Examination of a coupled supply- and demand-induced stress function for root water uptake modeling
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ABSTRACT
Vegetation water use is closely related to its biophysical functioning and is often under stress from various environmental factors. However, commonly used root water uptake models only consider the stress from root zone moisture availability. There is a need to incorporate the stress from both the above-ground factors and root zone water condition. In this study, a newly developed coupled supply- and demand-induced (S&D) root water uptake model is examined with measurements on two tree species, Guihua in the subtropical monsoon climate and Drooping Sheoak in the Mediterranean climate. The results show that the S&D model outperforms a supply-constraint water stress function (the S-shape model) for both studied species. The S&D model predicts 67% and 84% temporal variability in the measured water stress for Guihua and Drooping Sheoak, respectively. The improvement of the S&D model over the S-shape model is more significant for Guihua than for Drooping Sheoak, which might be associated with the specific climate conditions. A two-step parameterization approach is adopted in this study for the S&D model, and is recommended for future applications. These results further support the validity of the S&D model, and should be considered for the root water uptake modeling.

Key words | root water uptake, S&D model, S-shape model, transpiration

INTRODUCTION
Forest ecological systems are closely related to global change, because forests can influence climate through the exchanges of energy, water, carbon dioxide, and other chemical compositions with the atmosphere (Bonan 2008). Vegetation changes affect regional water balance (Yuan et al. 2012), and vegetation influences the water balance through root water uptake, transpiration and other means (Janeau et al. 2015). In the soil–plant–atmosphere system, plant roots play a key role in transporting water and nutrition. The root water uptake process reduces the potential for deep percolation although root induced macropores may increase hydraulic conductivity in soil, which facilitates percolation (Guan et al. 2010). Thus, plant root water uptake is an important process in the water cycle and soil water balance. It is a key subject of ecohydrology, land process modeling, and watershed hydrologic modeling.

According to the research scale, root water uptake models can be categorized into microscopic and macroscopic types (Yang & Hao 1999; Ji et al. 2006; Wang et al. 2011). A single radial root water uptake microscopic model with uniform water absorption characteristics was proposed by Gardner (1960). Based on this, a model of non-uniform root systems, including root hydraulic characteristics and soil-root-interface interaction, was developed (Cowan 1965; Molz 1976; Raats 1975). These models have not become dominant in application due to their numerous parameters and the requirement of complex root distribution representation.
A macroscopic model lumps the root zone into a root distribution function, which has broader applications in root zone soil water dynamic simulation for its simplicity. In such models, root water uptake is represented as a sink term in the root zone based on a root distribution function and water potential in different layers of the root zone. Two types of approaches have been developed. The first approach, proposed by Nimah & Hanks (1973), is based on a hydraulic gradient between soil and hydraulic resistance in the soil and root continuum. This approach has been adopted in root zone hydrological models such as LEACHM (Hutson & Wagenet 1991). It is difficult to parameterize the root resistance in such a model. The second approach, introduced by Feddes et al. (1978), treats root water uptake as a potential rate (depending on root distribution and the atmospheric demand) reduced by a stress function of soil water potential. This approach has been used in HYDRUS. The Feddes piecewise linear model (Feddes et al. 1978) and the S-shape non-linear model (van Genuchten 1987) are two commonly used water stress models. Both models simulate root water uptake as a potential rate (or the atmospheric demand) multiplied by a stress factor which is a function of root zone water condition. However, it is known that the stress on plant water use comes not only from the root zone moisture availability, but also from the atmospheric conditions which determine the evaporative demand (i.e., potential evapotranspiration) for root water uptake. Some land surface models consider these atmospheric factors (e.g., vapor pressure deficit, temperature and solar radiation), which are included in Jarvis-type canopy conductance models (Wang et al. 2014).

Thus, there is a need to incorporate the stress from the above-ground factors and root zone water availability into the root water uptake function to test whether root water uptake simulation can be improved. In fact, this has been attempted in HYDRUS (Simunek et al. 2005), in which two threshold soil water potentials (parameter \( h_3 \)) of the Feddes model are prescribed for two thresholds’ potential transpiration (PT) rates. This model is difficult to use for two reasons: (1) two thresholds do not provide flexibility to represent a spectrum of stress from varying atmospheric factors; and (2) the parameters are difficult to determine. Recently, Yang et al. (2013) proposed a new function for root water uptake modeling based on the S-shape model function in which, besides soil water potential, PT is used as a second factor to represent lumped stress from the atmospheric demand. In their model, the influence of both root zone water potential (which was determined by water supply) and the atmospheric demand are considered and represented. Thus, this model is now referred to as the coupled supply- and demand-induced stress function (the S&D model hereafter) for root water uptake modeling. The S&D model was previously tested with a short period of measurements on a tree species in a Mediterranean climate. It requires more rigorous testing over a longer period of measurements and in different environments.

The objective of this paper is to test the S&D model for two tree species in two climate zones (subtropical monsoon vs. Mediterranean type), by comparing the S&D modeling results with a supply-constraint water stress function (the S-shape model). A two-step parameterization method is suggested and discussed as well.

**METHODOLOGY**

**Experiments**

The experiments were performed at two sites with distinct climates, Changsha in the central south of China, and Adelaide in South Australia. The climate condition and studied tree species of the two sites are shown in Figure 1. Changsha (112.967°E, 28.183°N), the capital city of Hunan province in China, with an elevation of 70 m above sea level, has a subtropical monsoon climate characterized by hot and wet summers, and cold and dry winters. Precipitation is concentrated in spring and early summer, followed by a seasonal dryness in July and August, with a mean annual temperature of 17° C and mean annual precipitation of 1,360 mm. The experiment was conducted at a plantation site on the outskirts of the city, from April 19 to September 24 of 2013. Two *Osmanthus fragrans* (common name in China: Guihua) trees (labeled as No. 1 and No. 2) were chosen for this study. Guihua is a typical tree species in the subtropical monsoon climate zone.

The other site is on the campus of Flinders University (138.572°E, 35.039°S) in Adelaide, South Australia, with an elevation of 100 m. The climate of Adelaide is
Mediterranean type with long and hot summers, and mild and rainy winters, with a mean annual rainfall of 550 mm and mean annual temperature of 17.3°C. Drooping Sheoak (*Allocasuarina verticillata*) was selected as our study species, not only because it was a typical species in South Australia, but also because it is the species examined in Yang *et al.* (2015). The measurement was performed over two periods: January 21 to April 15 and October 29 to December 31 of 2012. Root zone hydrological studies often do not have direct soil water potential and transpiration measurements, in which the root water uptake function is often calibrated with measured root zone soil water content (Musters & Bouten 2000; Vrugt *et al.* 2001). Such exercises lump uncertainties from the determination of soil hydraulic properties, root distribution and root water uptake parameterization together, leading to difficulty in model calibration. Recent progress in monitoring stem water potential (Yang *et al.* 2015; Wang *et al.* 2014) provides a robust tool to separate parameterization of the root water uptake function from other parts of the root zone hydraulic properties.

Stem water potential was measured with thermocouple stem psychrometers (PSY1; ICT International Pty Ltd, Australia) at a 30-min interval. Details about this equipment can be found in Yang *et al.* (2015) and Wang *et al.* (2014). Previous studies (Ritchie & Hinckley 1975; Hinckley *et al.* 1978) have shown that water potential along the soil-plant continuum tends to be in equilibrium at dawn. Therefore, in this study, the predawn stem water potential was chosen as a surrogate for the root zone soil water potential to examine the water stress function for root water uptake modeling.

Transpiration was measured with the heat-pulse sap flow sensors at a 30-min interval. For each tree, two sets of sap flow probes were installed on the sunlit and shaded sides of the trunk, at a height of 0.7 m above ground. A software ‘sap flow tool’ obtained from the provider was used to calculate the daily transpiration; the whole tree transpiration was estimated from the average value of the two sides.

Micrometeorological conditions were measured from a standard automatic weather station, located in both experimental sites. Wind speed, relative humidity, air temperature and solar radiation were used to estimate PT using the Food and Agriculture Organization of the United Nations reference evapotranspiration (ET) equation.
(Allan et al. 1998),

\[
ET_0 = \frac{0.408 \Delta (R_n - G) + \gamma \frac{900}{T + 273} u_2 (e_s - e_a)}{\Delta + \gamma (1 + 0.54 u_2)} \tag{1}
\]

where \( ET_0 \) is reference evapotranspiration [mm day\(^{-1}\)], \( R_n \) is net radiation at the crop surface [MJ m\(^{-2}\) day\(^{-1}\)], \( G \) represents soil heat flux density [MJ m\(^{-2}\) day\(^{-1}\)], \( T \) is mean daily air temperature at 2 m height [\( ^\circ C \)], \( u_2 \) is wind speed at 2 m height [m s\(^{-1}\)], \( e_s \) and \( e_a \) are saturation vapour pressure [kPa] and actual vapour pressure [kPa], respectively, \( e_s - e_a \) is the saturation vapour pressure deficit (or VPD) [kPa], \( \Delta \) is the slope vapour pressure curve [kPa \( ^\circ C^{-1} \)], and \( \gamma \) is a psychrometric constant [kPa \( ^\circ C^{-1} \)].

It is difficult to accurately estimate transpiration and PT for individual trees. For transpiration estimates, a large uncertainty comes from the fact that an effective surface area required to convert volumetric sap fluxes to transpiration rates is not known. For PT, the uncertainty comes from the difficulty of accurately estimating radiation energy partitioning. We used \( ET_0 \) (Equation (1)), which was developed based on a type of densely distributed short grass, to represent the PT of the tree and adjusted the effective surface area so that the time series of PT envelops that of transpiration over the whole measurement period. Figures 2 and 3 show the calculated transpiration, PT estimated with \( ET_0 \) and precipitation measured with the automatic weather stations for Guihua and Drooping Sheoak, respectively. Since it is the ratio of transpiration (\( T \)) over PT, rather than true transpiration and true PT that is examined in this study, we consider this treatment of the data to be acceptable.

Leaf-scale data, including net photosynthetic rate, stomata conductance, transpiration rate and VPD of sunlit leaves and shaded leaves were measured by a Li-6400 photosynthetic analyzer from May 13 to August 30 in sunny days for Guihua No. 1. The measurements were taken about 2–5 times a day, from 8:00 to 16:00 h. Previous studies (Kemp et al. 1991; Gao et al. 2002) have established models to investigate the relationship between leaf-scale data, such as stomata conductance and leaf scale transpiration, and the soil water potential. This relationship is obtained based on leaf-level measurements on Guihua, and compared to that derived from the whole-tree measurements from sap flow meters and stem psychrometers.

**Theoretical background**

In the soil-plant-atmosphere continuum, suppose the change of water storage in the plant is negligible (Tyree & Yang 1990), the root water uptake rate equates to the plant’s actual transpiration rate. When a plant is under water stress, the actual transpiration is less than the PT. The equation of transpiration can be written as:

\[
T = \beta(h)^{-1} PT \tag{2}
\]

where \( T \) is the actual transpiration (mm day\(^{-1}\)), \( PT \) is the potential transpiration (mm day\(^{-1}\)), \( \beta(h) \) is the stress...
function, and \( h \) is the equivalent root zone soil water potential (MPa). \( h \) is not the mathematical average of water potential in the root zone, because roots uptake water preferentially from the wet part of the root zone to meet the atmospheric demand. As a result of this phenomenon, compensation root water uptake models have been developed (Li et al. 2001; Šimunek & Hopmans 2009; Willingen et al. 2012). Thus, \( h \) should represent the equivalent water potential of the whole root zone at which root water uptake stress currently occurs. Predawn stem water potential provides a good approximate of \( h \).

How to determine the stress function is key to the calculation of the actual transpiration or root water uptake rates. The S-shape function (Equation (3)), proposed by van Genuchten & Hoffman (1984), is commonly used for root zone hydrological simulation.

\[
\beta\left(\frac{h}{h_{50}}\right) = \frac{1}{1 + \left(\frac{h}{h_{50}}\right)^{\rho}}
\]

where \( h_{50} \) is the soil water potential (MPa) at which the water uptake rate is reduced by 50% from the potential rate, \( \rho \) is an empirical coefficient.

The S-shape function only considers the limitation from the ‘supply’ side. The results in Yang et al. (2013) show that the amount of water demanded by the atmospheric condition (i.e. PT), may pose stress on vegetation water use, and should be included in the stress function. Therefore, stress from both ‘supply’ and ‘demand’ sides is included in the S&D function:

\[
\beta\left(\frac{h}{h_{50}}, PT\right) = f\left(\frac{h}{h_{50}}\right)g\left(PT\right) = \frac{1}{1 + \left(\frac{h}{h_{50}}\right)^{\rho}}(aPT + b)
\]

where \( f \) is an S-shape function of root zone soil water potential, \( g \) is a linear function of PT, describing the stress from the atmospheric demand, PT means potential transpiration (mm day\(^{-1}\)), and \( a \) (day mm\(^{-1}\)) and \( b \) are fitted parameters.

**Model calibration and mathematical justification**

In order to examine the process of calibration and the applicability of the S&D model in different climate zones, we tested the model for both sites. For the Guihua site, we used one Guihua tree to parameterize the function and tested it with the second one. At the Drooping Sheoak site, due to only one Drooping Sheoak being measured, the odd-day data were used to fit the function and those of the even-day to test the effectiveness of the model.

A new stepwise parameterization method is adopted in this study. This is different from the method used by Yang et al. (2013) who calibrated the two parts in Equation (4) simultaneously. We found that determination of the four parameters simultaneously with all data did not come to consistent results for \( h_{50} \). This may be due to high correlation between PT and root zone water potential, particularly for
the Mediterranean climate. To avoid this problem, we calibrate the supply-induced stress first using the days with low PT values. We assume that in these low PT days, the atmospheric demand is small, the demand-induced stress is minimal and can be neglected. The data are fitted with the least sum of square method for the S-shape function, to obtain the parameter values of $h_{50}$ and $p$. After, these two parameters are determined, all data are fitted with the least sum of square method for the S&D model function to obtain the values of $a$ and $b$.

Although the S&D model is constructed based on our understanding of the environmental stress on transpiration, mathematically an overfitting problem may exist given that it has two more parameters than the S-shape model.

The Bayesian information criterion ($BIC$) (Schwarz 1978), considered to be the most strict statistical indicator to pose a penalty on additional parameters in a model (Hawkins 2003), was adopted to test if the S&D model is also mathematically sound. The $BIC$ can be calculated according to

$$BIC = n \log \left( \frac{SSE}{n} \right) + k \log (n)$$

where $SSE$ is the sum of square error, $n$ is the number of data points, and $k$ is the number of predictor parameters. A model with additional parameters is accepted if $BIC$ is smaller than that of a simpler model (e.g., Guan et al. 2013).

### Model validation and evaluation

To compare the S&D model and the S-shape model, two commonly used model evaluation indicators: root-mean-square error (RMSE) (Liu et al. 2015) and the Nash–Sutcliffe coefficient of efficiency (NSE) (Nash & Sutcliffe 1970; Legates & Mccabe 1999), are selected for the effectiveness evaluation of the two models. The calculation formula of the NSE is:

$$NSE = 1 - \frac{\sum_{i=1}^{n}(Q_m - Q_s)^2}{\sum_{i=1}^{n}(Q_m - \bar{Q_m})^2}$$

where $NSE$ is the Nash–Sutcliffe coefficient of efficiency, $Q_m$ is the measured value, $Q_s$ is the simulated value, $\bar{Q_m}$ is the average value of measurements and $n$ is the number of data. If $NSE = 1$, the result indicates the credibility of the model is perfect, while if $NSE = 0$, the result shows the effect of the model is nil.

### RESULTS AND DISCUSSION

#### Model parameterization

Relative humidity near 100% occurs during rainy days, and stem water potential responds sensitively to the rainfall events (Yang et al. 2013), therefore they are excluded from parameterization and examination of the water stress function.

Based on the relationship between predawn stem water potential and $T/PT$ for Guihua and Drooping Sheoak from field measurements, Equation (3) is fitted with Guihua No. 1 and Drooping Sheoak odd-day data. The results for $h_{50}$ and $p$ are shown in Table 1. With the same input data, Equation (4) is fitted stepwisely for four parameters of the S&D model, with the values of $h_{50}$, $p$, $a$ and $b$ shown in Table 1.

### Table 1 | The calibration and validation results for Guihua and Drooping Sheoak (n is the number of data points)

<table>
<thead>
<tr>
<th>Target trees</th>
<th>Calibration</th>
<th>Validation</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Models</td>
<td>$h_{50}$ MPa</td>
</tr>
<tr>
<td>Guihua No. 1</td>
<td>S-shape</td>
<td>-0.75</td>
</tr>
<tr>
<td></td>
<td>S&amp;D</td>
<td>-1.1</td>
</tr>
<tr>
<td>Guihua No. 2</td>
<td>S-shape</td>
<td>-1.1</td>
</tr>
<tr>
<td></td>
<td>S&amp;D</td>
<td>-1.1</td>
</tr>
<tr>
<td>Drooping Sheoak odd days</td>
<td>S-shape</td>
<td>-0.48</td>
</tr>
<tr>
<td></td>
<td>S&amp;D</td>
<td>-1.04</td>
</tr>
<tr>
<td>Drooping Sheoak even days</td>
<td>S-shape</td>
<td>-0.48</td>
</tr>
<tr>
<td></td>
<td>S&amp;D</td>
<td>-1.04</td>
</tr>
</tbody>
</table>

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The BIC value is −191.7 and −208.5 for Guihua No. 1 with the S-shape model and the S&D model, respectively, and −116.5 and −122.7 for the odd days of Drooping Sheoak with the S-shape model and the S&D model, respectively. This result supports the hypothesis that it is worthwhile to have the S&D model for root water uptake stress simulation.

The value of $h_{50}$ represents how plants are sensitive to water stress. As we can see from Table 1, the value of $h_{50}$ is −0.75 MPa and −0.48 MPa in the S-shape model for Guihua and Drooping Sheoak respectively. From the S&D model, the value of $h_{50}$ for Guihua and Drooping Sheoak is −1.1 MPa and −1.04 MPa, respectively. Previously, water stress has been examined for the Drooping Sheoak. The $h_{50}$ resulting from this study with the S-shape model (−0.48 MPa) is close to that (−0.52 MPa) of Yang et al. (2013). The $h_{50}$ by the S&D model in this study (−1.04 MPa) is quite different from the −0.49 MPa in Yang et al. (2013), but close to the −0.87 MPa in a study with a more rigorous model considering stress from both root zone and micrometeorological conditions (Wang et al. 2014). The value of $a$ for Guihua and Drooping Sheoak is −0.14 day mm$^{-1}$ and −0.09 day mm$^{-1}$, respectively. The value for Drooping Sheoak is close to −0.084 day mm$^{-1}$ in Yang et al. (2013). The value of $a$ represents the impact of PT: the more negative the value of $a$, the more sensitive the tree is to PT. Therefore, for the same amount of PT, water stress on Guihua is stronger than on Drooping Sheoak. This may be associated with the corresponding climatic conditions. The study area for Drooping Sheoak has a hot and dry summer, which causes large PT values (based on the measured data, PT is about 4.76 mm day$^{-1}$). We imagine trees in such an environment may adapt to the PT-induced stress, leading to a smaller PT dependency. While for the Guihua site, it is hot and relatively humid in summer. PT (based on the measured data, PT is about 3.43 mm day$^{-1}$) is not as high as that at the Drooping Sheoak site; trees in such an environment become more sensitive to PT-induced stress.

**Model testing**

**Testing with the leaf-scale measurements**

Leaves of the whole tree include sunlit leaves and shaded leaves, whose sensitivity to water potential is not the same due to different light conditions. Sunlit leaves receive more sunlight, leading to an increase in leaf temperature when the root zone water supply is limited (Han et al. 2006). A higher temperature increases stomata vapor pressure so that the leaves’ internal and external vapor pressure difference increases (Zhang et al. 2000), leading to increasing stress. On the other hand, shaded leaves receive less sunlight and the temperature difference between leaf and air is smaller. Thus, sunlit leaves may be more sensitive to the root zone soil water potential than shaded leaves. The $h_{50}$ fitted by a reasonable model for a whole tree would have a value between the value of $h_{50}$ in shaded leaves and sunlit leaves. We fitted the $h_{50}$ with the S-shape model (Figure 4); in the model function, $T$ is the actual leaf-level transpiration (mm h$^{-1}$), $T_0$ is the maximum leaf-level transpiration (mm h$^{-1}$), and $h_{50}$ and $p$ are empirical coefficients, as in Equation (2).

For the sunlit leaves, the fitted value of $h_{50}$ is −0.5 MPa (Figure 4). For the shaded leaves, the relationship between root zone soil water potential and leaf scale transpiration rate is not obvious and it is difficult to obtain the value of $h_{50}$ for such circumstances (Figure 5). The shaded leaves’ transpiration rates do not vary with root zone soil water potential over the measurement range, indicating that the value of $h_{50}$ may be lower than −2.5 MPa. The $h_{50}$ value of the whole tree should lie between the $h_{50}$ value of sunlit leaves and that of shaded leaves. Thus, the reasonable value of $h_{50}$ for Guihua should be lower than −0.5 MPa. Fitting the root water uptake function for Guihua No. 1, the value of $h_{50}$ is −0.75 MPa for the S-shape model and

\[
T = \frac{T_0}{1 + \left(\frac{h}{h_{50}}\right)^p} = \frac{4.70}{1 + \left(\frac{h}{0.5}\right)^{1.3}}
\]

**Figure 4 |** Fitting result of the relationship between root zone water potential and the sunlit leaf transpiration rates.
1.1 MPa with the S&D model, both are lower than -0.5 MPa, indicating both models reveal $h_{50}$ within the range estimated from leaf scale measurements.

Testing with whole tree measurements

The stress values estimated from the S&D model and S-shape model, based on data independent from those used for model calibration, are compared with the values calculated directly from the observations (Table 1). The S&D model is better than the S-shape model for both studied species. For Guihua in the subtropical monsoon climate zone we tested these two models with data from Guihua No. 2, and the NSE of the S&D model is 0.67, while that of the S-shape model is only 0.37. For Drooping Sheoak in the Mediterranean climate zone, we tested two models with data from even days; the NSE of the S&D model is 0.84, better than the S-shape model, which is 0.76 for the testing period.

Testing based on time series data

Another way to test the model performance is to compare simulated values with measured values in time series. The result of actual stress (actual ET over PT), model estimated stress by the S&D model and by the S-shape model, are shown in Figure 6 for Guihua and in Figure 7 for Drooping Sheoak.

For Guihua, the S&D model performs better than the S-shape model, particularly in the drought period (July to August). The estimated values from the S&D model agree well with the observed values, which explains why a plant suffers water stress from both the root zone soil water supply and the atmospheric demand.

In addition, the simulation results of both models are better in the dry period than the rainy period. Previous studies (van Genuchten & Hoffman 1984; Gavloski et al. 1992) have found that a plant suffers stress from many factors, including water stress, salt stress and meteorological factors. In the rainy period, water stress is not the major impact factor for transpiration, while in the dry period water stress is the main limiting factor for actual transpiration. This explains why both the S&D model and the S-shape model perform better in the dry period.
For Drooping Sheoak, the difference between the two models’ results is not as large as that for Guihua. The estimated water stress values from both models are in good agreement with the measured values. Nevertheless, the S&D method still provides slightly better estimation (Figure 7 and Table 1).

**About the model calibration approach**

The $h_{50}$ value fitted with the S&D model for Drooping Sheoak in this paper is $-1.04$ MPa, while Yang et al. (2013) gave $-0.48$ MPa. Both are based on data collected from the same site and same tree species, although in different years. It is very unlikely that this difference reflects the actual change in the response to environmental stress. More likely, the difference is an artifact due to the two calibration approaches as mentioned in the methodology section. In this study, a two-step calibration is adopted, while in Yang et al. (2013), the calibration was performed in one step. When this one-step approach is used for the data in this study, it results in a very large $h_{50}$ (in negative value: $h_{50} = -2.74$ MPa). This inconsistency indicates the one-step approach may not be appropriate. The good testing results for both tree species under two different climate conditions suggest the reliability and robustness of the two-step calibration approach adopted in this study.

**CONCLUSIONS**

In this study, the S&D model is examined with measurements on two tree species located in two different climatic areas. The results show that the S&D model outperforms the S-shape model for both studied species. It predicts 67% and 84% temporal variability in the measured water stress for Guihua in the subtropical monsoon climate and Drooping Sheoak in the Mediterranean climate, respectively. The improvement of the S&D model over the S-shape model is more significant for Guihua than for Drooping Sheoak, which might be associated with the specific climate conditions. The two-step parameterization approach adopted in this study for the S&D model appears to be more stable, and is recommended for future applications. These results further support the validity of the S&D model, which should be considered for root water uptake modeling.

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