Extension of the Cylindrical Root Model for Water Uptake to Non-Regular Root Distributions

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The water flow toward a single root is efficiently solved in cylindrical coordinates using the matrix flux potential. The upscaling of single root fluxes to whole root systems is commonly based on the assumption of regularly distributed and parallel aligned roots. To provide more accurate solutions for randomly distributed roots, the point to root distance probability density function (PDF) is transformed to an equivalent cylinder size PDF ($f_C$), which is used for upscaling steady-state and steady-rate cylindrical root models while simple analytical solutions are derived. The regular root distribution assumption leads to large overestimations (~50%) of root water uptake for randomly distributed roots. Several numerical comparisons with simulations of the two-dimensional (2D) Richards equation for five different soil textures and five root densities show the good performance of the derived solutions under both limiting and non-limiting soil hydraulic conditions. Moreover, an explicit analytical solution is given for negative-binomial clustered roots. Under this specific assumption, the solution can be transformed to an equivalent random solution with a modified root length density. Simulation of root water uptake of different 2D root maps generated by a Poisson cluster process shows the effectiveness of the derived approximation for clustered roots.

Abbreviations: 1D, one-dimensional; 2D, two-dimensional; 3D, three-dimensional; PDF, probability density function; SR, steady rate.

Nowadays, even with extended computing resources, valid mathematical approximations are still required for various computational problems in the vadose zone to tackle a number of environmental issues with physically based simulation models. When simulating water and nutrient dynamics of agricultural or natural systems, nutrient and water uptake processes of root systems are of paramount importance. It has become possible to compute the three-dimensional (3D) fluxes in soils and within root systems (Javaux et al., 2013). Even while work is in progress to speed up simulations within the root system and to improve the accuracy of computations (Meunier et al., 2017), such high-resolution 3D models are computationally demanding and are not yet feasible for large-scale applications. The need for simplifying root and soil water transport processes from 3D or 2D to one-dimensional (1D) is obvious and has been tackled (Couvreur et al., 2012, 2014).

One classical microscopic approach to approximate a complex 3D root system is the adoption of a radial-symmetric system of parallel aligned roots with half inter-root distances $r_m [L]$ and root length densities $L [L^{-3}]$ (Gardner, 1960, $r_m = (\pi L)^{-0.5}$; see Fig. 1). This 1D approach enables efficient approximations of root water uptake, while assuming steady-state or steady-rate soil water content changes in the root depletion zone (Cowan, 1965; Passioura and Cowan, 1968; de Willigen and Noordwijk, 1987; Raats, 2007; de Jong van Lier et al., 2008).

There have been only a few attempts to generalize these approaches to non-regularly distributed roots. Some explicit 2D approaches were based on Dirichlet tessellation (de Willigen and Noordwijk, 1987; Lafolie et al., 1991) or on root distances within a regular computational grid directly sampled from root maps (Beudez et al., 2013). However, these approaches are based on finite samples of spatial root distributions, which need to be large to allow generalizations.
Rappoldt (1990, 1992) proposed an interesting theory that transforms the distance distribution from arbitrary soil positions toward roots to an equivalent size distribution of cylinders. Van Noordwijk et al. (2001) adopted this approach and presented a method to assess the nutrient uptake efficiency from experimentally obtained root maps. Surprisingly, these theoretical results have not been put forward to search for simplifications of root water uptake modeling.

Based on the theory of Rappoldt (1992), we developed and tested a simple 1D root water uptake model that accounts for randomly distributed roots and does not require explicit information on the root distribution. Moreover, an extension for root clustering from a negative binomial point process was also developed.

Theory

Transformation of Probability Density Functions of Point Distances to Equivalent Cylinder Sizes

Randomly distributed parallel roots in a unit cube with normal orientation toward the cube top plane are considered (see Fig. 1). Viewing from the cube top plane and considering all roots marked with their cross-sectional midpoint, the statistical process leading to such a random point pattern over a plane is known as the 2D Poisson point process (Moltchanov, 2012). The distance probability density function from an arbitrarily chosen point in the top plane to the nearest root center is given as (Moltchanov, 2012)

\[
f_D = 2L \pi r_D \exp\left(-L \pi r_D^2\right)\tag{1}
\]

with the distance \(r_D\) [L] and the mean number of points (roots) per top plane area, which corresponds here to the root length density \(L\) [L⁻¹].

Rappoldt (1990, 1992) proposed to transform a distance PDF of point pattern to an equivalent size PDF of geometric bodies such as plane sheets, cylinders, and spheres (see Fig. 1). This theory forces the equivalence of widely scattered transport pathways in the soil with the well-defined diffusion pathways in plane sheets, cylinders, or spheres. Established single body (e.g., root) solutions of diffusion in planes, cylinders, and spheres can then be combined with the obtained equivalent size distribution of those bodies. While considering the nutrient uptake problem of cylindrically shaped depletion zones around the root, Rappoldt (1992) derived a general relation between the equivalent cylinder size PDF \(f_C\) and the point-distance PDF \(f_D\) from arbitrary points to root centers:

\[
f_C = 0.5 \left\{ f_D - r_D \frac{df_D}{dr_D} \right\} \tag{2}
\]

Applied to Eq. (1), this yields the size PDF of equivalent cylinders with radius \(r_C\):

\[
f_C = 2L^2 r_C^3 \pi^2 \exp\left(-L \pi r_C^2\right) \tag{3}
\]

The maximum density of Eq. (3) occurs at \(\sqrt{(1.5/L)}\) (Fig. 1, bottom) and its mean is about \(\sqrt{(1.777/L)}\), which is 33% larger than the commonly adopted mean half inter-root distance \(r_m = \sqrt{(1/L)}\) (Fig. 1, top) of regularly distributed roots. Following Rappoldt (1992), \(f_C\) can be made non-dimensional with the substitution \(\vartheta = L \pi r_C^2\):

\[
f_C^* = \frac{f_C}{2 \pi L r_C} = \vartheta \exp(-\vartheta) \tag{4}
\]

Application of an Equivalent Cylinder Size Probability Density Function to Root Water Uptake Modeling

Neglecting gravity and macropore flow, the soil water dynamic in a cylindrical shell around an inner root cylinder can be stated as

\[
\frac{\partial \theta}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r} \left[ r D(\theta) \frac{\partial \theta}{\partial r} \right] \tag{5}
\]

where \(r\) [L] is the radial distance from the root center and \(D(\theta)\) [L² T⁻¹] denotes the soil hydraulic diffusivity at the volumetric soil water content \(\theta\) [L³ L⁻³]. Using the Kirchhoff transformation of \(D(\theta)\) (Raats, 2007) the matrix flux potential \(M(\theta)\) [L² T⁻¹] can be defined with the permanent wilting point \(\theta_w\) [L³ L⁻³] as the lower integration limit:

\[
M(\theta) = \int_{\theta_w}^{\theta} D(\theta') d\theta' \tag{6}
\]

This allows Eq. (5) to be transformed to

\[
\frac{\partial \theta}{\partial t} + \frac{1}{r} \frac{\partial}{\partial r} \left[ M \frac{\partial \theta}{\partial r} \right] \tag{7}
\]

Assuming steady-state conditions (\(d\theta/dt = 0\)) and two boundary conditions at the root radius position \(r_0\): \(M(r_0) = M_0\) and
dM/dr|_{r_0} = 0.5(Sr_C^2/r_0) \) (Raats, 2007), Eq. [7] can be solved for the matrix flux potential at the radial position r within the equivalent cylinder with the outer radius r_C:

\[ M(r, r_C) = M_0 + 0.5S f \left( \frac{r}{r_0} \right) r_C^2 \]  

[8]

The chosen boundary conditions imply a unique water potential at the root surface and a root water uptake rate that is proportional to the cylinder volume. It also implies that the water potential at the outer boundary of large cylinders are higher (less negative) than the water potentials at the boundary of small cylinders.

The required volumetric soil water depletion rate \([L^3 L^{-3} T^{-1}]\) is related to the crop transpiration rate \([9]\) is physically consistent, e.g., from Coulomb's law the weighted integration of \([11]\) using the nondimensional size PDF \(f_{C*}\) is done with an approximate lower integration limit set to zero:

\[ M(\bar{\theta}) \approx \int_0^\infty f_{C*}(\bar{\theta}) S(\bar{\theta})d\bar{\theta} \approx M_0 + S \int_0^\infty \frac{\bar{\theta} \exp(-\bar{\theta}) \ln(0.5 \bar{\theta})}{2\pi L} d\bar{\theta} \]  

[12]

The integration yields

\[ M(\bar{\theta}) \approx M_0 + S \int_0^\infty \frac{\ln(a/(r_0 \sqrt{L})) + 0.4614}{\pi L} \]  

[13]

with the transpiration rate \(T = S \zeta R\) and the rooting depth \(z_R\). Setting \(a = 0.6075\) in Eq. [13] yields the best approximation of \(M(\bar{\theta})\) calculated with Eq. [10], with an error <0.2% across commonly observed ranges for \(r_0\) (0.01–0.05 cm) and \(L\) (0.1–5 cm cm\(^{-3}\)) (de Willigen et al., 2012). This obtained value compares well with the result \(a = 0.6065\) derived by de Jong van Lier et al. (2006) from the transient analytical solution of Eq. [5] under conditions of constant diffusivity \(D\), \(r_0 \ll r_m\), and large \(t\).

Any reference to root cylinder size \(r_C\) is integrated out in Eq. [13], while complete spatial randomness of root positions is now accounted for. The corresponding solution to a steady rate model of root water uptake by de Jong van Lier et al. (2008) is derived in the Appendix.

Substituting \(r_m = (\pi L)^{-0.5}\) for \(r_C\) in Eq. [11] and reassigning \(M(\bar{\theta}) = M(\bar{\theta})\), the solution of the bulk matrix potential for regularly distributed roots is obtained as

\[ M(\bar{\theta}) = M_0 + 0.5T \frac{\ln(a/(r_0 \sqrt{L})) + 0.4614}{\pi L \zeta R} \]  

[14]

Comparison of Eq. [13] and [14] reveals that the transpiration flux \(T\) enters the regular solution with a much lower weight \((0.5)\) compared with the random solution, which even decreases with increasing \(r_0\) and \(L\) due to the additive term (0.4614, see Eq. [13]). This implies significantly higher root surface to soil water potential gradients and earlier onset of soil water limitation for randomly positioned roots. Soil water limitation occurs always if \(M_0 = 0\) for prescribed transpiration rates and rooting depths. Under these conditions, Eq. [13] and [14] are solved for a soil-limited transpiration rate \(T\) with \(M_0 = 0\). Under non-limiting flow conditions \((M_0 > 0)\), Eq. [13] and [14] are solved for \(M_0\) with potential transpiration rates determined by atmospheric and plant physiological processes, which are not considered here.

### Extension to Root Clustering

Clustering of roots or the process of spatial over-dispersion of root center points is an intrinsic property of root systems because the root growth process results from branching and

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extensions of discrete spatially distributed meristems. From the various candidates of statistical models describing clustering, the negative-binomial distribution is analytically tractable and can be adopted to describe an over-dispersed spatial point process with mean \( L\pi r_D^2 \) and variance/mean ratio \( \nu > 1 \) (see Appendix). The distribution function of point distances \( F(r_D) \) is related to the probability \( P_0(r_D) \) of having zero root centers within a circle of radius \( r_D \) via

\[
F(r_D) = 1 - P_0(r_D) = 1 - \left( \frac{1}{\nu} \right)^{L\pi r_D^2 / (\nu-1)}
\]  

Differentiation of Eq. [15] with respect to \( r_D \) to obtain the distance PDF \( f(r_D) \) and the application of Eq. [2] and [4] yields the following nondimensional equivalent cylinder size PDF (see Appendix):

\[
f_C^*(\theta, \nu) = \vartheta \ln \left( \frac{1}{\nu} \right)^{\theta/(\nu-1)} \left( \frac{\nu-1}{\nu} \right)^2
\]  

Similar to the random case in Eq. [10], the integration over the mean matrix flux potentials \( M(\theta) \) of equivalent cylinders is

\[
M(\theta) = \frac{\int_{L_D}^{\infty} M(\vartheta) f_C^*(\vartheta, \nu) d\vartheta}{\int_{L_D}^{\infty} f_C^*(\vartheta, \nu) d\vartheta}
\]  

No analytical solution of Eq. [17] or optional simplifications (Eq. [11] and [12]) could be found. However, it was verified numerically that by introducing a modified clustered root length density \( f_C^*(\vartheta, \nu) \) of Eq. [16] always to the value 1, e.g., mode \( f_C^*(\vartheta, \nu) = 1 \), which is the case for randomly distributed roots. Because the maximum density of Eq. [16] is located at \( (\nu - 1)/\ln(\nu) \), \( g(\nu) \) is simply the inverse of this PDF mode

\[
\frac{\nu - 1}{\ln(\nu)} g(\nu) = L\pi r_0 = 1 \rightarrow g(\nu) = \frac{\ln(\nu)}{\nu - 1}
\]  

The effect of root clustering according to the negative binomial distribution with variance/mean parameter \( \nu \) is equivalent to the random solution (Eq. [10] and [13]) but using a modified root length density \( L_C^* \):

\[
M(\theta) \approx M_0 + T \ln \left( \frac{\nu r_0}{\nu \sqrt{\pi L_C^*}} \right) + 0.4614 \frac{\ln(\nu)}{\nu - 1}
\]  

Simulation Procedure

The Richards equation is solved in the two-dimensional \((x,y)\) spatial domain without effects of gravity. This can be stated as

\[
\frac{\partial \theta}{\partial t} = \nabla \cdot \left[ D(\theta) \nabla \theta(x,y) \right]
\]

Numerical solution is performed using MATLAB (R2018a) with the public domain class library OOPDE (Prüfert, 2015). A square box with side length of 25 cm is populated with roots having a radius of 0.1 cm, which are distributed according to a spatial Poisson point process with different root densities \( L = 0.25, 0.5, 1, 2, \) and 4 cm\(^{-3}\). This rather large root radius was chosen in order to use a large spatial domain with a sufficiently refined spatial grid. A root thinning step was performed to ensure that the distance between simulated root centers is at least 2.5\( r_0 \). The initial water content was set to the water content at field capacity (pF = 2), and the simulation proceeded at constant potential transpiration rates \( T \) representing high (0.6 cm d\(^{-1}\)) and medium (0.3 cm d\(^{-1}\)) atmospheric demands with an assumed rooting depth \( z_R \) of 50 cm. Simulations were repeated four times with different random root distributions.

An additional set of simulation runs was performed for clustered root systems according to a Poisson cluster process (Martinez and Martinez, 2015) with 25 child roots surrounding randomly distributed parent roots with different cluster sphere radii of 1, 2, and 3 cm. Simulations were run for \( L \) values of 0.25, 0.5, and 1 cm\(^{-3}\), a transpiration demand of 0.4 cm d\(^{-1}\), and a sandy soil. Ten different realizations of root-populated square boxes of each parameter set were simulated.

Simulations continued until the plant-available water content was almost depleted \( (\theta \sim \theta_w) \). At the outer square edge of the simulation domain, a zero-flux Neumann boundary condition was applied. For each single root, initially a Neumann-type flux condition based on the presumed transpiration rate was given. If the water content at the root surface approached the permanent wilting point, the Neumann-type boundary condition switched independently for each single root to a Dirichlet boundary condition with \( \theta_{root} = \theta_w \). Simulations were performed for a wide range of soil textures (five) taken from the Staring soil series (Kroes et al., 2009) (Table 1).

Assuming a van Genuchten type soil combined with the Mualem conductivity function, the hydraulic diffusivity is calculated as (van Genuchten et al., 1991)

\[
D(\theta) = \frac{(1-m)K_S \lambda^{1/m}}{\alpha m(\theta_S - \theta_w)} \left[ (1-S_e^{1/m})^{-m} + (1-S_e^{1/m})^m - 2 \right]
\]

<table>
<thead>
<tr>
<th>Soil Texture</th>
<th>( \alpha )</th>
<th>( \theta_S )</th>
<th>( \theta_w )</th>
<th>( n )</th>
<th>( \lambda )</th>
<th>( K_S )</th>
</tr>
</thead>
<tbody>
<tr>
<td>B3 sand</td>
<td>0.0144</td>
<td>0.02</td>
<td>0.46</td>
<td>1.534</td>
<td>-0.215</td>
<td>15.42</td>
</tr>
<tr>
<td>B11 clay</td>
<td>0.0195</td>
<td>0.01</td>
<td>0.59</td>
<td>1.109</td>
<td>-5.901</td>
<td>4.53</td>
</tr>
<tr>
<td>B13 silt</td>
<td>0.0084</td>
<td>0.01</td>
<td>0.42</td>
<td>1.441</td>
<td>-1.497</td>
<td>12.98</td>
</tr>
<tr>
<td>B8 loam</td>
<td>0.0099</td>
<td>0.01</td>
<td>0.43</td>
<td>1.288</td>
<td>-2.244</td>
<td>2.36</td>
</tr>
<tr>
<td>B18 peat</td>
<td>0.0197</td>
<td>0.02</td>
<td>0.77</td>
<td>1.288</td>
<td>-1.845</td>
<td>6.67</td>
</tr>
</tbody>
</table>
with \( m = 1 - 1/n, S_c = (\theta - \theta_c)/(\theta - \theta_c), S_s = \theta / S_c \), \( K_s \) is the saturated hydraulic conductivity \([L \cdot T^{-1}]\), and \( \theta_c \) and \( \theta_s \) are the residual and saturated volumetric soil water contents \([L^3 \cdot L^{-3}]\). The water retention was calculated as

\[
S_c(b) = \left[1 - (\alpha b)^m\right]^{-1}
\]

with soil water potential \( b (b > 0) \) \([L]\). Final simulation times were set as the time point of complete depletion of plant-available water contents at prescribed potential transpiration rates plus an additional 3 d.

**Post-processing**

The mean bulk water content \( \bar{\theta} \) and the mean matrix flux potential \( M(\bar{\theta}) \) were derived for all simulated grid nodes. Transpiration rates were calculated from simulated hourly changes of \( \bar{\theta} \) while accounting for root volume effects. Simulated mean root surface water potentials \( \bar{\theta}_{\text{root}} \) were derived from \( \bar{\theta}_{\text{root}} \) using Eq. \[22\].

Non-limiting soil hydraulic conditions were defined as states where the prescribed atmospheric transpiration demand was fulfilled by the current soil to root water flow. The matrix flux potential at the root surface using the steady-state model with regular root distributions is obtained from Eq. \[14\] with prescribed transpiration rates. These results are referred to as 1D Regular. Because simulations were performed with comparably large roots having a radius \( r_0 = 0.1 \) cm to facilitate dense spatial discretization, Eq. \[13\] was slightly reparameterized to retain its accuracy across an extended range of root system properties \((r_0 = 0.01–0.1 \text{ cm}; L = 0.1–10 \text{ cm}^{-3})\):

\[
M(\bar{\theta}) \approx M_0 + T \left[ \frac{\ln\left(\frac{\sqrt{r_0 \pi} L}{\pi L_{\text{a}}}ight)}{\pi L_{\text{a}}} + 0.4614 \right]
\]

\[ M_{\text{a}} = 0.30566 r_0 L_{\text{a}}^{0.7278} \pi L_{\text{a}} \]

This extended range equation with retained accuracy (error <0.2%) is referred to as 1D Random. Corresponding versions of steady-rate (SR) models with \( d\theta/dt = \) constant are derived in the Appendix and are referred to as 1D Random SR and 1D Regular SR. Finally, a clustered root system solution for the extended range is denoted as 1D Cluster:

\[
M(\bar{\theta}) \approx M_0 + T \left[ \frac{L_{\text{a}}^{0.4614}}{\sqrt{L_{\text{a}}}} \right]
\]

\[ M_{\text{a}} = L_{\text{a}}^{0.4614} \frac{\ln(v)}{\nu - 1} \]

The \( v \) parameter was directly estimated from the variance/mean ratio of 50,000 randomly chosen point-to-nearest-root-center distances obtained from 10 simulated root distributions for each scenario. Using the Poisson distance distribution (Eq. \[1\]), a transformation for distance \( (\nu_{\text{DF}}) \) to count-based estimates of \( v \) was derived as

\[ \nu = \nu_{\text{DF}} L^{0.5} \times 7.32 \]

Root water potentials are computed numerically from calculated \( M_0 \) using Eq. \[6\], \[21\], and \[22\].

With the onset of water limitation \((M_0 = 0)\), Eq. \[14\], \[13\], and \[24\] are solved for \( T \) with the new interpretation as the soil-limited transpiration rate. Because the final time was set prior to simulation runs, computed soil water limited transpiration rates are not always diminished to zero values.

A root system uptake efficiency \( \rho \) \([L^{-2}]\) might be defined as the flux \( S \) per matrix potential gradient \( S/(M(\bar{\theta}) - M_0) \), which yields, in the case of randomly dispersed roots (see Eq. \[13\]),

\[ \rho = \pi L \left[ \ln\left(\frac{\sqrt{r_0 \pi L}}{0.4614} + 0.4614 \right) \right] \]

while corresponding terms for regular and clustered roots are obtained from Eq. \[14\] and \[19\] accordingly.

**Results**

**Model Comparison under Non-limiting Soil Hydraulic Conditions**

The consideration of random root positioning largely improves the accuracy of estimated root water potentials (Table 2), while the steady-state model (Eq. \[23\]) performs slightly better than the steady-rate model (Eq. \[A6\]). Using the randomized version of the steady-state model, the root mean squared error is reduced by >70% during the week before the onset of soil water limitation. From the comparison of regular and random solution terms (Eq. \[14\] and \[13\]), a large underestimation of root surface water potentials was anticipated for approximations based on the regular root distribution assumption (Fig. 2). Detailed comparisons for a subset of soil types, leaf area densities, and a high transpiration demand (Fig. 2) show the very good correspondence between high-resolution two-dimensional simulations and the 1D Random type approximation for different soil textures, whereas the 1D Regular approximation did not perform as well over time. This behavior was also observed in all other combinations of root length density, soil type, and transpiration demand (results not shown).

<table>
<thead>
<tr>
<th>Model</th>
<th>RMSE</th>
</tr>
</thead>
<tbody>
<tr>
<td>1D Random (Eq. [23])</td>
<td>89</td>
</tr>
<tr>
<td>1D Regular (Eq. [14])</td>
<td>318</td>
</tr>
<tr>
<td>1D Random SR (Eq. [A6])</td>
<td>103</td>
</tr>
<tr>
<td>1D Regular SR (Eq. [A1])</td>
<td>381</td>
</tr>
</tbody>
</table>

Table 2. Root mean squared error (RMSE) between two-dimensional simulations of bulk root-to-soil water potential gradients and various one-dimensional (1D) approximations. Comparisons were made over 7 d prior to the onset of soil water limitation for five soil types, five root length densities, and two transpiration demands (\( \nu = 8450 \) h).
Model Comparison under Limiting Soil Hydraulic Conditions

Even under limiting hydraulic conditions, approximations accounting for random root distributions lead to more accurate predictions of the soil-limited transpiration flux (Table 3; Fig. 3), while improvements in accuracy amount to about 42%, with the largest improvements for sand and peat soils, which seems to be related to a low mean diffusivity (Table 3). For a subset of simulated treatments, the time point of soil water limitation was usually reached 1 to 2 d earlier in 1D Random than the 1D Regular approximation. Similar behavior was observed in all other combinations of root length density, soil type, and transpiration demand.

Table 3. Root mean squared errors in actual transpiration rates between two-dimensional simulations, two one-dimensional (1D) approximations and their steady-rate (SR) equivalents, and five soils. Comparisons were made over 8 simulated d, five root length densities, and two preceding atmospheric transpiration demands (n = 9650 h). Also shown is the simulated mean diffusivity $D = \frac{M(\bar{q}) - M(\bar{q}_{\text{root}})}{(\bar{q} - \bar{q}_{\text{root}})}$ during the stage of limiting hydraulic conditions.

<table>
<thead>
<tr>
<th>Model</th>
<th>RMSE</th>
<th>All soils</th>
<th>Sand</th>
<th>Clay</th>
<th>Silt</th>
<th>Loam</th>
<th>Peat</th>
</tr>
</thead>
<tbody>
<tr>
<td>1D Random (Eq. [23])</td>
<td>0.57</td>
<td>0.35</td>
<td>0.63</td>
<td>0.30</td>
<td>0.49</td>
<td>0.88</td>
<td></td>
</tr>
<tr>
<td>1D Regular (Eq. [14])</td>
<td>1.01</td>
<td>1.05</td>
<td>0.95</td>
<td>0.40</td>
<td>0.72</td>
<td>1.56</td>
<td></td>
</tr>
<tr>
<td>1D Random SR (Eq. [A6])</td>
<td>0.62</td>
<td>0.38</td>
<td>0.68</td>
<td>0.32</td>
<td>0.53</td>
<td>0.98</td>
<td></td>
</tr>
<tr>
<td>1D Regular SR (Eq. [A1])</td>
<td>1.08</td>
<td>1.19</td>
<td>0.98</td>
<td>0.41</td>
<td>0.75</td>
<td>1.64</td>
<td></td>
</tr>
</tbody>
</table>

Mean diffusivity $D = \frac{M(\bar{q}) - M(\bar{q}_{\text{root}})}{(\bar{q} - \bar{q}_{\text{root}})}$

During the stage of limiting hydraulic conditions.

Fig. 2. Simulated differences between root surface and bulk soil water potentials (MPa) for explicit two-dimensional (2D) simulations of randomly distributed roots and the steady-state model integrated over a random root distribution (1D Random, Eq. [23]) and the regular distribution (1D Regular, Eq. [14]). Different soils (sand, clay, and peat) and root length densities $L = 0.25$, 0.5, and 1.0 cm$^2$ are indicated. Other conditions were: transpiration rate $T = 6$ mm d$^{-1}$, root radius $r_0 = 0.1$ cm, and rooting depth $z_R = 50$ cm.

Fig. 3. Simulated actual transpiration rates for explicit two-dimensional (2D) simulations of randomly distributed roots and the steady-state model integrated over a random root distribution (1D Random, Eq. [23]) and the regular distribution (1D Regular, Eq. [14]). Different soils (sand, clay, and peat) and root length densities $L = 0.25$, 0.5, and 1.0 cm$^2$ are indicated. Other conditions were: transpiration demand $T = 6$ mm d$^{-1}$, root radius position $r_0 = 0.1$ cm, and rooting depth $z_R = 50$ cm.
Model Comparison for Clustered Root Systems

Solving an equivalent randomly distributed root system but using a reduced root length density (Eq. [24]) improved predictions for the simulated water transport of clustered root systems according to the Poisson cluster process (Table 4; Fig. 4 and 5). For the simulated sandy soil, root mean squared errors were almost halved during both states of soil water limitation (Table 4) when compared with the 1D Random solution (Eq. [23]).

Figure 6 shows calculated root system uptake efficiencies for regular, random, and clustered root systems. It reveals that the diminished water extraction ability of random root systems is even more reduced by the process of root clustering according to the negative-binomial distance PDF. Some simulated random and clustered 2D root maps are shown in Fig. 7.

Discussion

In this work, we generalized the frequently used single root cylinder water uptake model to a random and negative-binomial distribution of roots in the 2D plane. This was based on the weighted integration of the single root cylinder solution with an equivalent cylinder size PDF.

One crucial step is the use of the matrix flux potential as a true volumetric quantity like water content in Eq. [9] and [10]. It should be noted that this is only strictly valid under constant diffusivity when a change in the matrix flux potential with distance from the soil–root interface is proportional to the change in water content with distance. During a drying cycle, a gradient of diffusivities between the root surface and the outer radial distance develops, and usually a decrease in the calculated effective α parameter with increasing root to bulk soil diffusivity gradient is observed (results not shown). This is also indicated by an occasional overshooting of simulated water potential gradients toward the end of the period with non-limiting hydraulic conditions (see sand in Fig. 2).

While integrating over the equivalent cylinder size PDF, an invariant value for $M_0$ and $S$ had to be assumed because we could not find any relation for $M_0(r_c)$ or $S(r_c)$ to be integrated concurrently with $\mathcal{M}(r_c)$ (Eq. [10]). Several tests in the water-limited stage to use a unique mean matrix flux potential everywhere $\mathcal{M}(r_c) = \bar{M}$ and to perform the integration over a variable depletion rate $S$ per equivalent cylinder or to introduce some empirical function $S(r_c)$ yielded unreasonable results (not shown).

Table 4. Root mean squared errors between two-dimensional simulations and one-dimensional (1D) model calculations of clustered root systems (n = 9) for bulk root to soil water potential gradients (RMSEP_p) and actual transpiration (RMSET_T). Comparisons were made over 7 d prior to the onset of soil water limitation ($n = 1521$) and 14 d thereafter ($n = 3033$) for a sandy soil with root length densities $L = 0.25$, $0.5$, and $1$ cm cm$^{-3}$, variance/mean ratios ($\nu$) between 4 and 1.22, and transpiration demand $T = 4$ mm d$^{-1}$.

<table>
<thead>
<tr>
<th>Model</th>
<th>RMSEP_p</th>
<th>RMSET_T</th>
</tr>
</thead>
<tbody>
<tr>
<td>1D Random (Eq. [23])</td>
<td>231</td>
<td>0.59</td>
</tr>
<tr>
<td>1D Cluster (Eq. [24])</td>
<td>120</td>
<td>0.29</td>
</tr>
</tbody>
</table>

Fig. 4. Simulated differences between root surface and bulk soil water potentials for explicit two-dimensional (2D) simulations of clustered roots and a steady-state model integrated over a clustered root distribution (1D Cluster, Eq. [24]) and the random distribution (1D Random, Eq. [23]). Different root length densities $L = 0.25$, $0.5$, and $1.0$ cm$^{-2}$ and variance/mean ratios ($\nu$) are indicated. Other conditions were: transpiration rate $T = 4$ mm d$^{-1}$, root radius $r_0 = 0.1$ cm, and rooting depth $z_R = 50$ cm.
In general, any empirically based specification of candidate functions for \( M_0(\nu) \) or \( S(\nu) \) from 2D simulations would be problematic because equivalent cylinders are not explicitly observable. A more realistic boundary condition for \( M_0 \) with distributed root diameters could be obtained, however, if the flux \( S \) is specified at the root xylem site. Then \( M_0 \) would be a function of the root radial conductivity, \( S \), and root radius. Because 2D water flow simulations here were restricted to the root surface–soil path, this point requires more investigations with coupled simulations of water flow in the whole root system (Javaux et al., 2013).

The derived explicit analytical solution (Eq. [24]) for roots clustered according to a negative-binomial point process was obtained via matching its distribution mode to the mode of the Poisson point process (see Eq. [23]). An optimal point process model would cover the range from under- to over-dispersion of roots besides having a tractable point-distance PDF. Rappoldt (1992) derived a rather complex \( f_C^* \) PDF for a Poisson cluster process (Diggle, 1978) that requires numerical solution even for the size PDF. Because of this computational complexity, the simple analytical solution (Eq. [24]) is valuable if it will retain its predictive power under slight to medium deviations from the negative-binomial distribution assumption. Here, we tested Eq. [24] with root distributions generated by a Poisson cluster process, which proved to be a good 1D approximation (Table 4; Fig. 4 and 5).

Van Noordwijk et al. (2001) noted a so-called root position effect ratio value \( R_{\text{per}} = 0.3 \) for winter wheat (\emph{Triticum aestivum} L.) and sugar beet (\emph{Beta vulgaris} L.) crops in the plow layer. The calculation of their \( R_{\text{per}} \) is also based on the theory of equivalent cylinders, and it describes the fractional transport efficiency of the actual observed root distribution relative to the regular distribution (van Noordwijk et al., 2001). Using Eq. [13] and [14], \( R_{\text{per}} = 0.48 \) was computed for a random root distribution, which compares well with a random \( R_{\text{per}} = 0.5 \) given by van Noordwijk et al. (2015). Choosing a variance/mean ratio \( \nu = 2.4 \) (\( \nu = 1 \) denotes the random case) and using Eq. [24] would result in \( R_{\text{per}} = 0.3 \) and an additional 40% loss of transport efficiency due to root clustering.

Regarding soil water transport, the diffusion coefficient is several orders of magnitude larger than for nutrients, which facilitates water redistribution and makes a significant effect of colocation of higher root densities and water contents on root efficiency calculations unlikely if spatial discretization of the soil domain is chosen appropriately.

In some studies, root system efficiencies \( R_{\text{per}} \leq 0.05 \) (Faria et al., 2010; Casaroli et al., 2010) were estimated based on transpiration measurements. These low efficiencies are likely caused by additional processes occurring mostly downstream on the soil–root transport path: for example, root shrinkage caused gap formation between roots and soil (de Willigen et al., 2018) or loss of root xylem axial conductance due to cavitation (Sperry et al., 1998).

In principal, the variance/mean parameter \( \nu \) could be estimated from an elaborated spatial sampling and scaling (see Eq. [25]) of point to nearest root center distances using simulated 3D root systems.
(Schneepf et al., 2018). This opens a new perspective to combine 1D root water uptake modeling with 3D root growth simulations.

The distance PDF \( f_D \) (Eq. [1]) was easily derived for randomly distributed root center points in a 2D plane geometry (Fig. 1). Considering a 3D geometry, a more rigorous treatment was performed by Ogston (1958) for randomly distributed non-parallel straight fibers in three dimensions that yields for the distance distribution function (van Noordwijk et al., 2001)

\[
1 - F(r_D) = P_0(r_D) = \exp \left[ -\pi L \left( \frac{r_D^2}{3} + \frac{4}{3} \pi r_D^3 \right) \right] \tag{27}
\]

where \( \tau \) [L\(^{-1}\)] is the root tip number per unit root length. Disregarding root tips in Eq. [27] \( \tau = 0 \) because they contribute only little to water uptake owing to their very low axial conductivity (Melchior and Steudle, 1993) and after differentiation of Eq. [27] with respect to \( r_D \), the resulting PDF can be shown to be identical to Eq. [1] and all derivations made remain valid. It will still be interesting to see if the approximations that are provided in this work perform equally well for soil water transport simulations in the 3D domain.

The provided analytical solutions give insight into a complex transport process that is hard to obtain from water flow simulations alone because the simulated process is stochastic in nature and needs a dense spatial discretization across a very large soil area or volume. Choosing here a spatial simulation domain of 25 by 25 cm randomly populated with roots, a large root radius \( r_0 = 0.1 \) cm, and repeated simulation proved to be an effective compromise between computational complexity and accuracy.

\section*{Summary}

In this work we propose an extension of a widely adopted radial-symmetric root cylinder model for water uptake with respect to non-regular spatial root distributions. Simple analytical solutions are provided for randomly distributed (Eq. [23]) and clustered (Eq. [24]) roots throughout the 2D plane that are likely to be valid in three dimensions if the effect of root tips is neglected. Results from 2D water flow simulations support the obtained analytical solutions, while accuracy is higher during the non-limiting hydraulic stage of soil water depletion. Steady-state or steady-rate approaches performed almost equally well. Simulations and analytical solutions show that the common adoption of regularly distributed root systems leads to a substantial overestimation of root water uptake efficiency (~50%). Existing 1D soil to root water transport models based on the single root cylinder solution should be adapted to account for randomness and over-dispersion of roots.

\section*{Appendix}

\section*{Extending the Steady-Rate Model to Randomly Distributed Roots}

Assuming a steady-rate (SR) condition \( \left( \frac{dJ}{dt} = 0 \right) \) for the solution of Eq. [7], de Jong van Lier et al. (2008) derived the efficiency term \( \rho = S/M(\bar{r}) - M_0 \):

\[
\rho(r_m) = 4 \left[ \frac{r_m^2}{\pi} - a^2 \frac{r_m^2}{\pi L} + \left( \frac{a^2}{\pi L} \right)^2 \right] \ln \left( \frac{r_m}{r_0} \right) \left( \frac{r_m}{r_0} \right)^{-1} \tag{A1}
\]

with \( r_m = (\pi L)^{-0.5} \) and \( a = 0.55 \) (see below for estimation). This is referred to as the 1D Regular SR solution. Equation [A1] is based on the profile solution of matrix flux potential with radial distance \( r \):

\[
M(r) = M_0 + 4 \left[ \frac{r_0^2}{\pi} - r^2 + 2 \left( \frac{r_m^2}{\pi L} \right) \ln \left( \frac{r}{r_0} \right) \left( \frac{r}{r_0} \right)^{-1} \right] \tag{A2}
\]

Using variable transformations \( \varrho = \pi L r_C^2 \) with \( r_m = r_C \), Eq. [A1] is transformed to

\[
\rho(\varrho) = 4 \left[ \frac{r_0^2}{\pi} - \frac{a^2}{\pi L} + \left( \frac{a^2}{\pi L} \right)^2 \right] \ln \left( \frac{a^2}{\pi L} \right)^{-1} \tag{A3}
\]

Integral weighting of Eq. [A3] with the equivalent cylinder size PDF \( f_C(\varrho) \) \( \varrho \) \( \rho(\varrho)^{-1} d\varrho \) is performed by

\[
\bar{\rho}^{-1} = \int_0^\infty f_C(\varrho) \rho(\varrho)^{-1} d\varrho \tag{A4}
\]

with the solution (Euler–Mascheroni constant \( \gamma \approx 0.5772 \))

\[
\bar{\rho} = 4 \left[ \frac{r_0^2}{\pi} - 2 - \gamma - \ln \left( \frac{a^2}{\pi L r_0^2} \right) \right]^{-1} \tag{A5}
\]

\[
- 2 \gamma - 2 \ln \left( \frac{a^2}{\pi L r_0^2} \right) + 2 a^2 - 3 \right] \frac{1}{\pi L} \tag{A6}
\]

Allegorically to the steady-state case, the fractional distance \( a = 0.55 \) was obtained by equating Eq. [A5] to the integrals of Eq. [10] and [9] across the steady-rate profile function \( M(r) \) (Eq. [A2]) and is used for common ranges of \( r_0 \) from 0.01 to 0.05 cm and \( L = 0.25 \) to 5 cm cm\(^{-3}\). For an extended range of root properties \( r_0 = 0.01 \) to 0.1 cm and \( L = 0.25 \) to 10 cm cm\(^{-3}\), Eq. [A5] was slightly modified to

\[
\bar{\rho} = 4 \left[ \frac{r_0^2}{\pi} - 2 - \gamma - \ln \left( \frac{a^2}{\pi L r_0^2} \right) \right]^{-1} \tag{A6}
\]

\[
- 2 \gamma - 2 \ln \left( \frac{a^2}{\pi L r_0^2} \right) + 2 a^2 - 3 \right] \frac{1}{\pi L} \tag{A6}
\]

with \( a = 0.55 \), and is referred to as the 1D Random SR solution.
Deriving the Equivalent Cylinder Size Probability Density Function for the Negative-Binomial Distribution Distance Distribution

Setting the expected number of counts to \( \mu = \pi L r_D^2 \), the probability of finding no roots within a circle of radius \( r_D \) is, for a negative binomial distribution (Anscombe, 1949) of points,

\[
P_0(r_D) = 1 - F_D = \left( \frac{k}{k + \mu} \right)^k
\]

with variance/mean ratio \( v = \frac{\mu}{\nu - 1} \) [A7]

with resulting explicit size PDF

\[
f_C = 0.5 \frac{dF}{dr_D} = \frac{d^2F_D}{d^2r_D}
\]

with resulting explicit size PDF

\[
f_C = 2L^2C^3\pi^2 \ln \left( \frac{1}{v} \right) \frac{(\pi L r_D^2)(v-1)}{(v-2)^2}
\]

which is Eq. [16].

Abbreviations and Symbols

- \( D(\bar{\sigma}) \): soil water diffusivity, \( \text{cm}^2 \text{d}^{-1} \)
- \( F(r_D) \): probability distribution function of point to root center distances
- \( f_0(r_D) \): probability density function of point to root center distances, \( \text{cm}^{-1} \)
- \( f_C(r_D) \): probability density function of equivalent cylinder radiiuses, \( \text{cm}^{-1} \)
- \( f_C^*(\bar{\sigma}) \): nondimensional version of \( f_0 \)
- \( b \): soil water potential, \( \text{cm} \)
- \( K_s \): saturated hydraulic conductivity, \( \text{cm} \text{d}^{-1} \)
- \( L \): root length density, \( \text{cm} \text{cm}^{-3} \)
- \( M_0 \): matrix flux potential at root surface, \( \text{cm}^2 \text{d}^{-1} \)
- \( M(\mathbb{F}) \): matrix flux potential at mean soil water content \( \mathbb{F} \), \( \text{cm}^2 \text{d}^{-1} \)
- \( \mathcal{M}(r_c) \): mean matrix potential of an equivalent cylinder with outer radius \( r_c \), \( \text{cm}^2 \text{d}^{-1} \)
- \( P_0(r_D) \): probability of finding no point within a circle of radius \( r_D \)
- \( PWP \): permanent wilting point, \( \text{cm}^3 \text{cm}^{-3} \)
- PDF: probability density function, \( \text{cm}^{-1} \)
- \( \nu \): variance/mean ratio of point counts
- \( \bar{\sigma} \): nondimensional outer radius of root cylinder, \( \bar{\sigma} = \pi L r_c^2 \)
- \( r_0 \): mean root radius, \( \text{cm} \)
- \( r_c \): equivalent outer radius of root cylinder, \( \text{cm} \)
- \( r_m \): mean half distance between roots, \( \text{cm} \)
- RMSE: root mean squared error
- \( S \): rate of change of soil water content, \( \text{cm}^3 \text{cm}^{-3} \text{d}^{-1} \)
- \( S_z \): relative saturation
- \( T \): transpiration rate, \( \text{cm} \text{d}^{-1} \)
- \( \theta \): volumetric soil water content, \( \text{cm}^3 \text{cm}^{-3} \)
- \( \theta_r \): residual soil water content, \( \text{cm}^3 \text{cm}^{-3} \)
- \( \theta_s \): saturated soil water content, \( \text{cm}^3 \text{cm}^{-3} \)
- \( \theta_w \): soil water content at wilting point, \( \text{cm}^3 \text{cm}^{-3} \)
- \( z_R \): rooting depth, \( \text{cm} \)

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