length density have been implemented into the root growth module of HYDRUS-1D (Table 2) in addition to the Hoffman and van Genuchten (1983) root distribution function, which was available previously. The functions listed in the table are expressed using a normalized rooting depth,  $z_r$ . While the functions in Table 2 are dimensionless, they are always internally normalized in the HYDRUS models so that their integration over depth is equal to 1. In the HYDRUS models, the time-dependent actual rooting

Table 2. Root length density distribution  $b(z_r)$  models implemented in HYDRUS-1D.

Model	$b(z_r)†$	Reference
1	$2.938 - 2.462z_r$	modified after Zuo et al. (2004)
2	$4.522(1 - z_r)^{5.228} \exp[(9.644z_r)2.426]$	
3	$2.21 - 3.72z_r + 3.46(z_r)^2 - 1.87(z_r)^2$	Wu et al. (1999)
4	$(1 - z_r) \exp[-(P_z/z_m) z^* - z_r]$	Vrugt et al. (2001a)
5	$1 - z_r/3)^3$	Jones et al. (1991)

†  $z_r$ , normalized rooting depth;  $P_z$  and  $z^*$ , empirical parameters.

depth is an important input factor for these functions to calculate the root length density distribution. Of these functions, the root length density distribution model proposed by Vrugt et al. (2001b) is the most flexible model. Root length density distributions given by these functions represent the potential root length density distribution pattern, which would be obtained under optimal conditions when no restrictions of root growth, such as root senescence, were considered.

The actual root length density distribution is calculated similarly to the actual rooting depth. The actual increase in root length density (RLD<sub>ga</sub>) at each time step is derived from the potential increase (RLD<sub>gp</sub>), which is defined as the difference between the root length density distribution  $[b(z_r)]$  at the current ( $t_i$ ) and previous ( $t_i - 1$ ) time steps:

$$\text{RLD}_{gp}(t_i) = b(z_r, t_i) - b(z_r, t_{i-1}) \quad [15]$$

An increase in the potential root length density in each node can be reduced due to root senescence. This approach is used in HYDRUS-1D as well as in HYDRUS-2D. Similarly to the original version of the approach of Jones et al. (1991), the adapted version implemented into HYDRUS considers root senescence during the life of the plants. Only a few minor changes had to be made in the modeling approach of Jones et al. (1991) to make it compatible with HYDRUS. In HYDRUS, the root senescence (Sen) is calculated as

$$\text{Sen}(t_i) = r_d \text{RLD}_{gp}(t_i) \{1 + \max[1 - \theta_f(t_i), 1 - S_{AE}(t_i)]\} \quad [16]$$

where  $r_d$  is a scaling factor (0–1) defining the influence of root senescence. This approach assumes that root senescence can be increased due to low water availability or poor aeration. More information regarding the evaluation of root senescence was provided by Hartmann and Šimůnek (2015).

The actual root length density distribution  $b_a(t_i)$  is then calculated as

$$\begin{aligned} b_a(t_i) &= b_a(t_{i-1}) + \text{RLD}_{ga}(t_i) \\ \text{RLD}_{ga}(t_i) &= \text{RLD}_{gp}(t_i) - \text{Sen}(t_i) \end{aligned} \quad [17]$$

The implemented root growth module was used to simulate the impact of various environmental factors on root growth using two hypothetical examples.

## Experiment Description and Measurements

Jones et al. (1991) stated that their approach is only the first approximation of the effects of environmental factors on root growth that needs to be verified against experimental data. Experimental data from an aeroponic system (described below) were selected to evaluate the described approach to model the influence of temperature on the vertical penetration of the root system. The experimental setup in an aeroponic system with no soil and no water movement has the advantage of evaluating the effects of temperature on root growth while limiting the effects of other factors.

The experiment was conducted in a greenhouse with bell pepper at the Jacob Blaustein Institutes for Desert Research, in Midreshet Ben-Gurion, Israel (30°51'5" N, 34°47'0" E, altitude 480 m). The objective was to evaluate the effect of three different root zone temperatures on root and plant growth. Six bell pepper plants were cultivated from 7 Jan. to 20 Feb. 2015 in aeroponic pots mounted on top of the aeroponic systems. The aeroponic apparatus comprised circular pots made from plastic material with a diameter of 50 cm and a depth of 14 cm. Within each thermally isolated aeroponic pot, misters (Coolnet, Netafim Israel) were fixed to produce the desired fine mist sprayed directly onto the plant roots. The computer-controlled spraying varied from 8-s sprayings at 1-min intervals, depending on the growth stage (size) of the plants and the temperature of the greenhouse. Three different water temperatures were applied to each treatment, namely 7, 17, and 27°C. The air and root zone temperatures were measured daily. The air temperatures in the greenhouse were 25°C during the day and 18°C at night. The treatments were replicated twice, leading to six tanks in total. The maximum rooting depth of each plant was observed four times during the 44 d of plant growth. In the aeroponic systems, all other factors that affect the growth and development of roots were rendered insignificant during the treatment.

## Validation of the Temperature-Dependent Root Growth Modeling Approach

### Evaluated Models

The implemented modeling approach to simulate the temperature-dependent vertical root penetration was evaluated by comparing modeling results with the measured maximum rooting depths in the experimental aeroponic system with bell pepper. Because two approaches were implemented in HYDRUS to describe both time-dependent potential root growth and the temperature stress factor, four combinations are thus available to describe the temperature-dependent root growth. All four models were tested against measured maximum rooting depths to validate their ability to describe the temperature- and time-dependent vertical root penetration. The four combinations are summarized in Table 3. Were the these root growth models (see Table 3) able to properly

Table 3. Overview of four models (combinations of time-dependent potential root growth and the temperature stress factor equations) used in this study to evaluate the temperature-dependent root growth.

Model	Potential root growth	Temperature stress factor
A	Verhulst–Pearl logistic growth	Jones et al. (1991)
B	Verhulst–Pearl logistic growth	Yin et al. (1995)
C	Borg and Grimes (1986)	Jones et al. (1991)
D	Borg and Grimes (1986)	Yin et al. (1995)

simulate the influence of temperature on vertical root penetration, a single combination of model parameters for each model that could reproduce the measured maximum rooting depths for all temperature treatments would have to exist.

An overview of the model parameters that have to be specified for each model is given in Table 4. Table 4 shows that, depending on the model, four or six parameters have to be specified to model temperature-dependent root growth. In a complex soil water flow model such as HYDRUS, four to six additional parameters can significantly increase the calibration effort and parameter uncertainties. The temperature-dependent modeling approach was tested outside of the HYDRUS implementation and within a MATLAB environment. The goal of the evaluation was to determine whether the combination of the time-dependent root growth functions and the temperature stress functions were able to reproduce the measured rooting depths under the given boundary conditions.

## Sensitivity Analysis

A global sensitivity analysis was conducted using the Sobol' method to reveal the key parameters of each model and to determine the contribution of the uncertainty of each parameter to the uncertainty of the model output. The Sobol' method is based on variance decomposition and provides the impact of each parameter and its interactions with other parameters on the model output (Sobol', 1993). This type of global sensitivity analysis can be applied to nonlinear and non-monotonic models and is a widely used tool for sensitivity analysis studies. Its ability to account for interactions between model parameters is an important advantage of the Sobol' method (Rosolem et al., 2012).

Table 4. Parameters of the four models for calculating time- and temperature-dependent root growth.

Model	Parameters†
A	$L_m, r, T_{min}, T_{opt}$
B	$L_m, r, T_{min}, T_{opt}, T_c, ct$
C	$L_m, T_{min}, T_{opt}, t_m$
D	$L_m, T_{min}, T_{opt}, t_m, T_c, ct$

†  $L_m$ , maximum possible rooting depth;  $r$ , growth rate;  $T_{min}$ , minimum temperature when root growth starts;  $T_{opt}$ , optimum temperature for root growth;  $T_c$ , critical temperature for root growth;  $ct$ , shape of the bell function;  $t_m$ , time when the maximum rooting depth is achieved.



An overview of studies using the Sobol' method for sensitivity analysis in hydrological modeling was provided by Song et al. (2015). The method has already been applied with the HYDRUS software package by Li et al. (2012), Brunetti et al. (2016) (HYDRUS-1D), and Wang et al. (2016) (HYDRUS-2D).

Sobol' (1993) proposed that the total variance of the model output can be decomposed into component variances of individual parameters and their interactions. The first-order sensitivity index quantifies the main effect of the  $i$ th parameter,  $X_i$ . This sensitivity index denotes the part of the total variance due to  $X_i$  without considering the interactions with other parameters. The total-order sensitivity index additionally includes the proportion of the variance due to the interactions of  $X_i$  with the other parameters. The values of the indices vary from 0 to 1, where 0 stands for no influence and 1 for a high influence on the variance.

The first-order ( $S_i$ ) and total-order sensitivity ( $S_{ti}$ ) indices were approximated by a numerical Monte Carlo estimation proposed by Saltelli et al. (2010):

$$S_i = \frac{(1/N) \sum_{j=1}^N f(\mathbf{B})_j \left[ f(\mathbf{A}_B^i)_j f(\mathbf{A})_j \right]}{(1/N) \sum_{j=1}^N \left[ f(\mathbf{A})_j \right]^2 - f_o^2} \quad [18]$$

$$S_{ti} = \frac{(1/2N) \sum_{j=1}^N \left[ f(\mathbf{A})_j - f(\mathbf{A}_B^i)_j \right]^2}{(1/N) \sum_{j=1}^N \left[ f(\mathbf{A})_j \right]^2 - f_o^2} \quad [19]$$

where  $\mathbf{A}$  and  $\mathbf{B}$  denote two matrices of data sets generated using Sobol' quasi-random sequences, which consist of a sample of numbers between 0 and 1 distributed in a  $p$ -dimensional unit hypercube. In Eq. [18],  $\mathbf{A}_B^i$  denotes a matrix where all columns are from Matrix  $\mathbf{A}$  except for the  $i$ th column, which is from Matrix  $\mathbf{B}$ , and  $f_o$  is calculated as  $(1/N) \sum_{j=1}^N f(\mathbf{A})_j$ . Each matrix has the dimension  $N \times p$ , whereby  $p$  is the number of parameters and  $N$  denotes the number of required simulation runs. Each matrix thus consists of  $N$  sets of parameters.

The parameters were transformed into their defined parameter space based on the specified minimum and maximum values of the parameters (listed in Table 5). Parameter limits for rooting depths under favorable environmental conditions were taken from Borg and Grimes (1986). The limiting values of cardinal temperatures were specified based on information provided by Saha et al. (2010). The limits of parameter  $t_m$  were chosen in a way that common durations of vegetation periods would lie within these boundaries.

Parameters  $f(\mathbf{A})$  and  $f(\mathbf{B})$ , as well as  $f(\mathbf{A}_B^i)$ , represent the model output in the form of a chosen statistical metric. In this study, the root mean square error (RMSE) was chosen for the statistical metric:

Table 5. Upper and lower boundaries of the parameter space for the parameters of the four models considered in the sensitivity analysis and optimization.

Parameter†	Lower boundary	Upper boundary	Value for sensitivity analysis
$L_m$ , cm	70	150	110
$r$ , $d^{-1}$	0.1	1	0.15
$T_{min}$ , °C	0	19	8
$T_{opt}$ , °C	20	32	23
$T_c$ , °C	33	50	35
ct	0.01	100	0.15
$t_m$ , d	43	365	150

†  $L_m$ , maximum possible rooting depth;  $r$ , growth rate;  $T_{min}$ , minimum temperature when root growth starts;  $T_{opt}$ , optimum temperature for root growth;  $T_c$ , critical temperature for root growth; ct, shape of the bell function;  $t_m$ , time when the maximum rooting depth is achieved.

$$RMSE = \sqrt{\frac{\sum (L_{Obs} - L_{Sim})^2}{n}} \quad [20]$$

which describes the square root of the average squared differences between the observed ( $L_{Obs}$ ) and simulated ( $L_{Sim}$ ) rooting depths. The RMSE measure was selected to evaluate prediction errors because only one output of the root growth models, i.e., the rooting depth, was analyzed in the sensitivity analysis.

The number of parameter sets ( $N$ ) in the sensitivity analysis of the four models was set to 10,000. This number was initially set higher than in studies of Brunetti et al. (2016) and Zhang et al. (2013) to avoid a time-consuming convergence analysis of the sensitivity analysis and to achieve a higher accuracy of the sensitivity analysis, which increases with an increasing number of model runs. The  $p$  parameter depends on the considered model and is either four (for Models A and C) or six (for Models B and D). To calculate the sensitivity indices for all  $i = 1, \dots, p$  parameters, Matrix  $\mathbf{A}_B^i$  has to be evaluated  $p$  times. The total number of model runs required to calculate the sensitivity indices for all parameters of each model were  $M = N(2 + p)$ . Archer et al. (1997) suggested using bootstrap confidence intervals (Efron and Tibshirani, 1993) to evaluate a suitable accuracy of the sensitivity estimates. For this reason, each estimation of the sensitivity indices was repeated 500 times to evaluate the 25th and 75th percentiles of the sensitivity indices. The small number of repetitions is due the fact that the sensitivity analysis of four models, each including four or six parameters, requires a high level of computational effort. Evaluated percentiles were used only as an additional parameter to assess the sensitivity indices (Archer et al., 1997).

Rather than using experimental data, which may be subject to various errors and effects of various factors, the sensitivity analysis was performed using a hypothetical data set in which observed rooting

depths  $L_{Obs}$  were generated by running all four models (Table 3) with a predefined parameterization. The cardinal temperatures  $T_{min}$ ,  $T_{opt}$ , and  $T_c$  were set to 8, 23, and 27°C, respectively. A complete list of parameter values for the model runs is provided in Table 5. The boundary conditions were similar to those of the aeroponic experiments. The temperature was set to 22°C during the first 14 d and to either 7, 17, or 27°C during the remaining time period of 150 d. Additionally, a fourth scenario was considered with a temperature of 37°C after the first 2 wk to make sure that the specified cardinal temperatures would lie within the applied boundary conditions to determine their influence on the model output. Each model was thus executed four times with four different temperature boundary conditions to generate data for  $L_{sim}$  in Eq. [20].

### Parameter Optimization

The Differential Evolution Adaptive Metropolis (DREAM) algorithm (Vrugt et al., 2009; Vrugt, 2016) was used for optimizing the model parameters and for model calibration. The DREAM algorithm is based on Bayesian statistics; it runs multiple different Markov chains to generate a random walk through the search space. Based on a proposal distribution, the sampler evolves to the posterior distribution by iteratively finding solutions with stable frequencies stemming from the fixed probability distribution (Laloy and Vrugt, 2012). The Gaussian likelihood function was used to summarize the distance between model simulations and corresponding observations. The residuals were assumed to be independent (uncorrelated) and normally distributed while the measurement error was neglected. The latest MATLAB implementation of DREAM (Vrugt, 2016) was used for model parameter optimization.

Eight Markov chains were run with a set of 5000 generations. The initial state of each chain was sampled from a Latin hypercube. The parameter space of each parameter was defined by using the same boundaries as were used for the sensitivity analysis (see Table

5). These parameter limits also define the search domain for the predominantly physically based parameters (Vrugt, 2016). The calculation time for the DREAM optimization of a single model was approximately 10 min, with no parallelization needed on a machine with the following specifications: Intel Core i7–4710HQ CPU with 2.50 GHz of RAM and 12 GB of storage.

## Results and Discussion

We evaluating the effects of different factors on root growth with two examples using the new root growth module in HYDRUS-1D and HYDRUS-2D. Then we analyzed the collected experimental data and the evaluation of the temperature-dependent root growth modeling approach. Therefore, we first collected data on the experimental outcomes. Second, we carried out the sensitivity analysis to evaluate the sensitivity of the modeling results to various input parameters and identified which parameters need to be fitted and which can be set to values from the literature. Third, we used the DREAM optimization approach to analyze the collected experimental data while considering the results of the sensitivity analysis.

### Applications of the Root Growth Module

We used two hypothetical examples that demonstrate the implemented root growth model and the impact of various environmental factors on root growth. In the first example, we used HYDRUS-1D and simulated optimal root growth as well as root growth restricted due to low water availability, temperature, texture, and bulk density. In the second example, we used HYDRUS-2D to again simulate optimal root growth and then root growth affected by a nonuniform distribution of water contents due to asymmetrical irrigation.

#### HYDRUS-1D Examples

Figure 2 shows examples of the development of simulated root systems under the influence of various environmental factors (Scenarios 1–4) compared with the potential development of the

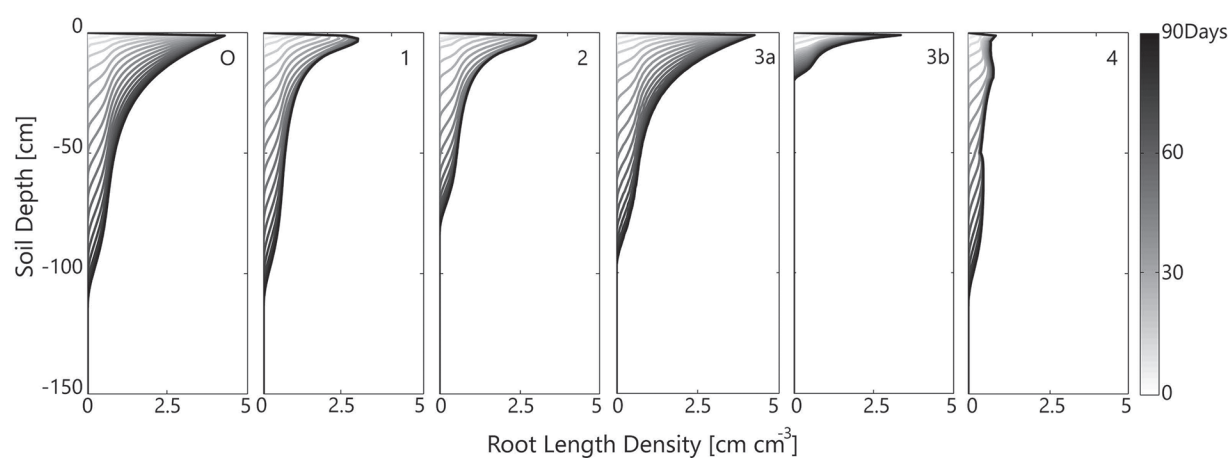


Fig. 2. Simulated potential (0) and actual (1–4) root length density distributions at different times (different shades of gray): (1) under drought conditions, (2) under the influence of texture and bulk density, (3a and 3b) under the influence of different root zone temperatures, and (4) in a heterogeneous soil system.

root system, independent of environmental factors (Scenario 0). The soil profile was considered to be homogenous, consisting of 10% sand, 50% silt, and 40% clay and having the bulk density of  $1530 \text{ kg m}^{-3}$ . The parameters for the soil hydraulic functions of van Genuchten (1980) and Mualem (1976) were estimated from the textural information using the Rosetta module of HYDRUS-1D. Time-dependent root growth was simulated using the function of Borg and Grimes (1986). Model 2 from Table 2 was selected to describe the potential root length density distribution. The maximum potential rooting depth ( $L_m$ ) was set to 120 cm, and root growth was considered for 90 d ( $t_m$ ). The upper and lower boundary conditions were set to atmospheric boundary conditions with surface runoff and free drainage, respectively.

In Scenario 1, the development of the root length densities was simulated for drought conditions, which may cause aeration stress and root senescence (both options were enabled in this simulation). Potential evaporation and transpiration rates were set to increase stepwise at the beginning (up to 28 d) and remain constant at the end of the simulation. Irrigation took place at irregular intervals (only every 3–6 d) and covered only 25% of the potential evapotranspiration. Due to low water availability, the root system was underdeveloped compared with the reference simulation when no restrictions on root growth were considered (Scenario 0). The root length density in this scenario is reduced compared with Scenario 0, mainly close to the soil surface because the drought stress is highest in soil horizons with the highest root water uptake.

Scenario 2 considered the effects of texture and bulk density (the option of the soil strength stress factor was additionally enabled) on the development of the root length densities and vertical root penetration. The results show that due to the increased soil strength (a high clay content and a high bulk density), the potential maximum rooting depth of 120 cm was not reached. The additional stress due to the soil strength negatively influenced the vertical penetration of roots, in addition to the effects of root senescence due to the drought stress in Scenario 1.

Scenario 3 considered the influence of different root zone temperatures on the root length density development. In this case, only the option to consider the influence of temperature on root growth was enabled. The development of the root system was simulated using the root growth function of Borg and Grimes (1986) in combination with the temperature stress function of Jones et al. (1991). The parameters  $T_{\min}$ ,  $T_{\text{opt}}$ , and  $t_m$  were set to  $5^\circ\text{C}$ ,  $35^\circ\text{C}$ , and 90 d, respectively. The temperature throughout a soil depth of 150 cm was set to a constant value of  $10^\circ\text{C}$ . The temperature at the soil surface was set to  $25^\circ\text{C}$  during the first 14 d and to 30 and  $7^\circ\text{C}$  in Scenarios 3a and 3b, respectively, until the end of the simulation. The results show that the root system in Scenario 3b, which was exposed to temperatures close to  $T_{\min}$ , was underdeveloped compared with the root system in Scenario 3a, which was exposed to temperatures close to  $T_{\text{opt}}$ . The root system under conditions that were close to the

optimum temperature showed greater growth rates and thus reached deeper depths and developed greater root length densities than the root system under non-optimum temperature conditions.

Finally, an additional soil horizon, consisting of 24% sand, 64% silt, and 12% clay and having the bulk density of  $1290 \text{ kg m}^{-3}$ , was specified between 20 and 50 cm in Scenario 4. The same stress factors as in Scenario 2 were enabled. The results for this scenario show that, due to the different properties of the additional soil horizon, which affect water availability and  $\text{O}_2$  supply, the development of the root length density distribution can be highly influenced. The results show that the root length density can be spatially altered due to a spatial distribution of stress factors. In this case, unfavorable growing conditions led to a reduction of root length density in the middle layer.

## HYDRUS-2D Examples

Figure 3 shows the simulated potential and actual two-dimensional development of the root system in a homogeneous soil consisting of 50% sand, 20% silt, and 30% clay and having a bulk density of  $1510 \text{ kg m}^{-3}$ . The parameters for the soil hydraulic functions of van Genuchten (1980) and Mualem (1976) were estimated using the Rosetta module of HYDRUS-2D. The lower boundary condition was set to free drainage. The simulation time was set to 60 d, and root growth was considered until the end of the simulation. Potential transpiration was set to  $0.1 \text{ mm d}^{-1}$  between the first day and Day 11. From Days 12 to 29, potential transpiration was set to  $1 \text{ mm d}^{-1}$ ; from Day 30 until the end of the simulation, it was set to  $2 \text{ mm d}^{-1}$ . Irrigation was applied at a rate of  $2 \text{ mm d}^{-1}$  between Days 30 and 50 only in the top left corner (10 cm), while the rest of the soil surface remained unirrigated. Potential evaporation was specified only for the unirrigated soil surface, with a rate of  $0.1 \text{ mm d}^{-1}$  from the beginning until Day 15,  $1 \text{ mm d}^{-1}$  between Days 16 and 18, and  $2 \text{ mm d}^{-1}$  from Day 19 until the end of the simulation. In addition to water availability and aeration, the texture and bulk density were also considered influences on root growth. Only one plant in the middle of the domain was specified with a potential rooting depth in the vertical direction of 100 cm and 30 cm in the horizontal direction. The root length density function of Vrugt et al. (2001a, 2001b) predicts an axially symmetrical shape of the potential root length density distribution.

Asymmetrical irrigation results in an unequal development of the root system. The root system is more developed on the left-hand side of the transport domain than the right-hand side due to greater water availability. Additionally, the root system simulated under the influence of growth restrictions showed a smaller rooting depth than the reference simulation when no restrictions on root growth were considered.

## Experimental Outcomes

The observed maximum rooting depths significantly differed among the three treatments. After 44 d, the average rooting depths

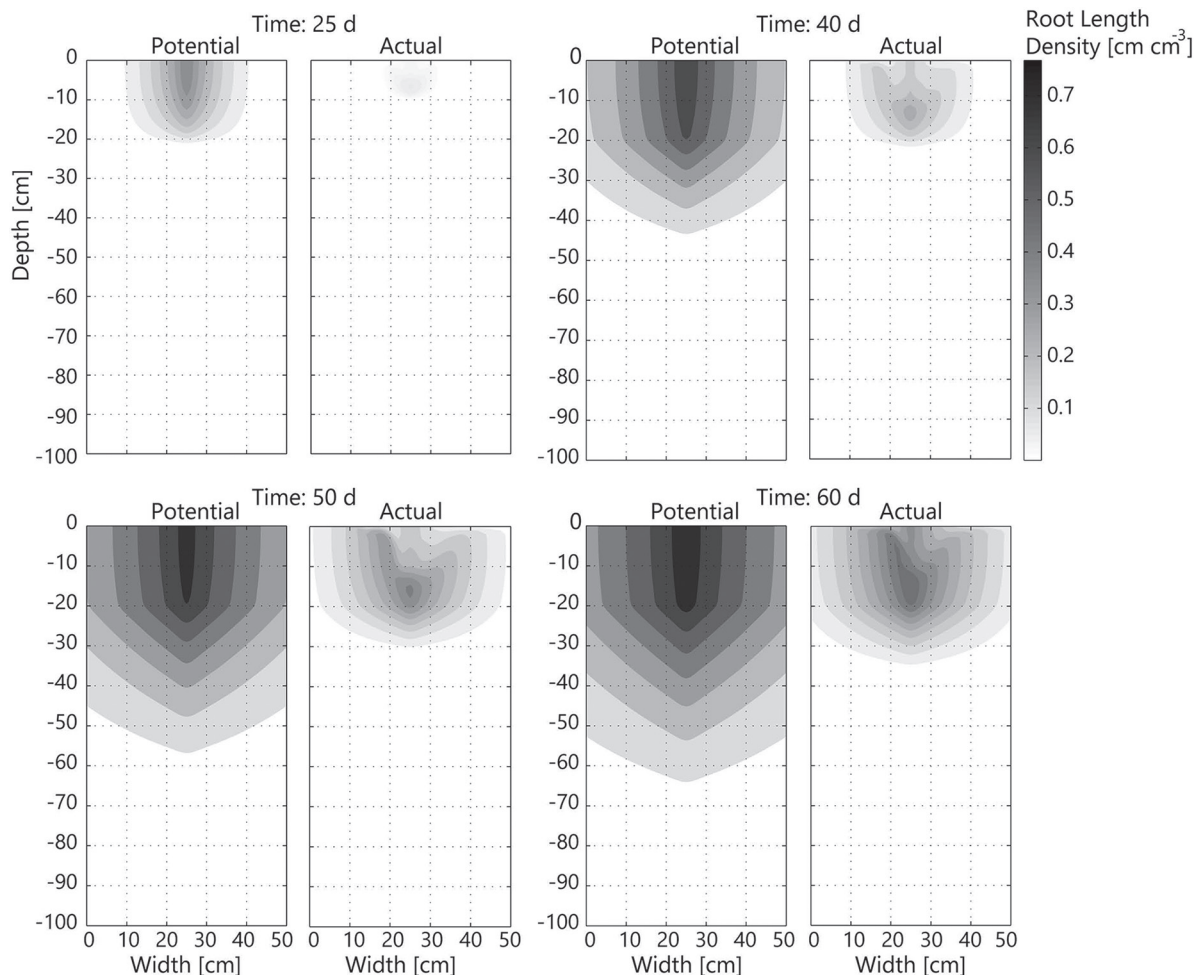


Fig. 3. Potential and actual two-dimensional root system development at different times when irrigation was applied in the top left corner.

for the treatments with root zone temperatures of 7, 17, and 27°C were 19, 47, and 72 cm, respectively. The biomass above ground showed the same trend.

### Sensitivity Analysis

The results of the global sensitivity analysis in the form of the total- and first-order sensitivity indices of all parameters of the four root growth models are shown in Fig. 4. The light gray bars represent the contribution of each individual parameter to the variance of the model output (the first-order sensitivity). The dark gray bars represent the individual parameter contributions, as well as the contributions of their interactions with the other parameters to the variance of the model output.

The results of the sensitivity analysis (Fig. 4) reveal that the differences among the influences of different parameters in Models A and C are more pronounced than between different parameters in Models B and D. The differences between the sensitivity indices of different parameters of Models B and D are not very different from each other. Figure 4 reveals that the plant-specific cardinal temperatures  $T_{opt}$ ,  $T_{min}$ , and  $T_c$  and the plant-specific parameter  $L_m$  (the maximum rooting depth reached when no

environmental stresses are present) have only a minimal impact on the model outcome. Because these parameters are biologically based and specific for a particular crop cultivar, their values can be found in the literature and do not have to be calibrated. For example, Yan and Hunt (1999) provided cardinal temperatures for sorghum [*Sorghum bicolor* (L.) Moench], wheat, barley, bean (*Phaseolus vulgaris* L.), and maize, and Li et al. (2008) provided a list of sources for cardinal temperatures for winter wheat. Borg and Grimes (1986) provided an overview of  $L_m$  for several crops.

Specifying parameters that do not exert a large influence on the model output using values found in the literature reduces the number of calibrated parameters and thus the complexity and effort of the calibration task. By defining a limit of 0.3 for the total sensitivity index to neglect the parameter influence, the number of calibrated parameters of Model A can be reduced from four to two. Based on the results in Fig. 4, the number of calibrated parameters of Model B can be reduced from six to one. However, because no information about parameters  $r$  and  $ct$  could be found in the literature, these parameters need to be considered within the model calibration. The number of calibrated parameters could thus only be reduced to two for Model B. Yan and Hunt (1999) suggested

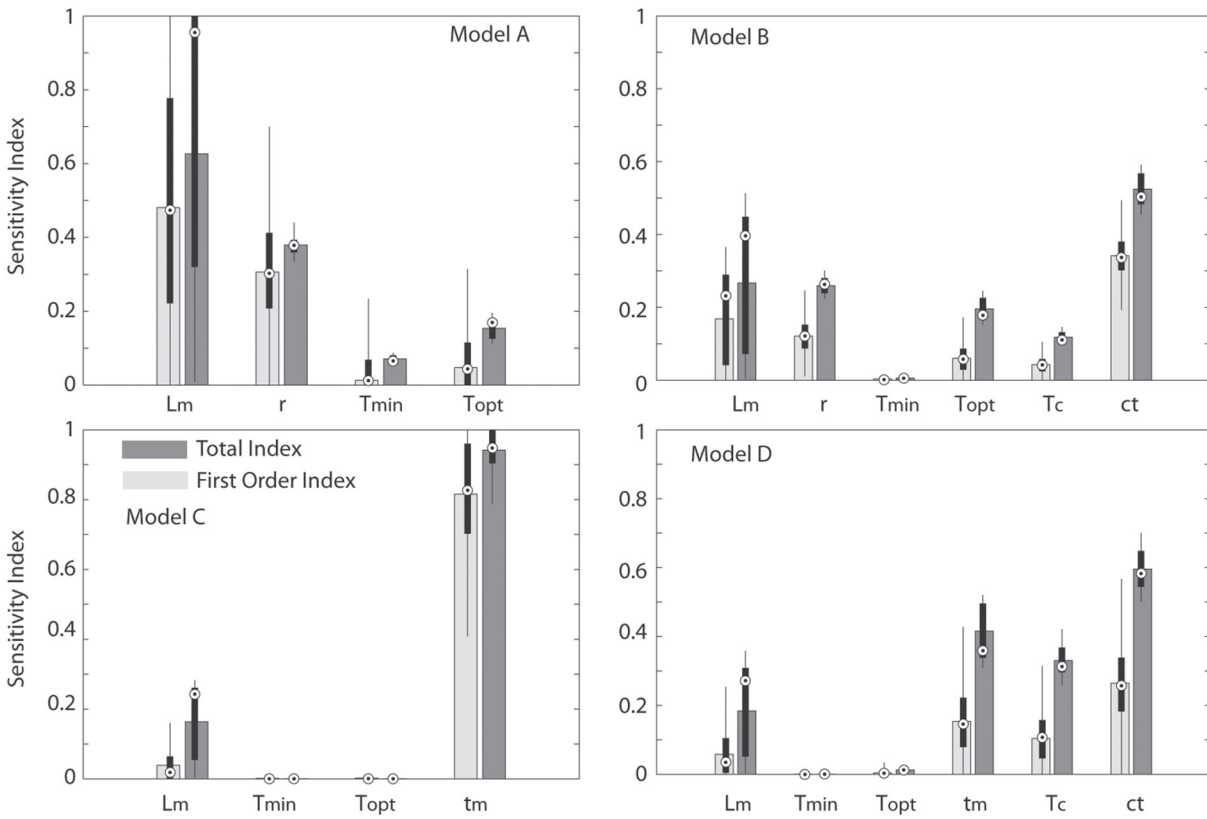


Fig. 4. Total- and first-order indices for all parameters of the four root growth models. The bars represent the mean value of all evaluations, and the boxplots indicate the value of the median and the 25th and 75th percentiles;  $ct$  is the shape coefficient of the bell function,  $L_m$  is the maximum possible rooting depth,  $r$  is the growth rate,  $t_m$  is the time when the maximum rooting depth is achieved,  $T_{min}$  is the minimum temperature for root growth, and  $T_{opt}$  is the optimum temperature for root growth.

that reasonable results can be found by setting  $ct$  to 1. They also suggested that it may be possible to set  $T_{min}$  to  $0^{\circ}\text{C}$ , which could be acceptable for all crops except for summer crops.

The results of the global sensitivity analysis for Models C and D (when the sinusoidal growth function of Borg and Grimes [1986] is used) show that the parameter  $L_m$  is less important than in Models A and B. In these models, the parameter defining the time when plants reach maturity,  $t_m$ , demonstrates a high influence on the model output. Based on the results of the sensitivity analysis, the number of calibrated parameters can be reduced from four to a single parameter for Model C and from six to three for Model D, while the other parameters can be specified using values from the literature. In contrast to the other models, the results presented in Fig. 4 suggest the parameter  $T_c$  should be considered as a calibration parameter for Model D. Due to the lack of knowledge about the value of  $ct$ , this parameter should still be considered in the model calibration.

### Parameter Optimization

The optimized parameter values of all four modeling approaches are listed in Table 6. In addition to these, the table also provides an overview of the goodness of fit obtained by individual models determined by the RMSE. This value indicates how well

the rooting depths simulated by the models using the optimized parameter sets fit the observed maximum rooting depths.

Figure 5 visualizes the maximum rooting depths measured for all temperature treatments in the aeroponic system and simulated using the four models and the optimized parameter sets in Table 6. The upper left figure shows the simulation results for all four models compared with the average observed maximum rooting depths (averaged for six plants) in each tank. These averaged values were used as data in the comparison within the optimization task.

Table 6. Parameter values for all four models optimized using the DREAM optimization algorithm, including the maximum possible rooting depth ( $L_m$ ), the growth rate ( $r$ ), the minimum temperature when root growth starts ( $T_{min}$ ), the optimum temperature for root growth ( $T_{opt}$ ), the critical temperature for root growth ( $T_c$ ), the shape of the bell function ( $ct$ ), and the time when the maximum rooting depth is achieved ( $t_m$ ). The RMSE shows the goodness of fit of the model output to the measured data using the optimized parameter sets.

Model	$L_m$	$r$	$T_{min}$	$T_{opt}$	$T_c$	$ct$	$t_m$	RMSE
	cm	$\text{d}^{-1}$	$^{\circ}\text{C}$				d	cm
A	70	0.3	1.9	31.8	–	–	–	7.6
B	71.6	0.31	2.9	30.7	37	0.22	–	7.9
C	76.5	–	4.6	32	–	–	50.3	3.1
D	144.6	–	9.3	22.5	45.5	11.8	65	2.1

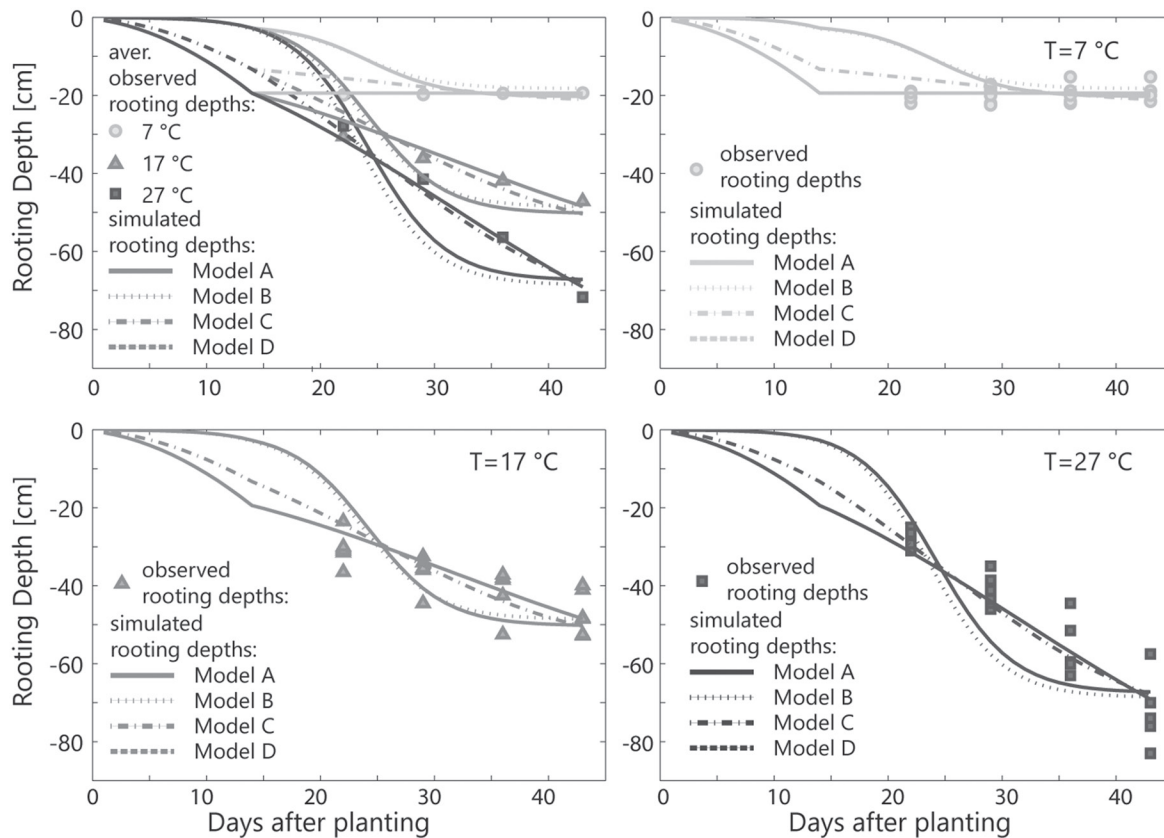


Fig. 5. Comparison of the rooting depths simulated using the parameter sets from Table 6 (all parameters were optimized) with those measured in the aeroponic system. Data (simulated and average observed) displayed in the upper left figure (for all three temperatures) were used to calculate the goodness of fit. The upper right, lower left, and lower right figures display the measured (for all six plants) and simulated rooting depths for temperatures  $T$  of 7, 17, and 27°C, respectively.

The other three subplots show a comparison between the simulated rooting depths and the measured maximum rooting depths of all six plants for all three temperature treatments.

Figure 5 and the RMSE in Table 6 indicate that Models C and D fitted the observed data very well. Models A and B did not seem to capture the root growth dynamics as well as the other two models. This is underscored by the RMSE values listed in Table 6. The graphs produced by Models A and B are quite similar, and both resulted in an RMSE of 7 to 8 cm. In contrast, Models C and D produced RMSE values below 4 cm. The best correspondence between the model and the data, with the smallest RMSE of only 2 cm, was achieved with Model D, which uses the growth function of Borg and Grimes (1986) and the stress reduction function of Yin et al. (1995). However, despite the slightly worse performance of Model C, the results show that both temperature stress approaches can be used to simulate temperature-dependent root growth when used in combination with the time-dependent root growth function of Borg and Grimes (1986).

Table 7 lists the optimization results when the numbers of calibration parameters were reduced based on the results of the sensitivity analysis. In this case, the parameters with a total-order sensitivity

index lower than 0.3 were set equal to values from the literature. The parameters describing cardinal temperatures were taken from Reddy and Kakani (2007), who investigated cardinal temperatures of bell pepper for pollen germination. Due to the low sensitivity of cardinal temperatures on the model output, these temperatures could also be used to model the root growth, even though this has not yet been scientifically documented. The value for  $L_m$  was taken from Borg and Grimes (1986). Based on the results of the

Table 7. Optimized parameter sets obtained when the insensitive parameters were specified with values taken from the literature, including the maximum possible rooting depth ( $L_m$ ), the growth rate ( $r$ ), the minimum temperature when root growth starts ( $T_{min}$ ), the optimum temperature for root growth ( $T_{opt}$ ), the critical temperature for root growth ( $T_c$ ), the shape of the bell function (ct), and the time when the maximum rooting depth is achieved ( $t_m$ ). Italic values indicate insensitive parameters that were not considered within the optimization process.

Model	$L_m$	$r$	$T_{min}$	$T_{opt}$	$T_c$	ct	$t_m$	RMSE
	cm	d <sup>-1</sup>	°C				d	cm
A	70	0.49	12	30	-	-	-	12
B	90	0.6	12	30	40	1.7	-	12.3
C	90	-	12	30	-	-	52	6.7
D	90	-	12	30	49	0.7	63	5.4

sensitivity analysis, the parameter  $T_{min}$  was still considered as a calibration parameter in Models A and B.

The optimization results shown in Table 7 indicate that despite the reduction in the number of calibrated parameters, the evaluated root growth models, especially Models C and D, produced an acceptable correspondence with the measured data and associated goodness of fit. The other two models (A and B) show a larger increase in the RMSE, which indicates a drop in the goodness of fit. Simulated rooting depths for all temperature treatments using the four root growth models and the optimized parameter sets from Table 7 are shown in Fig. 6.

Figure 6 and the RMSE in Table 7 indicate that Model D also fit the observed data very well, even when three of the six model parameters were specified using values taken from the literature and not calibrated. Model C, which only had one calibration parameter, provided a sufficient reproduction of the observed maximum rooting depths.

## Summary and Conclusions

We implemented an adapted root growth modeling approach based on Jones et al. (1991) in the HYDRUS software packages. The modeling approach describes root growth and root system

development under the influence of environmental factors such as soil hydraulic properties, soil strength, water availability, chemical conditions, and temperature. The implementation of growth and stress functions in the HYDRUS software opens the opportunity to derive parameters of these functions from laboratory or field experimental data using inverse modeling. This option was then demonstrated using experimental data from an aeroponic system for the temperature stress part of the root growth model.

The impact of temperature on root growth was described using two stress response functions, both combined with two, time-dependent root growth functions. The four resulting combinations were tested against rooting depth data measured using an aeroponic system experiment. Because the experiment was not initially set up to evaluate the described root growth module, the collected data were not fully suitable to identify model parameters with high accuracy. For example, the use of a wider temperature range would help to better identify cardinal temperatures and the maximum potential rooting depth ( $L_m$ ). Nevertheless, the results indicate that the temperature-dependent root growth approaches are well capable of reproducing real root growth data. All four of the tested root growth models reproduced the measured rooting depth data very well, with RMSE values ranging between 2.1 and 8 cm. Especially the results of the root growth model referred to as Model D, which combined the Borg and Grimes (1986) root

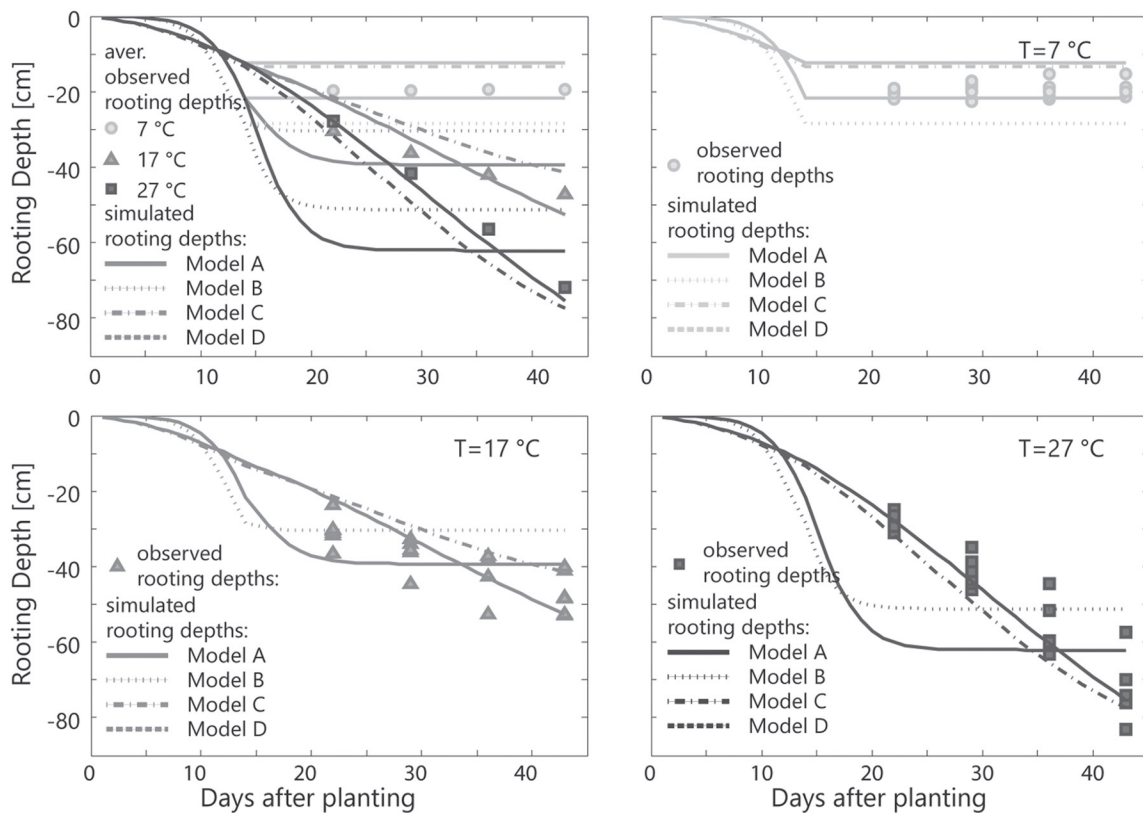


Fig. 6. Comparison of the rooting depths simulated using the parameter sets from Table 7 (only sensitive parameters were optimized) with those measured in the aeroponic system. Data (simulated and average observed) displayed in the upper left figure (for all three temperatures) were used to calculate the goodness of fit. The upper right, lower left, and lower right figures display measured (for all six plants) and simulated rooting depths for temperatures  $T$  of 7, 17, and 27°C, respectively.

growth function with the Yin et al. (1995) temperature stress function, showed an excellent agreement with the observed rooting depth data. The results indicate that the implementation of the time-dependent root growth function of Borg and Grimes (1986) into the HYDRUS software was beneficial because this function captured the actual root growth better than the originally implemented Verhulst–Pearl logistic growth function. However, a complete evaluation of the two proposed (theoretical and heuristic) approaches simulating root growth still requires further testing under dynamic stress conditions that would occur under field conditions, e.g., by using data provided by Aidoo et al. (2018).

A sensitivity analysis revealed that the biologically based parameters of the models, such as the cardinal temperatures and the maximum rooting depth, tend to have a small impact on the model outcome. Because of the low sensitivity of the model outputs to the uncertainties originating from these parameters, it seems reasonable to approximate these parameters with values from the literature and to reduce the number of parameters that need to be calibrated. We have shown that when values from the literature are used for the model-insensitive parameters, the number of calibrated parameters can be reduced for Model A from four to two, for Model C from four to one, for Model B from six to four, and for Model D from six to three. The reduced number of calibrated parameters leads to a reduced complexity of the calibration task and a reduced uncertainty in optimized parameters, especially in connection with the HYDRUS programs. The small number of additional calibration parameters makes the modeling approach of temperature-dependent root growth a convenient add-on to the HYDRUS models. However, the implementation of the influence of other stress factors (other than temperature) on the vertical root penetration, as well as on the root length density distribution, into the HYDRUS models still needs to be validated against experimental data.

## Acknowledgments

This research was partially supported by the Bayer Fellowship Program in the form of the Jeff Schell Scholarship, the Israel Ministry of Agriculture and Rural Development (Eugene Kandel Knowledge Centers) as part of the “Root of the Matter: The root zone knowledge center for leveraging modern agriculture,” and the BonaRes project (BOMA03037514) of the Federal Ministry of Education and Research (BMBF), Germany.

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