A macroscopic soil-water transport model to simulate root water uptake in the presence of water and disease stress

Srinivasa Rao Peddintia,⁎, B.V.N.P. Kambhammettuab, Ranjith S Ladb, Jiří Šimůnек, R.M. Gadeb, J. Adinarayana\textsuperscript{d}

\textsuperscript{a}Department of Civil Engineering, Indian Institute of Technology Hyderabad, Telangana, India
\textsuperscript{b}Department of Plant Pathology, Dr. Panjabrao Deshmukh Krishi Vidyapeeth, Akola, Maharashtra, India
\textsuperscript{c}Department of Environmental Sciences, University of California Riverside, Riverside, CA 92521, USA
\textsuperscript{d}Center of Studies in Resource Engineering, Indian Institute of Technology Bombay, Powai, India

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\section*{ABSTRACT}

Macroscopic modeling approaches based on the solution of the Richards equation with root water uptake (RWU) as a sink term can help in understanding soil-water-plant interactions within the rhizosphere. However, these models currently cannot capture the differences in RWU attributed to variations in plant health. Errors in simulating RWU from unhealthy plants are significant when disease-causing fungus inhibits water uptake rather than other usually considered plant stresses. We developed RWU reduction functions to simulate plant transpiration under combined water and disease stress conditions using linear and non-linear response models. The developed functions were implemented in the numerical model HYDRUS (2D/3D) to simulate water uptake from a root system in a radially symmetrical flow domain. Field experiments were conducted in the Vidarbha region of central India for one crop cycle on four citrus trees with varying disease intensities (healthy to severely diseased). The proposed model was rigorously tested by comparing its results with measured soil water contents and plant transpiration fluxes under various water and disease limiting conditions. Error in simulating RWU fluxes from unhealthy trees by ignoring the disease stress factor was found to be significant (15% for slightly diseased to 26% for the severely diseased tree). Parameters of the spatial root distribution and the disease stress response functions were optimized for each scenario using a genetic algorithm approach. Our results indicate that calibration targets to validate uptake reduction functions should be chosen cautiously based on the dominant stress experienced by the plant root system.

\section*{1. Introduction}

The plant root system is a primary pathway for the exchange of water and energy between the soil environment and the atmosphere (Zheng and Wang, 2015). The morphology, spatial distribution, and water uptake mechanism of the root system controls several hydrological fluxes, including evapotranspiration, soil moisture, and drainage (Canadell et al., 1996). Accurate quantification of root water uptake (RWU) and characterization of its temporal variability can help in optimizing irrigation schedules and improving crop productivity for sustainable development (Schröder et al., 2009). The assessment of RWU can also help in understanding the movement of nutrients and other chemicals in the vadose zone for solute transport studies (Somma et al., 1998; Vrugt et al., 2001b). Several variably-saturated water flow models that simulate soil-water-plant interactions within the rhizosphere, including SWAP (Kroes et al., 2000) and HYDRUS (Šimůnek et al., 2008, 2016) can analyze the role of site-specific irrigation and management practices on crop production (Skaggs et al., 2006). However, these models work on the assumption that the plant is healthy and do not impose any stress on RWU resulting from the disease severity.

Based on the representation of complex structure and geometry of roots in the soil-water flow equation, RWU from the vadose zone can be modeled using two approaches, i.e., microscopic and macroscopic. In the microscopic approach, the geometry of individual roots is approximated by an infinitely long cylinder of uniform radius and water-absorbent properties (e.g., Gardner, 1960; Philip, 1957). The soil-water flow equation is then analytically solved in a radial domain with the flow into the root driven by a product of the water potential gradient and the soil hydraulic conductivity (Šimůnek and Hopmans, 2009).
However, this method considers steady-state conditions that rarely exist in field situations (Feddes and Raats, 2004; Yadav et al., 2009). Also, this method requires detailed knowledge of the geometry of the root system, which is difficult to measure and hence limits its application to simple root systems (Deb et al., 2013; Vrugt et al., 2001b). In the macroscopic approach, the Richards equation is numerically solved with RWU represented by an empirical sink term, averaged over the system of roots (Vrugt et al., 2001b):

$$\frac{\partial \Theta}{\partial t} = \nabla [K(h-z)] - S(x, y, z, t)$$  \hspace{1cm} (1)

where $\Theta$ is the volumetric water content (cm$^3$ cm$^{-3}$), $K$ is the unsaturated hydraulic conductivity tensor (cm s$^{-1}$), $h$ is the soil water matric potential (the pressure head) (cm), and $S$ is an empirical sink representing RWU (cm$^3$ cm$^{-3}$ s$^{-1}$). The macroscopic approach is widely used in numerical models since it requires easy to measure and/or estimate parameters, including the soil water potential, plant transpiration, and root density (Wang et al., 2015). The sink term $S$ in Eq. (1) defines the volume of water removed by RWU from a flower volume of soil per time. This can be represented using: i) water transfer models that are based on the water pressure head gradient at the soil-root interface and a depth-dependent root density function (e.g., Feddes et al., 1974; Gardner, 1964; Molz, 1981) or ii) transpiration based models that depend on the atmospheric demand and a spatially varied root distribution function (e.g., Belmans et al., 1983; Šimůnek et al., 1994; Wu and Cosgrove, 2000; Zuo et al., 2004). In the former case, the root density function is primarily dependent on soil hydraulic properties, whereas in the latter case, it represents root morphology and architecture in the spatial domain (Skaggs et al., 2006). Owing to a simple representation and reliable estimation of the atmospheric demand from meteorological parameters, the transpiration based RWU functions are commonly adopted (Gardner, 1960) and have the form:

$$S_p(x, y, z, t) = \beta(x, y, z) \cdot T_{pot} \cdot L$$  \hspace{1cm} (2)

where $S_p$ is the potential RWU that could occur from a water-unlimited, saline-free, and healthy root system, $\beta(x, y, z)$ is a normalized root density distribution function (cm$^{-2}$), $T_{pot}$ is potential transpiration (cm s$^{-1}$) that depends on meteorological conditions and leaf properties (van den Berg et al., 2002), and $L$ is the surface area associated with transpiration (cm$^2$). Several empirical equations were proposed in the literature to model $\beta(x, y, z)$ (e.g., Feddes and Zaradny, 1978; Hao et al., 1997; Vrugt et al., 2001b; Wu and Cosgrove, 2000). These functions largely differ in terms of representing the shape (linear, exponential, or trapezoidal) and scale parameters of the root system. Actual RWU under prevailing agrometeorological conditions can be obtained as:

$$S_a(x, y, z, t) = \Gamma(h, \Phi) \cdot S_p(x, y, z, t)$$  \hspace{1cm} (3)

where $S_a$ is actual RWU occurring from a natural root system, and $\Gamma(h, \Phi)$ is a dimensionless stress response function ($0 \leq \Gamma(h, \Phi) \leq 1$) representing the stress factors that reduce potential RWU due to non-optimal conditions that exist during crop growth, such as:

a) the water stress, $\alpha(h)$, that reduces RWU due to sub-optimal soil water pressure head ($h$), and can be modeled using either a piece-wise linear reduction function (Feddes and Zaradny, 1978) or a continuous $S$-shape reduction function (van Genuchten and Jury, 1987), and b) the salinity stress, $\alpha(\Phi)$, that reduces RWU due to the osmotic head ($\Phi$), and can be modeled considering the relation between the whole-plant water use and yield loss (van Genuchten and Hoffman, 1984; Maas and Hoffman, 1977)

Almost all water uptake reduction functions proposed in the literature are based on abiotic (drought, salinity, nutrient) stresses encountered by a plant. However, the plant water consumption can also be hampered by biotic (bacteria, viruses, fungi) stresses, which primarily reduce the ability of roots to absorb water by lowering the crop water consumption and associated yield (Rejeb et al., 2014). For the same irrigation and water management conditions, it is well known that a diseased tree consumes less water than a healthy tree. It is difficult to modify existing abiotic stress functions to account for both abiotic and biotic stresses, as the inter-dependence of these stresses can result in different RWU patterns (Atkinson and Urwin, 2012; Fujita et al., 2006). The effect of soil-borne diseases on the uptake mechanism was never explored from the hydrological perspective, hence questioning the applicability of existing models to simulate RWU from disease-affected trees (Peddinti et al., 2018). In the co-existence of multiple uptake reduction factors of varying strengths, it is crucial to dynamically quantify appropriate stresses that a plant experiences so that effective management strategies can be implemented. Peddinti et al. (2018) highlighted the role of plant health in simulating RWU from disease citrus trees. However, they failed to develop stress response functions that consider plant health conditions for the use with numerical models and irrigation scheduling.

The Vidarbha region in Maharashtra, India, is the leading producer of mandarin oranges (Citrus reticulate), accounting for 40% of the country’s citrus production with a yield of 6 t ha$^{-1}$, far below the nation’s average (Peddinti et al., 2018). The low citrus production in Vidarbha is primarily attributed to improper management activities that result in the formation and propagation of a water mold disease called ‘root rot’ (Phytophthora spp.). Under favorable conditions (high soil moisture and cold temperature), the disease-causing fungus produces a large number of motile zoospores that move towards the roots. These zoospores contact the root system, then encyst, germinate, and enter the root tip, resulting in the rot of the entire rootlet (Savita and Nagpall, 2012). These root pathogens can damage the tree by decreasing the root density, and water and nutrient uptake (Dunlaw, 1971). It is almost impossible to identify early-stage symptoms of this disease, which originates in the rhizosphere (Jegtap et al., 2012). Late-stage impressions of a disease-affected tree are seen at the surface with symptoms including leafless branches, yellow foliage, shoot dieback, reduced fruit size and yield, thin canopy, and reduced water and nutrient uptake (Zekri and Rouze, 2007). The disease intensity can be estimated by measuring the population density of Phytophthora spp. in the soil surrounding the root zone and is expressed on a scale of 0 (healthy) to 4 (severely diseased) (Gade et al., 2006; Gade and Koche, 2012). The disease intensity has a strong negative correlation with biomass and crop yield (Choudhari et al., 2018). A disease-affected tree inhibits RWU, resulting in higher soil water contents, a condition favorable for further growth of disease-causing fungus. In order to evaluate alternate irrigation and management practices for citrus trees of different health conditions, it is imperative to accurately represent RWU from disease-affected trees using numerical tools.

The objectives of this research are: i) to formulate linear and non-linear disease stress response functions and implement them in a numerical model to simulate RWU from citrus trees, ii) to evaluate the applicability of disease stress response functions in the presence and absence of water stress conditions, and iii) to derive optimal root distribution and disease sensing parameters for use with numerical models and the operational management of citrus trees.

2. Materials and methods

2.1. Experimental setup and data acquisition

Factorial field-scale experiments were conducted on four matured citrus trees of varying health conditions located in the Nagziri village of Maharashtra, India (latitude: 21° 27′ 5″ N, longitude: 78° 9′ 12″ E, elevation: 460 m asl). Agrometeorological conditions at the experimental site were discussed in Peddinti et al. (2018). The selection of trees was made based on the visual disease symptoms at the surface (Gade and Koche, 2012). These include a healthy tree with no yellowing (T1), a tree with 10–25% yellowing of leaves with oozing lesions of 1 cm$^2$ area (T2), a tree with 25–50% yellowing of leaves with oozing lesions of 2.5 cm$^2$ area (T3), and a tree with more than 50% yellowing

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The residual and saturated soil water contents \( \theta_r \) and \( \theta_s \) are estimated using gravimetric measurements at selective depths. Plant transpiration was measured using SFM1 sap flow meters (ICT International, Armidale, NSW, Australia) that were placed in the tree trunk at the height of 0.5 m above the ground in four citrus trees (Fig. 1). The sap flow meter utilizes a heat-ratio method to measure high, low, and reverse sap flows using a set of three 35 mm stainless steel needles placed at 5 mm spacing. Sap flows were monitored at 15 min interval and accumulated over each day. The hydraulic gradient across the root zone was estimated using tensiometers placed along the vertical axis (Fig. 1), and drainage fluxes across the bottom boundary were estimated using Darcy’s law (Whitaker, 1986).

### 2.2. Laboratory estimation of soil properties

Undisturbed soil samples were collected in cylindrical cores (height: 13 cm, diameter: 10 cm) from a representative depth of 30 cm surrounding each experimental plot. These samples were used to estimate soil physical and electrical properties in the laboratory under controlled conditions (Table 1). Texturally, the soil is classified as vertisol, having high expansive clay content and water-holding capacity with a swell index of 55% (Virmani et al., 1982). Soil suctions and moisture contents during the drying phase were estimated using dew point potentiometer and gravimetric methods, respectively. The van Genuchten-Mualem model (van Genuchten, 1980) shape parameters \( \alpha \) and \( n \) were estimated using the RETC code (van Genuchten et al., 1991) that considers the constitutive relationships given by:

\[
\theta(\psi) = \begin{cases} 
\theta_r + \frac{\theta_s - \theta_r}{1 + (\frac{\psi}{\psi_0})^n} & \psi < 0 \\
\theta_s & \psi \geq 0
\end{cases}
\]

(4)

where \( \psi_0 \) is the residual saturated soil water content \( (\text{cm}^3\text{cm}^{-3}) \) respectively; \( \alpha \) is the reciprocal of air entry \( \psi \text{ (cm}^{-3}\text{)} \); \( n \) is a pore-size distribution index \((-\) with \( m = 1 + \frac{1}{n} \text{ (cm}^{-3}\text{)} \). The non-linear relation between electrical resistivity and soil moisture was developed following ASTM guidelines (ASTM G57-06, 2012). A simplified form of Waxman and Smits (1968) was fitted to the data using the constitutive relation given by:

\[
\sigma = a \psi^b + b
\]

(5)

where \( \sigma \text{ (S}\text{cm}^{-1}\text{)} \) is the electrical conductivity of a soil sample; \( a \text{ (S}\text{cm}^{-1}\text{)} \) is the soil volumetric water content, with \( a \text{ (S}\text{cm}^{-1}\text{)} \), \( b \text{ (S}\text{cm}^{-1}\text{)} \) and \( c \text{ (S}\text{cm}^{-1}\text{)} \) being the best-fit parameters. A comprehensive description and methodology for laboratory estimation of pedo-physical and pedo-electrical relations can be found in Peddinti et al. (2018). Inoculum dynamics for the four trees (T1 through T4) were observed at weekly intervals to characterize disease intensity. Soil cores from four corners of each tree, located at 75 cm distance from the trunk, were pooled to make the composite soil. About 10 cm\(^2\) of soil from the homogeneous sample was added to 90 ml of 0.025 percent agar, and 1 ml of the slurry was plated on Phytophthora selective medium (Tsao and Stephen, 1977). Plates were then incubated at 27 °C for three days and Phytophthora colonies were counted using a microscope and reported as a propagule count per cc of soil, \( PC \) (Gade and Koche, 2012).

### 2.3. Root water uptake model

For isolated trees such as citrus in large monocultures, the process of
water uptake is complex and hence requires a three-dimensional representation of the spatial root distribution (Green and Clothier, 1998). The distribution of soil moisture following the irrigation of citrus trees has been found to be symmetric in the X-Y plane, and hence considering an isotropic distribution of RWU in the lateral direction is appropriate (Peddinti et al., 2018). Since the root distribution function proposed by Vrugt et al. (2001a) can be readily tested with numerical tools such as HYDRUS and has the scale and shape parameters that can be readily modified, it is ideal for characterizing the root morphology and simulating RWU. Keeping these points in view, we have adopted the two-dimensional axisymmetric form of the root distribution function proposed by Vrugt et al. (2001a) to model RWU of the citrus trees in the study area:

$$\beta(r, z) = \left[1 - \frac{Z}{Z_m}\right] \left[1 - \frac{r}{R_m}\right] \exp\left(-\frac{z^*}{h} - \frac{r^*}{p}\right)$$

where $\beta(r, z)$ is the shape function describing the spatial root distribution (cm$^{-3}$); $Z_m$ and $R_m$ are the maximum rooting depth (cm) and the maximum radial distance (cm) respectively; $z^*$ and $r^*$ are the empirical parameters that control the position of the maximum uptake intensity (cm), and $p$ and $p_*$ are the empirical parameters that control the shape of the root distribution ($-\)$. These empirical parameters are constrained to provide zero RWU at $z = Z_m$, $r = R_m$, and maximum RWU at $z^*$ and $r^*$. Normalized RWU from the citrus root system, $S_p$ (cm$^3$cm$^{-3}$s$^{-1}$), considering the atmospheric demand, is given by:

$$S_p(r, z) = \beta(r, z) \times T_p \times L_t$$

2.4. Uptake reduction functions

Eq. (7) is applicable to estimate potential RWU from a healthy tree subjected to stress-free conditions. In the presence of uptake reduction stresses, actual RWU, $S_a$ (cm$^3$cm$^{-3}$s$^{-1}$) is given by:

$$S_a(r, z) = \Gamma(h, \Phi, PC) \cdot S_p(r, z)$$

where $\Gamma(h, \Phi, PC)$ is the total stress experienced by the plant root system, involving both biotic and abiotic components. The integration of the above equation over the spatial domain gives cumulative actual RWU from the root system, which is equal to actual plant transpiration, $T_a$ (Vrugt et al., 2001b; Šimůnek and Hopmans, 2009). Commonly used abiotic uptake reduction factors include the water stress $\alpha(h)$ and the salinity stress $\alpha(\Phi)$, which depend on the pressure head and the osmotic head, respectively (Fujimaki et al., 2008). When the assumption of disease-free conditions is violated, biotic pathogens in the rhizosphere can cause an additional reduction in RWU, and the plant is said to experience the disease stress $\alpha_{PC}$ (PC). In reality, all these stresses can coexist during the crop cycle; hence, their integrated effect on RWU needs to be simulated. The combined effect of all possible uptake reduction factors can be described using either additive or multiplicative approaches of individual stresses experienced by the plant. It is still under debate, which approach can best describe the plant water uptake more accurately (Fujimaki et al., 2008; Šimůnek and Hopmans, 2009).

2.4.1. Water stress response function

To account for the reduction in RWU resulting from changes in soil moisture between irrigations, piece-wise linear and non-linear response functions are often used (Feddes and Zaradny, 1978; van Genuchten and Jury, 1987). The piece-wise linear model is parameterized using four thresholds of the soil water pressure head between a permanent wilting point and full saturation, with $h_4 < h_3 < h_2 < h_1$. The water stress response function $\alpha(h)$ used in this study is given as (Feddes and Zaradny, 1978):

$$\alpha(h) = \begin{cases} 1 & h > h_4 \\
\frac{h - h_4}{h_4 - h_3} & h_4 \geq h \geq h_3 \\
\frac{h - h_3}{h_3 - h_2} & h_3 \geq h \geq h_2 \\
\frac{h - h_2}{h_2 - h_1} & h_2 \geq h \geq h_1 \\
0 & h \leq h_1 \text{ or } h \geq h_3 
\end{cases}$$

2.4.2. Disease stress response function

Peddinti et al. (2018) concluded that ignoring plant health conditions in the numerical models can result in significant deviations in simulated RWU fluxes, particularly from disease-affected trees. In this research, the disease level of a citrus tree is quantified using the population density of Phytophthora spp. (i.e., propagule count, PC) per a unit volume of soil (cfu g$^{-1}$) and is represented on a scale of 0 (healthy with no yellowing) to 4 (severely affected with more than 50% yellowing and leaf fall) (Gade et al., 2006). Several researchers have concluded that PC changes during crop growth stages have a strong correlation with soil moisture and yield loss (Bright et al., 2004; Gade and Koch, 2012). We considered the yield data from 30 mature citrus trees of the region with varying disease intensities to obtain a functional form of the water uptake reduction function due to plant disease conditions, $\alpha_{PC}$ (Fig. 2). Because of the differences in frequency and amount of irrigation between crop growth stages, we defined stage
specific parameters while formulating the disease stress response function. For the observed citrus trees, the range in PC is highest during the growth stage (20–35), followed by the flowering stage (9–20), and the harvest stage (4–15). Increased frequency and irrigation amounts during the growth stage has resulted in swamplike environment and high soil moisture, a condition favorable for further growth of disease-causing bacteria. First, we proposed a segmented linear function of the form:

\[ \alpha = \begin{cases} 
\frac{PC_{\min}}{PC_{\max}} & \text{if } PC_{\min} < PC < PC_{\max} \\
\frac{PC_{\max} - PC_{\min}}{PC_{\max} - PC_{\min}} & \text{otherwise}
\end{cases} \]

Fig. 2. Plots of piece-wise linear (left) and S-shaped nonlinear (right) uptake reduction functions fitted to the observed data of a stage-specific propagule count (PC) of disease-causing fungus (Refer to Eqs. (10) and (11) for mathematical representation).

Table 2
Schedule of irrigation and ERT data acquisition activities performed during the experiment.

<table>
<thead>
<tr>
<th>Case/Scenario</th>
<th>Date of observation</th>
<th>Start–End Times of the ERT Survey</th>
<th>Start–End Times of Irrigation</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>(Indian Standard Time)</td>
<td>T1 – T2 T3 T4</td>
<td>(Indian Standard Time)</td>
</tr>
<tr>
<td>Case I</td>
<td>10.09.2017</td>
<td>09:00–09:20 09:30–09:50 11:00–11:20 11:30–11:50</td>
<td>Rain (2 mm) on 12.09.2017</td>
</tr>
<tr>
<td>Case II</td>
<td>26.09.2017</td>
<td>10:30–11:00 16:15–16:45 17:00–17:30 12:00–12:30</td>
<td></td>
</tr>
<tr>
<td></td>
<td>27.09.2017</td>
<td>18:00–18:30 17:30–17:50 16:30–17:00 15:40–16:10</td>
<td></td>
</tr>
<tr>
<td></td>
<td>28.09.2017</td>
<td>10:00–10:30 12:00–12:30 13:00–13:30 11:00–11:30</td>
<td></td>
</tr>
<tr>
<td></td>
<td>29.09.2017</td>
<td>11:30–12:00 10:30–11:00 09:45–10:15 09:00–09:30</td>
<td></td>
</tr>
<tr>
<td></td>
<td>29.10.2017 (AI)</td>
<td>17:15–17:45 16:15–16:45 15:45–16:15 16:10–16:30</td>
<td></td>
</tr>
<tr>
<td></td>
<td>31.10.2017</td>
<td>09:45–10:15 10:30–11:00 09:00–09:30 08:30–08:55</td>
<td></td>
</tr>
<tr>
<td>Case IV</td>
<td>14.11.2017</td>
<td>15:30–16:00 16:15–16:45 15:00–15:25 17:00–17:30</td>
<td></td>
</tr>
<tr>
<td></td>
<td>16.11.2017</td>
<td>09:00–09:30 11:30–12:00 10:00–10:30 12:15–12:45</td>
<td></td>
</tr>
<tr>
<td></td>
<td>28.12.2017</td>
<td>08:00–08:30 10:30–11:00 08:45–09:15 09:30–10:00</td>
<td></td>
</tr>
<tr>
<td>Case VI</td>
<td>17.02.2018</td>
<td>16:00–16:30 16:30–17:00 17:30–18:00 18:15–18:50</td>
<td></td>
</tr>
<tr>
<td></td>
<td>18.02.2018</td>
<td>11:00–11:30 11:30–12:00 12:15–12:45 13:00–13:30</td>
<td></td>
</tr>
</tbody>
</table>
where $\min$ is the lowest possible uptake factor that is possible from a disease-affected tree, $PC_{\min}$ and $PC_{\max}$ are the minimum and maximum thresholds for $PC$ that results in unit and $\min$ uptake factors, respectively, and $\gamma$ is the slope of the linear function (note that $\gamma$ can be evaluated directly from $PC_{\min}$, $PC_{\max}$, and $\alpha_{\min}$). Similarly, a nonlinear or S-shaped continuous smooth function is postulated to simulate the effects of plant health on RWU:

$$\alpha(PC) = \frac{1}{1 + (\frac{PC}{PC_{50}})^{p_3}}$$

(11)

where $PC_{50}$ and $p_3$ are the empirical parameters, with $PC_{50}$ representing the soil $PC$ at which $\alpha(PC)$ becomes 0.5.

### 2.4.3. Combined water and disease stress

We assume that the two stress functions 'disease' and 'water' are solely caused by changes in $PC$ and water potential, respectively, and are independent of each other. Even though $PC$ has an indirect relationship with the soil water potential, this relationship is yet unexplored, and hence difficult to implement with Eq. (9). Since the soil water potential is explicitly included in the water stress function, this assumption seems to be meaningful. In reality, plants show different degrees of sensitivity to water and disease stress conditions (Rejeb)

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Table 3: Parameters of the optimal root distribution for citrus trees of varying health conditions considering the root distribution function proposed by Vrugt et al. (2001b).

<table>
<thead>
<tr>
<th>Tree</th>
<th>$Z_m$ (cm)</th>
<th>$R_m$ (cm)</th>
<th>$z^*$ (cm)</th>
<th>$r^*$ (cm)</th>
<th>$p_z$ (-)</th>
<th>$p_r$ (-)</th>
</tr>
</thead>
<tbody>
<tr>
<td>T1</td>
<td>47.51</td>
<td>162.11</td>
<td>38.52</td>
<td>108.73</td>
<td>3.44</td>
<td>3.32</td>
</tr>
<tr>
<td>T2</td>
<td>43.22</td>
<td>151.58</td>
<td>36.73</td>
<td>101.18</td>
<td>3.44</td>
<td>3.32</td>
</tr>
<tr>
<td>T3</td>
<td>39.19</td>
<td>146.67</td>
<td>32.33</td>
<td>92.47</td>
<td>3.44</td>
<td>3.32</td>
</tr>
<tr>
<td>T4</td>
<td>35.88</td>
<td>129.98</td>
<td>26.81</td>
<td>87.55</td>
<td>3.44</td>
<td>3.32</td>
</tr>
</tbody>
</table>

Note: Parameter ranges considered during optimization process are as follows: $z_m(0–100 \text{ cm})$; $R_m(0–250 \text{ cm})$; $z^*(1–100 \text{ cm})$; $r^*(1–250 \text{ cm})$. 

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Fig. 3. Three-dimensional volumetric water content distributions measured using ERT around four experimental trees (from healthy (T1) to severely diseased (T4)) before irrigation (top row) and after irrigation (bottom row). The high soil water content around the severely ill tree (T4) reflects the low water uptake produced by the plant. Irrigation was given on 27-09-2017.

Fig. 4. An axisymmetric flow domain used in HYDRUS (2D/3D) for numerical simulations of RWU in experimental plots with water and disease stress function.
We assumed that the effects of water and disease stress on the uptake reduction are independent and hence their integrated effect
\( \Gamma(h, PC) \) can be obtained using a multiplication rule (Skaggs et al., 2006; Šimůnek and Hopmans, 2009):

\[
\Gamma(h, PC) = \sigma(h) \cdot \sigma(PC)
\]

(12)

where \( \Gamma(h, PC) \) ranges from 1 (healthy, water-unlimited) to 0 (severe disease, water-stress) and is always less than or equal to \( \sigma(h) \) and \( \sigma(PC) \).

2.4.4. Numerical implementation

The proposed linear and non-linear disease stress response functions (Eqs. (10) and (11)) were implemented in HYDRUS (2D/3D) (Šimůnek et al., 2016, 2008) to simulate either individual or simultaneous effects of water and disease stresses on RWU. Both static \( (Z_{\text{min}} , R_{\text{max}} , p_1 , p_2 , z^* , r^*) \) and dynamic \( (PC_{\text{min}}, PC_{\text{max}}, a_{\text{min}} or PC_{\text{co}}, p_1) \) parameters of the RWU function were varied during model calibration to minimize the discrepancy between measured and simulated soil water contents as well as plant transpiration fluxes.
2.5. Model calibration and performance evaluation

The proposed model was calibrated for different water (pre and post irrigation) and disease limiting conditions (T1 to T4) using the spatial distribution of water contents and whole-plant transpiration fluxes. A global sensitivity analysis was performed using the Sobol’s method (Sobol, 2001) to reveal critical parameters of each function and to determine the contribution of the uncertainty of each parameter to the uncertainty of the model output. The first-order \( S_i \) and total-order \( S_{ti} \) sensitivity indices were approximated by a numerical Monte Carlo estimation proposed by Saltelli et al. (2010). The static root distribution parameters and the stage-specific disease stress function parameters were transformed into their defined parameter intervals based on the specified minimum and maximum values. Parameter limits on the rooting depth and radial distance were observed from the ERT profiles, whereas the other root distribution parameters were taken from the literature. A total of 1000 parameter sets were considered to develop the first-order and total-order sensitivity indices.

Optimization was performed using a genetic algorithm (GA) to reveal the optimal set of the most sensitive parameters (Vrugt et al., 2001b). GAs were developed based on the evolution theory, inspired by natural selection and genetics, and aimed to solve complex optimization problems. The root distribution and disease stress response function parameters were optimized by calibrating the model against soil water contents and plant transpiration fluxes, respectively. Since the inverse module of HYDRUS (2D/3D) is not set to optimize these parameters, the GA toolbox in MATLAB was coupled with the forward computational module of HYDRUS (2D/3D) to perform the calibration. The GA was run with 1000 initial parameter sets, a penalty factor of 10, a population size of 1000, a crossover fraction of 0.5, and a mutation rate of 0.05 during optimization. Two-point cross over and uniform mutation functions were used with the GA solver (Goldberg and Holland, 1988). Eight Markov chain runs with a set of 1000 generations were utilized to minimize the errors in HYDRUS (2D/3D) simulated water contents. Model performance was evaluated using the statistical indices that include the root mean square error (RMSE), and coefficient of determination (R²).

### Table 4
Parameters of the optimal disease stress reduction functions (piece-wise linear and S-shaped nonlinear) for citrus trees of varying health conditions.

<table>
<thead>
<tr>
<th>Stage</th>
<th>T2</th>
<th>T3</th>
<th>T4</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>S-Shaped</td>
<td>Linear</td>
<td>S-Shaped</td>
</tr>
<tr>
<td></td>
<td>( PC_{50} ) (cfu g⁻¹)</td>
<td>( p_3 ) (–)</td>
<td>( PC_{\text{min}} ) (cfu g⁻¹)</td>
</tr>
<tr>
<td>Flowering</td>
<td>19.55 7.78 11.42</td>
<td>21.55 0.25</td>
<td>17.67 8.11</td>
</tr>
<tr>
<td>Growth</td>
<td>32.21 13.23 23.77</td>
<td>36.28 0.22</td>
<td>30.51 12.37</td>
</tr>
<tr>
<td>Harvesting</td>
<td>13.65 4.88 9.42</td>
<td>14.62 0.25</td>
<td>12.32 6.18</td>
</tr>
</tbody>
</table>

Note: Parameter ranges considered during optimization process are as follows: \( PC_{50} \) (0–100 cfu g⁻¹); \( p_3 \) (0–50); \( PC_{\text{min}} \) (1–100 cfu g⁻¹); \( PC_{\text{max}} \) (1–100 cfu g⁻¹); \( \gamma \) (0–5).

Fig. 7. Scatter plots between observed and HYDRUS (2D/3D) simulated (considering linear and non-linear response models) transpiration fluxes (cm d⁻¹) from the experimental citrus trees of varying health conditions (from healthy (T1) to severely diseased (T4)).
of determination ($R^2$) (Cai et al., 2018).

3. Results and discussion

3.1. Analysis of soil moisture profiles from ERT

Spatiotemporal patterns of the soil water content surrounding the citrus tree were obtained by performing 3D ERT experiments before and after each irrigation application. During each watering, citrus trees were flood irrigated to a depth of about 35–40 mm to replicate the field practices. Six irrigation applications were considered during the monitoring period (Table 2), and a typical ERT-generated soil moisture profile is presented in Fig. 3. Before the interpretation of the results, ERT data quality and noise reduction were ensured using reciprocal errors and stacking (Sreeparvathy et al., 2019). Calibrated time domain reflectometry (TDR) probes placed at four depths (15, 30, 45, and 60 cm below the ground level) were used to correlate with ERT measurements. ERT derived soil moisture data was in agreement with TDR observations ($R^2 = 0.65$, RMSE = 0.03 cm$^3$ cm$^{-3}$, error range: 0.04 to 0.08, n = 21) and hence were considered as observed soil water contents for use with HYDRUS (2D/3D) calibration.

It can be observed that irrespective of the health condition, soil moisture profiles are visibly distinct between pre- and post-irrigation scenarios. Since no lithological anomalies were reported, these changes in soil water contents can be attributed to the root zone activity (Cassiani et al., 2015; Peddinti et al., 2018). Before irrigation (water stress conditions), the soil moisture front that separates the active root zone from the bottom soil layers is clearly visible from the ERT profiles (Fig. 3). The depth of the soil moisture front was decreasing from 47 cm for a healthy matured tree (T1) to 35 cm for a severely diseased citrus tree (T4). As the disease intensity progresses (from T1 to T4), the root zone is observed to be attenuating in radial and depth directions. For the same applied irrigation water and evaporation losses, relatively high soil water contents under a diseased tree following irrigation (no water stress condition) were observed due to less RWU. Low photosynthetic activity of diseased trees due to a reduction in LAI and chlorophyll contents could be an additional cause. Even though healthy and unhealthy trees have recorded similar temporal moisture patterns, their values differed significantly. ERT results led to the conclusion that ignoring the health condition of a tree in the numerical model can result in high RWU from diseased trees (due to the absence of the water stress), which is in contrary to the field measurements.

3.2. Numerical simulations with HYDRUS (2D/3D)

An axisymmetric form of the Richards equation for water flow under unsaturated conditions around the citrus tree, with RWU represented by an external sink term, was numerically solved. The finite element mesh, along with the applicable boundary conditions, is shown in Fig. 4. The generated mesh with a mesh refinement around the root zone consisted of 9884 nodes, 346 1D elements, and 17,420 2D elements. The model refinement is chosen to achieve a tradeoff between computational cost...
and numerical convergence. The flow domain has a length of 250 cm in the radial direction and 100 cm in the depth direction. The upper boundary of the flow domain represents the land surface subjected to atmospheric and irrigation fluxes and was assigned an atmospheric boundary condition. Since the groundwater table depth (4–6 m) is well below the root zone, the bottom boundary was assigned a free drainage boundary condition to allow gravitational drainage fluxes following irrigation, which were estimated using Darcy’s equation. All remaining boundaries were assumed to represent no-flow conditions. The upper boundary conditions were assigned using a daily time step for 110 days (09 Sep. to 27 Dec. 2017). Daily meteorological data was obtained from an automatic weather station (AWS) located at about 30 m from the experimental site. The reference evapotranspiration ($ET_0$) was estimated using the FAO based Penman-Monteith equation (Allen et al., 1998) and is in the range of 2 to 8 mm/day. $ET_0$ was further partitioned into evaporative ($E_0$) and transpiration ($T_0$) demands using the methodology proposed by Ritchie (1972) and is validated using flux partitioning methodology (Peddinti and Kambhammettu, 2019). RWU is considered as a system-dependent boundary condition and is adjusted during the simulation depending on the state variables (water and disease stresses). RWU is equal to potential transpiration from a healthy, irrigated plant and is limited by the lack of soil moisture and/or plant health conditions. Two disease stress response functions (linear and non-linear models) were incorporated into the HYDRUS (2D/3D) code using time-varying stage-specific PC values.

Since HYDRUS (2D/3D) does not have a dedicated calibration tool for root distribution and disease sensing parameters, it was coupled with the GA tool in MATLAB to perform calibration and parameter estimation. The variance-based sensitivity analysis using Sobol’s algorithm was performed to reveal the contribution of individual parameters and their interactions on simulated soil water and transpiration fluxes. The detailed results of the sensitivity analysis are available as Supplementary Material. Model parameterization and optimization were performed by considering model sensitive parameters. Root distribution parameters that are sensitive to soil water simulations and their optimal values for each experimental tree are given in Table 3. It can be observed that the parameters defining the shape of the spatial root distribution ($p_r$ and $n_r$) are insensitive to model simulations. As discussed below in Section 3.5, the $g(r, z)$ function for different experimental trees is governed exclusively by scale parameters in the depth and radial directions.

The ERT domain was discretized in such a way that the grid cells of ERT and HYDRUS (2D/3D) coincide as much as possible to minimize the interpolation errors. Model calibration was achieved by matching i) simulated soil water contents with ERT measurements and ii) simulated whole-plant transpiration fluxes with SAP flow measurements. A good agreement between simulated and observed soil water contents was achieved during water limiting (pre irrigation) and water available (post irrigation) conditions (Fig. 5). Overall, HYDRUS (2D/3D) was able to capture the soil moisture profiles for T1 ($R^2 = 0.71; \text{RMSE} = 0.032; n = 230$), T2 ($R^2 = 0.74; \text{RMSE} = 0.026; n = 230$), T3 ($R^2 = 0.69; \text{RMSE} = 0.039; n = 230$), and T4 ($R^2 = 0.78; \text{RMSE} = 0.021; n = 230$) scenarios.

3.3. Evaluation of disease stress response functions

To be consistent with the commonly used water and salinity stress response models, we developed piece-wise linear and S-shaped non-linear disease stress response functions (Fig. 2) for use with HYDRUS (2D/3D) simulations. However, the PC of disease-causing bacteria was observed to change dynamically during the crop cycle and was controlled by soil water contents and crop phenology (Fig. 2). Hence, we divided the crop cycle into three stages (flowering (DOY90-135), growth (DOY136-287), and harvest (DOY288-365)) to define the stage-specific functional parameters. Daily plots of RWU from the experimental plots using the two models are presented in Fig. 6. Both models produced similar RWU patterns during the simulations, with marginally different magnitudes. During the simulation, daily RWU was in the range of 0.05 to 0.46 cm/d using a linear stress function, and 0.01 to 0.34 cm/d using a nonlinear stress function (lumped over all experimental trees). The linear stress response function yielded slightly higher RWU (0.20 ± 0.08 cm/d) in comparison to the non-linear model (0.16 ± 0.06 cm/d). Cumulative RWU from the four experimental trees (T1 through T4) using a linear stress response function were found to be 28.07, 25.48, 20.84, and 13.54 cm, respectively, and their counterparts using a nonlinear stress response function were found to be 20.34, 19.91, 17.75, and 11.54 cm, respectively. RWU from the linear stress response function was in close agreement with observed transpiration fluxes in comparison to the non-linear model.

Daily RWU fluxes simulated using a linear stress response function from a healthy citrus tree (T1) for growth and harvest stages were 0.29 ± 0.06 cm/d and 0.18 ± 0.03 cm/d, respectively, and the corresponding values from a severely diseased citrus tree (T4) were 0.146 ± 0.04 cm/d and 0.08 ± 0.01 cm/d, respectively. Similarly, daily RWU fluxes simulated using a non-linear stress response function from a healthy citrus trees (T1) for the growth and harvest stages were 0.21 ± 0.04 cm and 0.12 ± 0.01 cm/d, respectively, and the corresponding values from a severely diseased citrus tree (T4) were 0.13 ± 0.03 cm/d and 0.07 ± 0.01 cm/d, respectively. Temporal patterns of RWU averaged over each crop stage can be approximated by a unimodal distribution with low RWU during the flowering stage, highest during the growth stage, followed by a decreasing trend towards the harvest. Interestingly, this pattern coincides with the PC (Fig. 2) and irrigation frequency. This indicates that plant transpiration is sensitive to the PC and applied irrigation water with varying strengths. Hence, the application of irrigation water to disease-affected trees during the crop growth stage is more crucial for the effective management of citrus trees.

Parameters of the disease stress response function were optimized for each crop growth stage using linear and nonlinear functions and are presented in Table 4. It can be observed that differences between optimized parameters are relatively small between different experimental plots for a given growth stage and relatively large between different growth stages. This indicates that it is important to consider time-variable disease sensing parameters (such as $PC_{\text{min}}, P_0, P_{\text{max}}, PC_{\text{max}}, \sigma_{\text{min}}$) to effectively simulate RWU from diseased trees. Scatter plots of actual transpiration (RWU) simulated using the two disease stress reduction models along with observed whole-plant transpiration fluxes are shown in Fig. 7. Results showed that the RWU fluxes simulated using the piece-wise linear stress response function are clustered around the 1:1 line for all scenarios (T2 through T4), even though there is some scatter and bias in the estimates. It can be observed that the magnitude of underestimation of RWU fluxes (deviations from the 1:1 line) when the non-linear stress response function is used diminishes towards severely disease-affected trees (T4). This indicates that for severely diseased trees, both linear and non-linear stress functions give similar predictions close to observed RWU fluxes. In other words, the bias in estimated daily RWU fluxes is high for a slightly diseased tree (T2) and gradually diminishes as the disease severity progresses. We attribute this change to variations in model parameters.

3.4. Propagation of the error in simulated RWU due to ignorance of disease stress

To quantify the error and its magnitude in the estimated RWU fluxes from unhealthy trees as a function of disease intensity, HYDRUS (2D/3D) simulations were repeated without considering the disease stress response function. A healthy citrus tree (T1), for which the disease stress function is not applicable, had slightly higher simulated transpiration fluxes (Fig. 8). In reality, the ubiquitous influence of low PC from healthy trees might inhibit RWU, resulting in low observed transpiration. To match with, HYDRUS (2D/3D) adjusts its root distribution

### Table 3: Model parameterization and optimization

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$p_r$</td>
<td>0.5</td>
</tr>
<tr>
<td>$n_r$</td>
<td>2</td>
</tr>
<tr>
<td>$g(r, z)$</td>
<td></td>
</tr>
</tbody>
</table>

### Table 4: Parameters of disease stress response function

<table>
<thead>
<tr>
<th>Scenario</th>
<th>Linear Stress Function</th>
<th>Non-Linear Stress Function</th>
</tr>
</thead>
<tbody>
<tr>
<td>T1</td>
<td>0.29 ± 0.06 cm/d</td>
<td>0.13 ± 0.03 cm/d</td>
</tr>
<tr>
<td>T2</td>
<td>0.18 ± 0.03 cm/d</td>
<td>0.07 ± 0.01 cm/d</td>
</tr>
<tr>
<td>T3</td>
<td>0.21 ± 0.04 cm/d</td>
<td>0.12 ± 0.01 cm/d</td>
</tr>
<tr>
<td>T4</td>
<td>0.146 ± 0.04 cm/d</td>
<td>0.08 ± 0.01 cm/d</td>
</tr>
</tbody>
</table>

### Figure 2: Piece-wise linear and S-shaped disease stress response functions

- Piece-wise linear function for RWU
- S-shaped disease stress function for RWU

### Figure 3: Flow domain discretization

- Grid cells of ERT and HYDRUS (2D/3D)
- Flow domain discretization

### Figure 4: Calibration of soil water contents

- Simulated soil water contents with ERT measurements
- Observed soil water contents

### Figure 5: Soil moisture profiles

- T1, T2, T3, T4 soil moisture profiles

### Figure 6: Daily RWU fluxes

- Linear stress response function
- Non-linear stress response function
parameters, yet achieving significantly deviated RWU fluxes. A similar, yet significant deviation was observed for other disease-affected trees (T2 through T4), indicating that consideration of a compensation mechanism to lower simulated RWU is essential. The error in simulated RWU from unhealthy trees when ignoring the α(PC component (i.e., the difference in box plots of ‘without disease stress’ and ‘observed transpiration’) was found to be in the range of 15 to 26%. It can be observed that for diseased trees of varying intensities (T2 through T4), actual transpiration simulated by considering the disease stress response function matched almost perfectly with the observed values, having the same range and median values.

3.5. Spatial distribution of RWU from citrus trees

The spatial representation of root water uptake, β(r,z), from the experimental trees is illustrated in Fig. 9. It can be observed that the zone of maximum RWU is located in a thin soil layer that varies from 0.2 m for T4 to about 0.32 m for T1. This zone can be designated as an external sink region that drives soil water flow towards active roots. A healthy citrus tree (T1) has a larger rooting depth and radius compared to the other three diseased trees. It can be observed that the shape of the root distribution function remains the same for all experimental trees. This indicates that the health condition of a tree has a significant impact on the scale parameters of the root distribution function. The close spacing of contours for a diseased tree indicates that pathogens are inhibiting the water uptake mechanism, thereby minimizing the spatial extent of RWU. We also conclude that measured plant transpiration fluxes are more useful than measured water content for calibration of soil–water-plant models from diseased trees.

3.6. Limitations of research

The proposed disease stress functions are applicable to citrus orchards family with similar agro-climatic conditions, and hence cannot be generalized to other plants. We assumed that the two stress functions are independent of each other when evaluating their combined effect on RWU simulations, which may not be accurate in reality. We could not compare the simulated transpiration fluxes with observations during the flowering stage due to the absence of sap flow measurements. The proposed idea can be taken further to develop similar disease stress response functions applicable to different crops of various agro-climatic conditions.

4. Summary and conclusions

This research provides an insight into soil-water-disease interactions of citrus trees using combined experimental and numerical studies. Field experiments were conducted at four citrus trees of varying health conditions located in the Vidarbha region of India to monitor hydrological and root water uptake fluxes in response to irrigation. Soil water contents and RWU within the rhizosphere were monitored using 3D ERT measurements and sap flow meters, respectively. ERT results revealed that a diseased tree consumes less water, resulting in higher soil water contents in the root zone, a condition favorable to further growth of the fungus. An axisymmetric form of the Richards equation with the root distribution function proposed by Vrugt et al. (2001a) was then numerically solved using HYDRUS (2D/3D). The reduction in RWU due to the disease stress was modeled using piece-wise linear and S-shaped non-linear functions, and their applicability to simulate RWU was evaluated in the presence of the water stress. Parameters of the disease stress response function were specified by defining thresholds of PC of bacterial pathogens for each crop growth stage. Optimal root distribution and disease stress function parameters for each scenario were obtained using a genetic algorithm. Errors in simulating RWU from unhealthy trees by ignoring the disease stress condition was observed to be in the range of 15–26%. Our results indicate that model calibration using plant transpiration data can accurately quantify RWU fluxes from diseased trees.

Declarations of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.jhydrol.2020.124940.

References


