Supporting Information

Article title: Diurnal variation in the isotope composition of plant xylem water biases the depth of root-water uptake estimates

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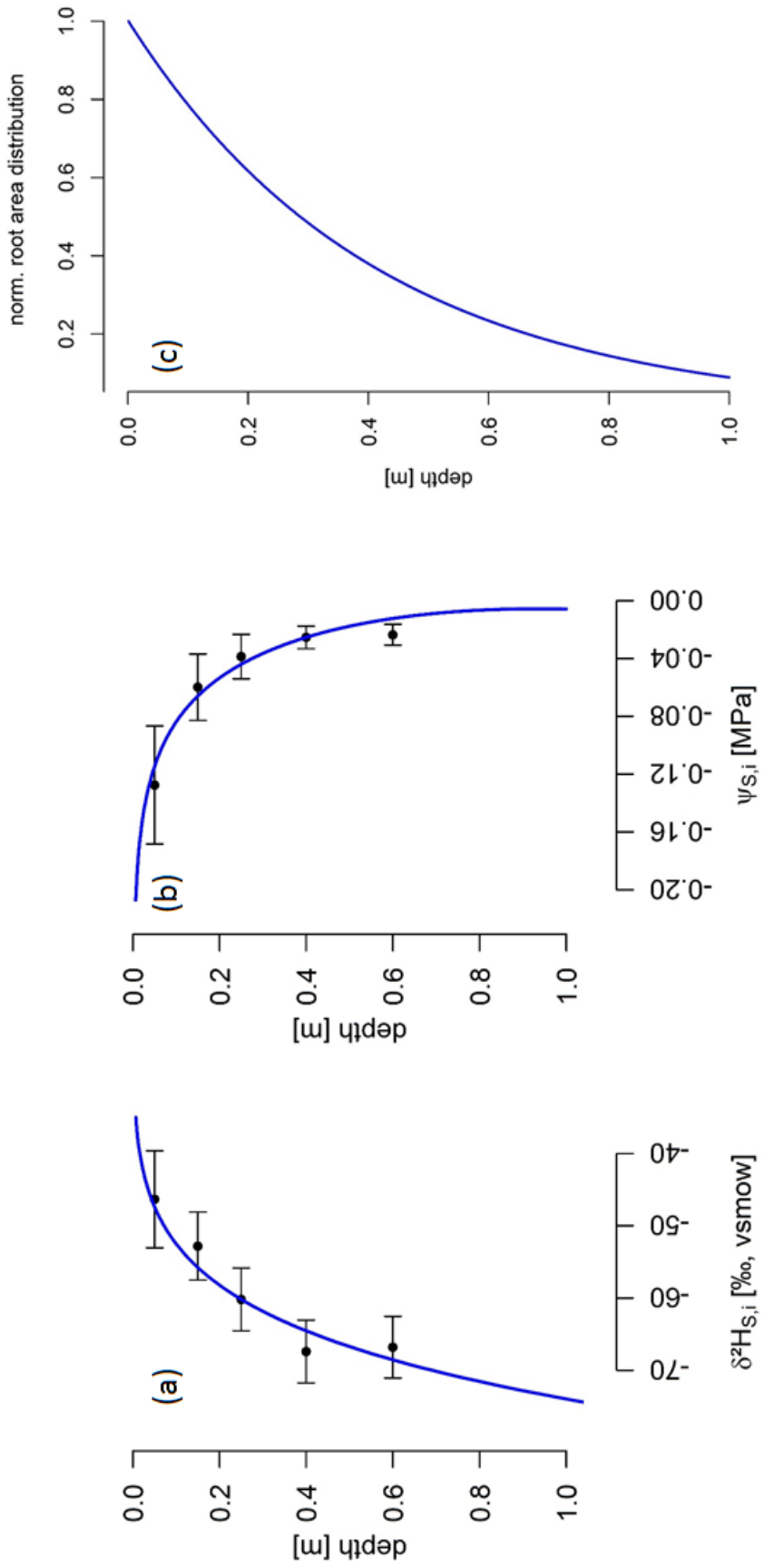
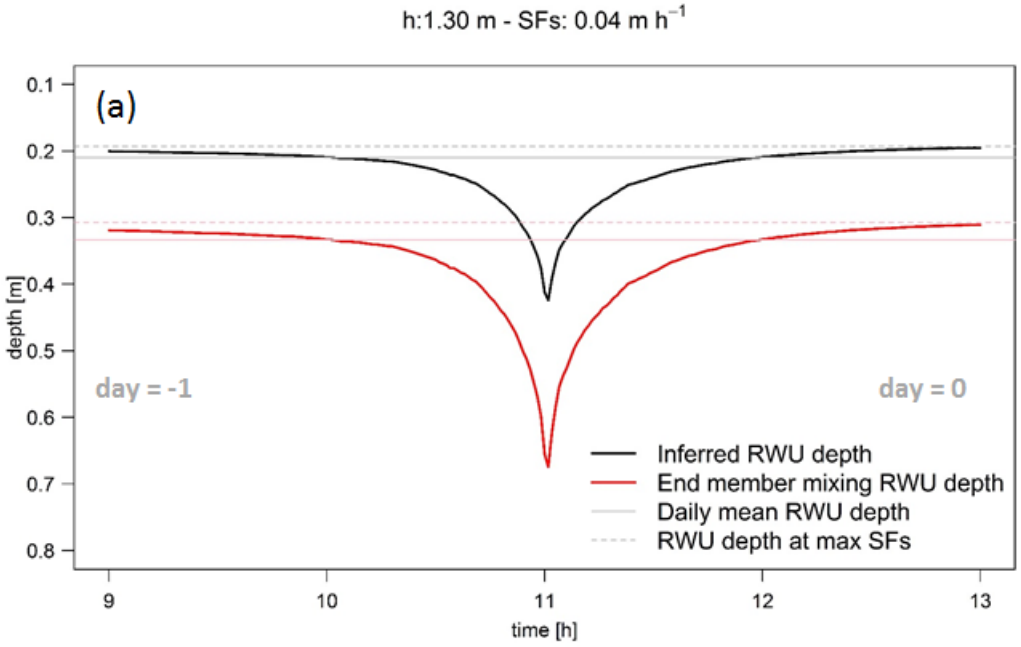

(a)
depth [m]
0.0
0.2
0.4
0.6
0.8
1.0
$\delta^2H_{S,i}$ [‰, vsmow]
-70
-60
-50
-40
(b)
depth [m]
0.0
0.2
0.4
0.6
0.8
1.0
$\psi_{S,i}$ [MPa]
-0.20
-0.16
-0.12
-0.08
-0.04
0.00
(c)
depth [m]
0.0
0.2
0.4
0.6
0.8
1.0
norm. root area distribution
0.2
0.4
0.6
0.8
1.0

Fig. S1. Panel a: Soil depth profile of deuterium isotope composition of soil water ($\delta^2H_{S,i}$), data from Meißner et al. (2012). Panel b: Soil water potential ($\Psi_{S,i}$) over the soil depth, data from Meißner et al. (2012). Panel c: The relative absorptive root area distribution with soil depths adapted from Jackson et al. (1995) and normalized to the topsoil. All equations and corresponding parameters for the fitted curves can be found in Table S1.


h:1.30 m - SFs: 0.04 m h^{-1}
(a)
depth [m]
time [h]
day = -1
day = 0
Inferred RWU depth
End member mixing RWU depth
Daily mean RWU depth
RWU depth at max SFs

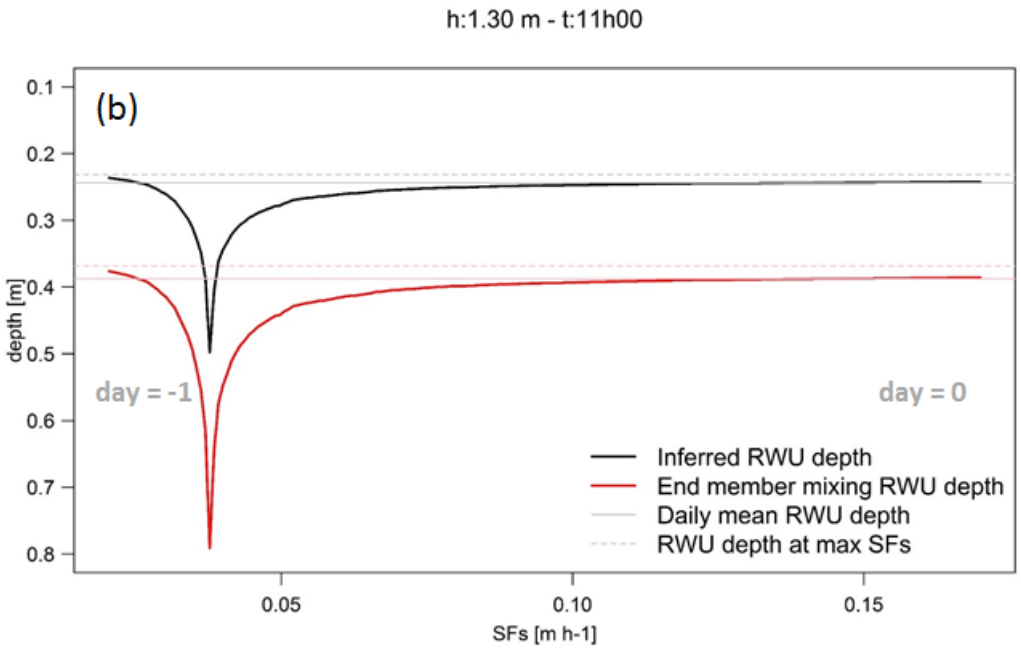

h:1.30 m - t:11h00
(b)
depth [m]
SFs [m h-1]
day = -1
day = 0
Inferred RWU depth
End member mixing RWU depth
Daily mean RWU depth
RWU depth at max SFs

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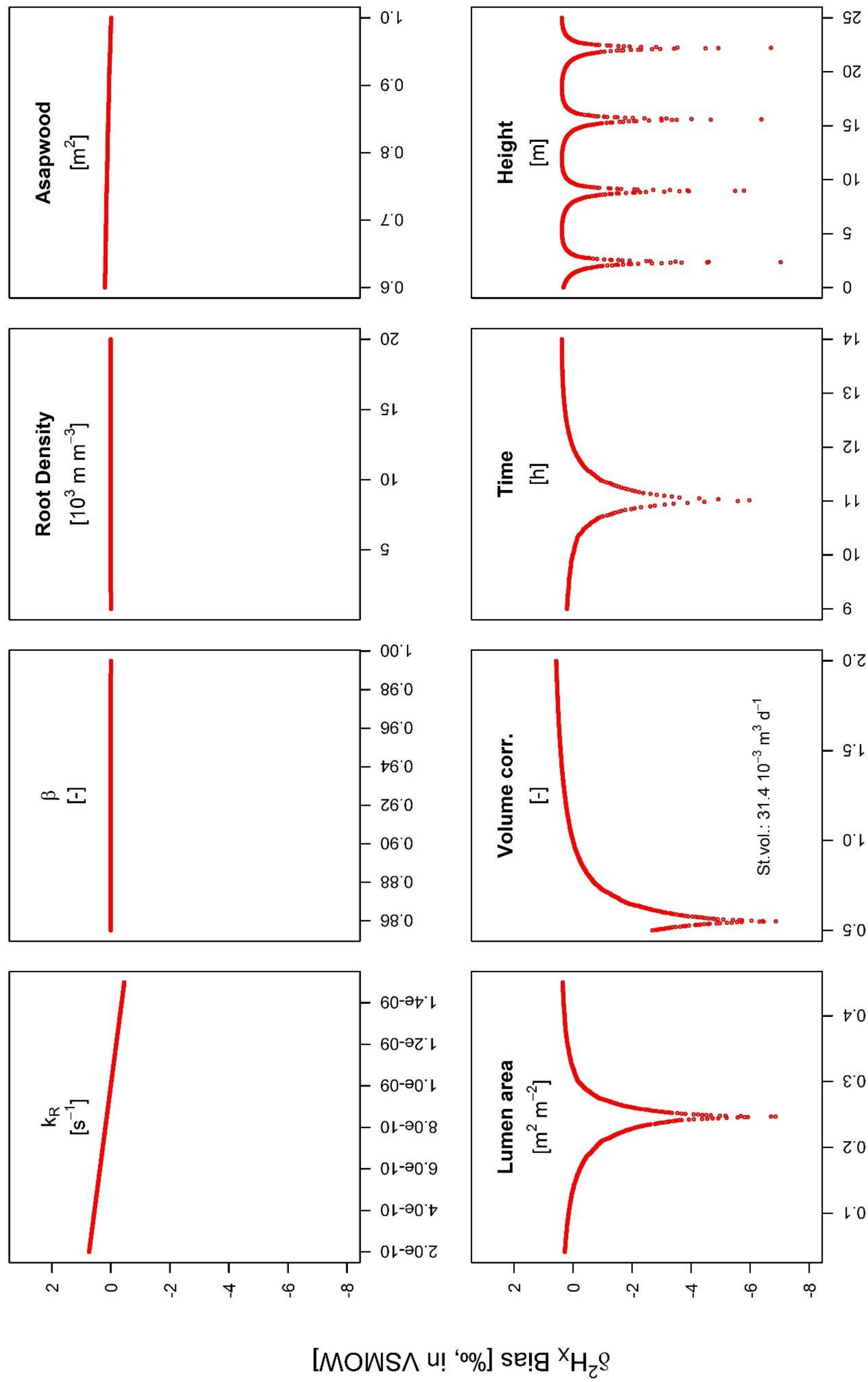
Fig. S2. Differences between the root water uptake (RWU) depth derived from using either the direct inference (black line) or the end member mixing (red line) approach. **Panel a:** The derived RWU depth for a tree sampled at standard tree coring height (i.e. 1.30 m) having a sap flux density (SF_S) of 0.04 m h^{-1} (i.e. SF_V = 0.28 m h^{-1}), over the common sampling period (9:00 until 13:00). **Panel b:** The derived RWU depth considering a tree sampled at standard tree coring height (1.30 m) at 11:30, but which differs in SF_S. The grey and pink solid lines represent daily mean RWU depth while the grey and pink dashed lines represent the RWU depth at peak sap flow activity, respectively, for the direct inference and end member mixing model approach. day= -1 and day= 0 indicate whether the derived RWU depth error corresponds to the previous or current day of measurement.



k_R [s^-1]
β [-]
Root Density [10^3 m m^-3]
Asapwood [m^2]
Lumen area [m^2 m^-2]
Volume corr. [-]
St.vol.: 31.4 10^-3 m^3 d^-1
Time [h]
Height [m]
δ2Hx Bias [‰, in VSMOW]

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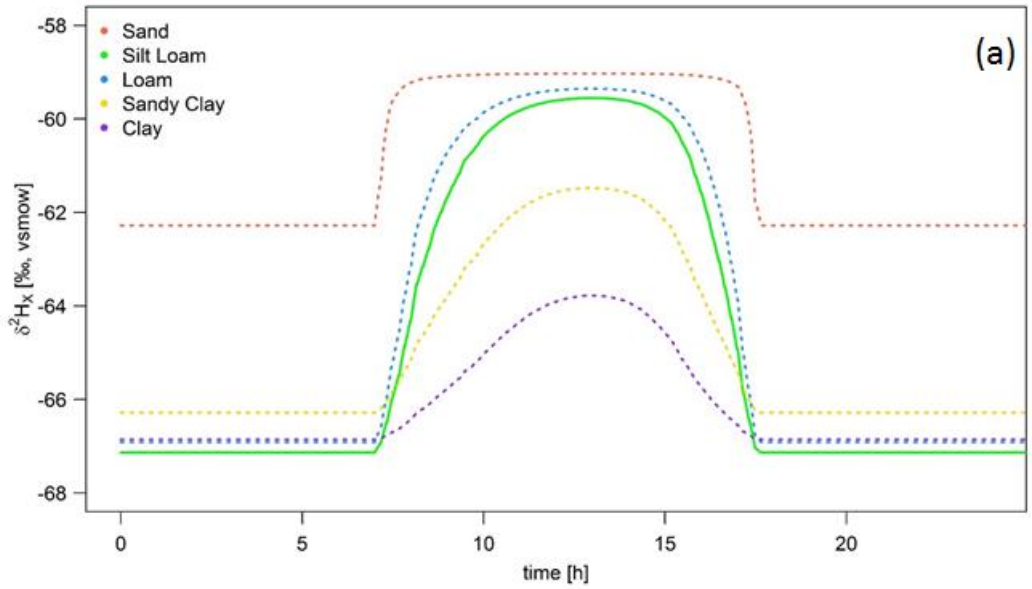
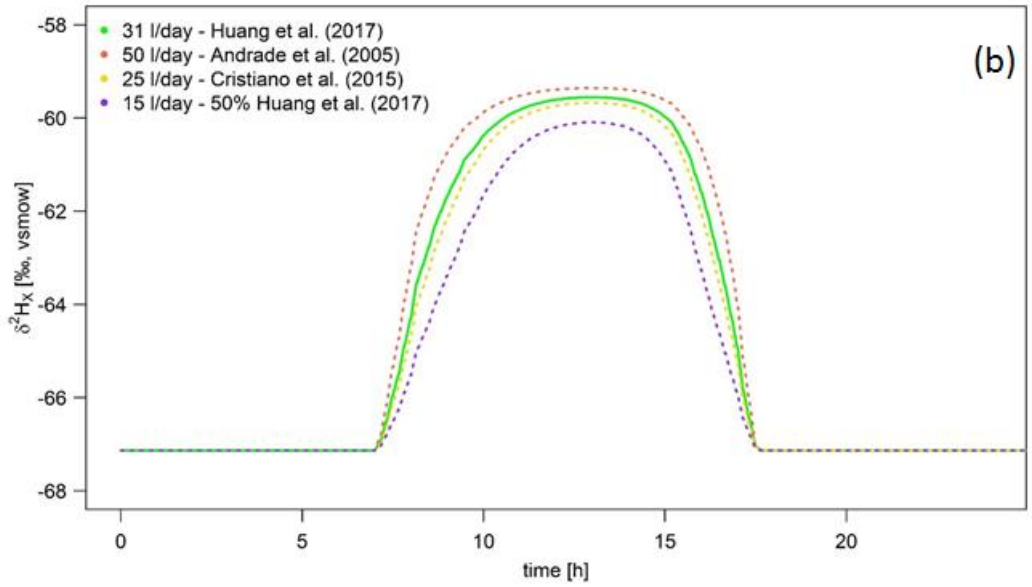
Fig. S3. Sensitivity analysis where all parameters are varied one-at-the-time as compared to the standard parameterization (see Table S1). For each studied variable, 1000 model runs were performed, studying the resulting δ^2H_X bias in comparison with the standard run. Each time, the studied parameter value was assigned randomly from a defined probability distribution or range using a Latin Hypercube scheme (see Table S2). Together the effective root radial conductivity (k_R, in s^{-1}), the β (-) and root density (in 10^3 m m^3) form an informative proxy for the soil to root resistance. The lumen fraction (in m^2 m^{-2}), sapwood area (*Asapwood*, in m²) and the total diurnal transported sap flow volume, i.e. net root water uptake (Volume corr., factor of standard run volume), provide an informative proxy for the sap flux density. (see Table S1). Time (in h) and height (in m) respectively represent the timing of sampling and the height of sample collection.


Sand
Silt Loam
Loam
Sandy Clay
Clay
(a)
-58
-60
-62
-64
-66
-68
δ²H_X [‰, vsmow]
0
5
10
15
20
time [h]


31 l/day - Huang et al. (2017)
50 l/day - Andrade et al. (2005)
25 l/day - Cristiano et al. (2015)
15 l/day - 50% Huang et al. (2017)
(b)
-58
-60
-62
-64
-66
-68
δ²H_X [‰, vsmow]
0
5
10
15
20
time [h]

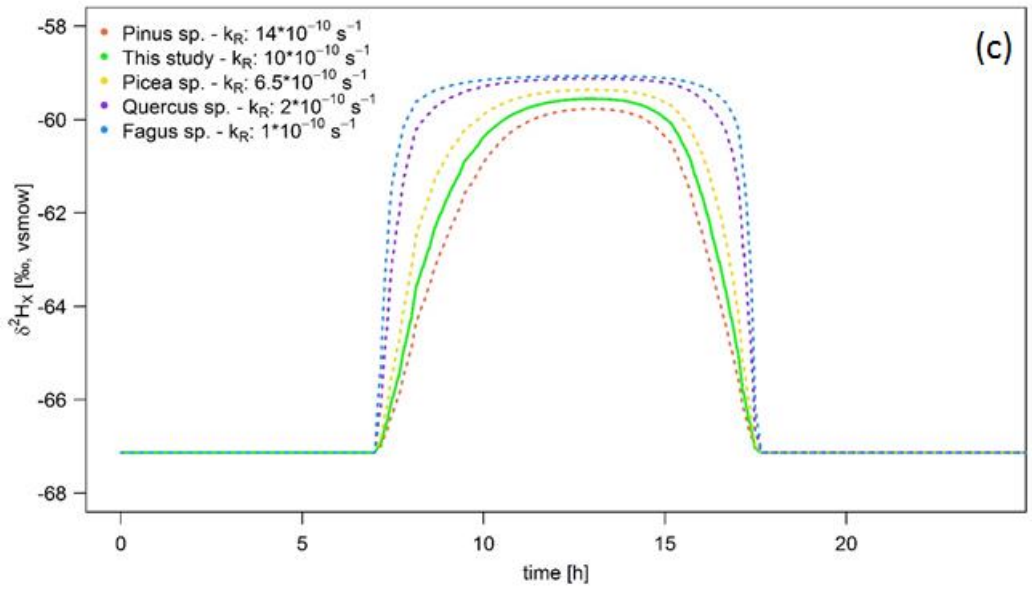

Pinus sp. - k_R: 14*10^-10 s^-1
This study - k_R: 10*10^-10 s^-1
Picea sp. - k_R: 6.5*10^-10 s^-1
Quercus sp. - k_R: 2*10^-10 s^-1
Fagus sp. - k_R: 1*10^-10 s^-1
(c)
-58
-60
-62
-64
-66
-68
δ²H_X [‰, vsmow]
0
5
10
15
20
time [h]

Fig. S4. Model sensitivity to (bio)physical parameters. The standard model run is shown by the solid green line in all panels. **Panel a:** fixed soil moisture and depth profile in isotope composition of soil water ($\delta^2 H_{S,i}$), but with different soil types influencing the soil conductivity and soil water potential gradient in the soil ($\Psi_{S,i,t}$). Parameterization for each soil type is derived from Clapp & Hornberger (1978). **Panel b:** Impact of altering volumes of water taken up by the plant. **Panel c:** Effect of altering values of the effective root radial conductivity (k_R) values. Values are species-specific and are derived from literature (Sands *et al.*, 1982; Rüdinger *et al.*, 1994; Steudle & Meshcheryakov, 1996; Leuschner *et al.*, 2004). In each panel all other parameters follow the standard plant parameterization (Table S1).

Species	Max. diurnal $\delta^{18}O_X$ range [‰, in vsmow]	Growth form	Color code
Q. Spruce	2.8	Tree	
P. euphratica	1.1	Tree	
P. fruticosa	1.8	Shrub	
R. soongorica	6.8	Shrub	
P. viviparum	3.2	Herb	
S. capillata	6.5	Herb	

Fig. S5. High temporal field measurements of oxygen isotope composition of plant xylem water ($\delta^{18}O_X$) of two tree (red, stem samples), two shrub (blue, stem samples) and two herb (green, root samples) in the Heihe River Basin (northwestern China) shown for the respective measurement period. Timing and location of sampling are provided in the panel title. The full colored envelope per respective species delineates the acceptable variance from the stem mean (i.e. 0.3‰) according to the standard assumption of no variance along the length of a lignified plant. Grey vertical lines mark the transition of days. The table provides the maximum measured diurnal $\delta^{18}O_X$ range per species.

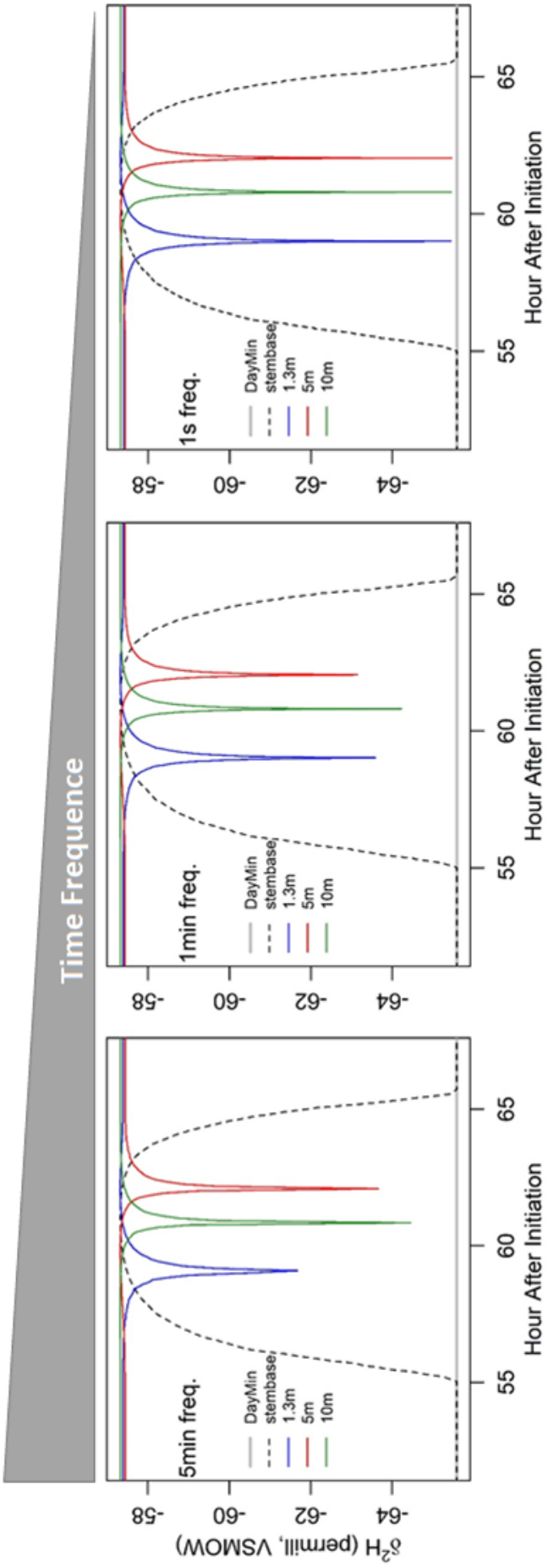

Time Frequence
δ2H (permill, VSMOW)
-64
-62
-60
-58
55
60
65
Hour After Initiation
5min freq.
1min freq.
1s freq.
DayMin
stembase
1.3m
5m
10m

Fig. S6. Model simulations performed with varying temporal resolutions, i.e. 5min, 1min and 1sec.

Table S1. An overview of the model standard parameterization of the present model, including sap flow, with corresponding references to literature.

Abbr.	Parameter	Unit	Value	Source
A_{Rtot}	The plants' total absorptive root area	m^2	$e^{0.88 \cdot \ln\left(\pi \cdot \left[\frac{DBH \cdot 10^2}{2}\right]^2\right) - 2}$	Čermák *et al.* (2006) $A_{Rtot} = 23.825\ m^2$
$A_{R,i}$	The absorptive root area distribution over soil layer *i*	m^2	$A_{Rtot} \cdot \beta^{100 \cdot z_i} \cdot (1 - \beta^{100 \cdot \Delta z})$	A_{Rtot} multiplied by the integrated root distribution of each soil layer adapted from Jackson *et al.* (1996)
			β =0.976	Huang *et al.* (2017)
$A_{SAPWOOD}$	Sapwood area	m^2	$\frac{1.582 \cdot [DBH \cdot 10^2]^{1.764}}{10^4}$	Meinzer *et al.* (2001)
Ax	Total lumen area	m^2	$LF \cdot A_{SAPWOOD}$	
B_i	The overall root length density per unit of soil, not necessarily limited to the studied plant.	$m\ m^{-3}$	$R_0 \cdot \beta^{100 \cdot z_i} \cdot \ln(\beta)$	Adapted from Huang *et al.* (2017) R_0= -438 688 β =0.976
DBH	Diameter at breast height	m	0.213	Huang *et al.* (2017)
$\delta^2 H_{S,i}$	Deuterium isotope composition of soil water of the sampled soil layers	in ‰, VSMOW	$a + (z_i + b)^c$	Adapted from Meißner *et al.* (2012) …a: -73.98008 …b=0.001 …c=0.148735;
Δz	The thickness of each soil layer	m	0.001	
f_t	Temporal resolution	s^{-1}	1/60	
k_R	The effective root radial conductivity	s^{-1}	10^{-9}	Huang *et al.* (2017)

Table S1 (continuation)

Abbr.	Parameter	Unit	Value	Source
$K_{S,i}$	The soil hydraulic conductivity defined per soil depth	m s^{-1}	$K_{s,max} \cdot \left(\frac{\Psi_{sat}}{\Psi_{S,i,t}}\right)^{2+\frac{3}{b}}$	Huang *et al.* (2017)
			$K_{s,max}$= 7.2·10^{-6} m s^{-1}	Clapp & Hornberger (1978) [Table 2, silt loam soil]
			Ψ_{sat}= -0.786 m H_2O	Clapp & Hornberger (1978) [Table 2, silt loam soil]
			b = 5.30	Clapp & Hornberger (1978) [Table 2, silt loam soil]
LF	Lumen fraction per unit sapwood area	m^2 m^{-2}	0.136	Zanne *et al.* (2010) [Table 2]
SF_t	Instantaneous sap flow at time t	m^3 s^{-1}		Adapted from Huang *et al.* (2017) [derived from scenario 6, day 11]
$\Psi_{S,i,t}$	Water potential at a specific soil layer depth *i* and time *t*	m H_2O	$(a + b \cdot log(z_i) - c \cdot z_i^2) \cdot CT$	Adapted from Meißner *et al.* (2012) a: 19.8455·10^{-3} b: 44.8909·10^{-3} c: 25.5594·10^{-3} CT: 101.97 (i.e. conversion factor between MPa and m H_2O)

z_i the soil depth of the i^{th} soil layer (in m)

Table S2. An overview of the defined distribution and ranges used for the sensitivity analysis whose results are displayed in Fig S4.

Model Variable	Description	Unit	Distribution	Specification
Variables that provide an informative proxy for the soil to root resistance				
k_R	The effective root radial conductivity	s^{-1}	Uniform	St.=$10 \cdot 10^{-10}$, min = $2 \cdot 10^{-10}$, max = $15 \cdot 10^{-10}$
Root density	Integral of B_i for entire soil depth by changing R0 (see Table S1)	m	Uniform	St.= 4000, min = 1000, max = 20000
β	Factor defining root length density profile (see Table S1)	[-]	Uniform	St.= 0.976, min = 0.855, max = 0.995
Variables that provide an informative proxy for the sap flow velocity of a plant				
$A_{SAPWOOD}$	Sapwood area	m^2	Uniform	St.= 0.979, min = 0.6, max = 1
Lumen Fraction	Lumen fraction	$m^2\ m^{-2}$	Uniform	St.=0.136, min = 0.0411, max = 0.451
Volume corr.	Correcting factor of the daily total transported sap flow volume which in the standard run corresponds to 31.4 10^{-3} m^3	[-]	Uniform	St.= 1, min = 0.5, max = 2.0
Variables related to the sample collection protocol				
Height	Height of sampling	m	Uniform	St. = 1.3, min = 0, max = 25
Time	Timing of sampling	h	Uniform	St. = 12, min = 9; max = 14

With: *St.* parameter value of the standard run, *min* and *max* the minimum and maximum assigned value