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Assessment of the interactions between soil–biosphere–atmosphere (ISBA) land surface model soil hydrology, using four closed-form soil water relationships and several lysimeters

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Supplement

S1 Solution method for liquid soil moisture

According to the Richards equation, the ISBA governing equation for water transfers within the soil is written as follows:

$$\frac{\partial w_i}{\partial t} = \frac{1}{\Delta z_i}[F_{i-i} - F_i + \frac{S_i}{\rho_\omega}] \quad \text{with} \quad F_i = \tilde{k_i}(\frac{\psi_i - \psi_{i+1}}{\Delta \tilde{z}_i} + 1) \tag{S1.1}$$

where ω_i ($\mathrm{m}^3.\ \mathrm{m}^{-3}$) is the volumetric water content of the layer i, ψ_i (m) the water pressure head, $F_i(m.s^{-1})$ the water flux term, Δz_i (m) the layer thickness, $\Delta \tilde{z}_i$ (m) the thickness between two consecutive layer midpoints or nodes, and S_i $(kg.m^{-2}.s^{-1})$ the soil-water source/sink term. $\tilde{k_i}(m.s^{-1})$ is the interfacial hydraulic conductivity computed as the geometric means over two consecutive nodes of the soil hydraulic conductivity (Decharme et al., 2011) :

$$\tilde{k_i} = \sqrt{k_i(\psi_i) \times k_{i+1}(\psi_{i+1})} \tag{S1.2}$$

S1.1 Numerical method

The Eq.(S1.1) is solved with a Cranck-Nicholson implicit time scheme defined as follow :

$$\frac{\Delta \omega_i}{\Delta t} = \frac{1}{\Delta z_i}[\varphi(F_{i-1}^{t+1} - F_i^{t+1}) + (1-\varphi)(F_{i-1}^{t} - F_i^{t}) + \frac{S_i}{\rho_\omega}] \tag{S1.3}$$

where $\Delta \omega_i = \omega_i^{t+1} - \omega_i^t$ is the change in water content over the model time step Δt (s) and $\varphi = 0.5$ which results in the Cranck-Nicholson time scheme used in ISBA. Note that φ can be set to 1 to use a backward difference scheme or to 0 to use an explicit time scheme. Next, we use a linearization method in which the flux terms at time $t+1$ in Eq.(S1.3) are approximated via a one-order Taylor series expansion of the form :

$$F_i^{t+1} = F_i^t + \frac{\partial F_i}{\partial \omega_i}\Delta \omega_i + \frac{\partial F_i}{\partial \omega_{i+1}}\Delta \omega_{i+1} \tag{S1.4}$$

where the flux F_i is a function of the water content in layers i and i+1 as shown later. The substitution of Eq.(S1.4) into Eq.(S1.3) results in a system of linear equations in $\Delta\omega$ that can be expressed as follow :

$$a_i \Delta \omega_{i-1} + b_i \Delta \omega_i + c_i \Delta \omega_{i+1} = f_i \tag{S1.5}$$

where f_i is the forcing function including all explicit terms. This system can be solved using a tridiagonal matrix written as :

$$\Delta\hat{\omega} = \mathbf{A}^{-1}\hat{f} \quad \text{with} \quad \mathbf{A} = \begin{pmatrix} b_1 & c_1 & 0 \\ a_i & b_i & c_i \\ 0 & a_N & b_N \end{pmatrix} \tag{S1.6}$$

where $\Delta\hat{\omega}$ and $\hat{f}$ are vectors of length N (the number of soil layer), and **A** the N×N coefficient matrix. The non-zero elements, represented by a, b and c, are then defined as follow :

$$\begin{cases} a_i = -\varphi \frac{\partial F_{i-1}}{\partial \omega_{i-1}} \\ b_i = \frac{\Delta z_i}{\Delta t} - \varphi(\frac{\partial F_{i-1}}{\partial \omega_i} - \frac{\partial F_i}{\partial \omega_i}) \\ c_i = \varphi \frac{\partial F_i}{\partial \omega_{i+1}} \end{cases} \tag{S1.7}$$

The forcing function is written as :

$$f_i = F_{i-1}^t - F_i^t + \frac{S_i}{\rho_\omega} \tag{S1.8}$$

S1.2 Flux derivatives

The flux derivatives in Eq.(S1.4) are calculated as follow using the flux term of Eq.(S1.1) :

$$\frac{\partial F_i}{\partial \omega_i} = \frac{\partial \tilde{k_i}}{\partial \omega_i} \frac{\psi_i - \psi_{i+1}}{\Delta \tilde{z}_i} + \frac{\tilde{k_i}}{\Delta \tilde{z}_i} \frac{\partial \psi_i}{\partial \omega_i} + \frac{\partial \tilde{k_i}}{\partial \omega_i} \tag{S1.9}$$

$$\frac{\partial F_i}{\partial \omega_{i+1}} = \frac{\partial \tilde{k_i}}{\partial \omega_{i+1}} \frac{\psi i - \psi_{i+1}}{\Delta \tilde{z}_i} - \frac{\tilde{k_i}}{\Delta \tilde{z}_i} \frac{\partial \psi_{i+1}}{\partial \omega_{i+1}} + \frac{\partial \tilde{k_i}}{\partial \omega_{i+1}} \tag{S1.10}$$

The matrix potential derivatives for each model approaches (or closed-form equations) are given by :

– for $BC66$ the derivative is relatively simple :

$$\frac{\partial \psi_i}{\partial \omega_i} = -\frac{b_i \psi_i}{\omega_i} \tag{S1.11}$$

– for $VG80$ using Mualem (1976) condition the derivative is more complex and require an integration by parts :

$$\frac{\partial \psi_i}{\partial \omega_i} = \frac{\psi_i}{\omega_i(1-n_i)} \frac{S_i^{-1/m_i}}{S_i^{-1/m_i} - 1} \quad \text{with} \quad S_i = \frac{\omega_i}{\omega_{sat_i}} \tag{S1.12}$$

– for BCVG, i.e. $VG80$ using Burdine (1963) condition, an integration by parts is also required :

$$\frac{\partial \psi_i}{\partial \omega_i} = \frac{\psi_i}{\omega_i(2-n_{bi})} \frac{S_i^{-1/m_{bi}}}{S_i^{-1/m_{bi}} - 1} \tag{S1.13}$$

The derivatives of the interfacial hydraulic conductivity (S1.2) for each model approaches are given by :

– for $BC66$:

$$\frac{\partial \tilde{k_i}}{\partial \omega_i} = \frac{(2b_i + 3)\tilde{k_i}}{2\omega_i} \tag{S1.14}$$

– for $BCVG$:

$$\frac{\partial \tilde{k_i}}{\partial \omega_i} = \frac{(2\lambda_{bi} + 3)\tilde{k_i}}{2\omega_i} \tag{S1.15}$$

– for $VG80$:

$$\frac{\partial \tilde{k_i}}{\partial \omega_i} = \frac{\tilde{k_i}}{2\omega_i}(l_i + 2X_i) \quad \text{with} \quad X_i = \frac{S_i^{1/m_i}[1 - S_i^{1/m_i}]^{-1/n_i}}{1 - [1 - S_i^{1/m_i}]^{m_i}} \tag{S1.16}$$

– for VG_c, the derivative is the same than Eq.(S1.16) $\forall \psi \leq \psi_c$, but :

$$\frac{\partial \tilde{k_i}}{\partial \omega_i} = \frac{\tilde{k_i}}{2\omega_i}(l_i + \frac{2S_i}{(\alpha_i - \psi_{c_i})\Gamma_i}) \quad \forall \psi > \psi_c \tag{S1.17}$$

S1.3 Upper boundary condition

The upper boundary condition in ISBA represents the water that infiltrates the soil surface. According to Eq.(S1.1), the governing equation for the first soil layer is written as follow :

$$\frac{\partial w_1}{\partial t} = \frac{1}{\Delta z_1}[F_0 - F_1 + \frac{S_1}{\rho_\omega}] \quad \text{with} \quad F_1 = \tilde{k_1}(\frac{\psi_1 - \psi_2}{\Delta \tilde{z_1}} + 1) \tag{S1.18}$$

F_0 $(m.s^{-1})$ is the soil infiltration taken equal to the flux of water reaching the soil surface. F_0 is treated as an explicit term and the expression of the Cranck-Nicholson for Eq(S1.18) is given by :

$$\frac{\Delta \omega_1}{\Delta t} = \frac{1}{\Delta z_1}[F_0 - (\varphi F_1^{t+1} + (1-\varphi)F_1^t) + \frac{S_1}{\rho_\omega}] \tag{S1.19}$$

The non-zero elements of the tridiagonal matrix and the forcing function are then defined as follow :

$$\begin{cases} a_1 = 0 \\ b_1 = \frac{\Delta z_1}{\Delta t} + \varphi \frac{\partial F_1}{\partial \omega_1} \\ c_1 = \varphi \frac{\partial F_1}{\partial \omega_2} \\ f_1 = F_0 - F_1^t + \frac{S_i}{\rho_\omega} \end{cases} \tag{S1.20}$$

S1.4 Lower boundary condition

According to Eq.(S1.1), the governing equation for the last soil layer, N, is written as follow :

$$\frac{\partial w_N}{\partial t} = \frac{1}{\Delta z_N}[F_{N-1} - F_N + \frac{S_N}{\rho_\omega}] \tag{S1.21}$$

where F_{N-1} is defined according to Eq.(S1.1) while F_N depends on the choise of the lower boundary condition.

Seepage face case - As long as the last layer remain unsaturated, a prescribed flux boundary with $F_N = 0$ is imposed at the lower boundary. When the last layer is saturated, a prescribed pressure head boundary with $\psi = \psi_{sat}$ for BC66 or $\psi = 0$ for other models is assumed at the lower boundary.

Free drainage case - It is the usual lower boundary condition in ISBA assuming that the water table lies far below the last soil layer. So, the pressure head gradient is equal to zero and the flux of the last layer is equal to the hydraulic conductivity, $F_N = k_N(\psi_N)$. For this lower boundary condition, only the flux derivative change and are expressed as follow :

$$\begin{cases} \frac{\partial F_N}{\partial \omega_i} = \frac{\partial k_N}{\partial \omega_N} \\ \frac{\partial F_N}{\partial \omega_{N+1}} = 0 \end{cases} \tag{S1.22}$$

For all model versions, the flux derivative in the last layer of ISBA is given by :

- for $BC66$:

$$\frac{\partial F_N}{\partial \omega_N} = \frac{(2b_N + 3)k_N}{\omega_N} \tag{S1.23}$$

- for $BCVG$:

$$\frac{\partial F_N}{\partial \omega_N} = \frac{(2\lambda_{bN} + 3)k_N}{\omega_N} \tag{S1.24}$$

- for $VG80$:

$$\frac{\partial F_N}{\partial \omega_N} = \frac{k_N}{\omega_N}(l_N + 2X_N) \quad \text{with} \quad X_N = \frac{S_N^{1/m_N)}[1 - S_N^{1/m_N}]^{-1/n_N}}{1 - [1 - S_N^{1/m_N}]^{m_N}} \tag{S1.25}$$

- for VGc the derivative is the same than Eq.(S1.25) $\forall \psi \leq \psi_c$, but :

$$\frac{\partial k_N}{\partial \omega_N} = \frac{k_N}{\omega_N}(l_N + \frac{2S_N}{(\alpha_N - \psi_{c_N})\Gamma_N}) \quad \forall \psi > \psi_c \tag{S1.26}$$

S2 Summary of lysimeter characteristics

Table S1. Description of the available observations at the both experimental stations and for each lysimeter: observation period, mean annual precipitation (precip) and drainage water (drain). For each type of data, the available depths are indicated. Quality of measurements is given as percentage of missing data: meteo gap for the meteorological forcing, defect for the lysimeters measurements.

Experimental station		**GISFI**				**OPE**		
Lysimeters		**G1**	**G2**	**G3**	**G4**	**O1**	**O2**	**O3**
Period		2011 – 2016	2009 – 2016		2011 – 2016	2014 – 2019		
Mean annual	precip (mm.year^{-1})	727				876		
	drain (mm.year^{-1})	317	337	115	170	312	304	363
Depths (cm)	total water mass	full column				full column		
	volumetric water content	100 – 150	50 – 100 – 150		50	20 – 50 – 100 – 150		
	matric potential	100 – 150	50 – 100 – 150		50	20 – 50 – 100		
	drainage	200				200		
	temperature	50 – 100 – 150				20 – 50 – 100 – 150		
Data quality	meteo gap (%)	12				10		
	defect (%)	16	8	23	0	0		

Table S2. Table of parameters estimates for each lysimeter and each depth.

Lysimeters	$Depth$	ω_{sat}	ψ_{sat}	b	α	n	n_b	k_{sat}	l
Units	m	m^3/m^3	m	$-$	m^{-1}	$-$	$-$	$10^{-6} m.s^{-1}$	$-$
G1	1,0	0,415	0,10	40,0	10,00	1,025	2,025	1,0	-2,0
	1,5	0,434	0,15	17,0	6,67	1,060	2,063	1,0	-2,0
G2	0,5	0,420	0,12	11,0	6,67	1,090	2,090	2,0	-2,0
	1,0	0,420	0,10	11,0	10,00	1,090	2,095	2,0	-2,0
	1,5	0,360	0,07	30,0	14,28	1,035	2,033	2,0	-2,0
G3	0,5	0,373	0,10	9,5	7,69	1,100	2,200	1,0	-5,0
	1,0	0,370	0,15	11,0	6,67	1,090	2,090	1,0	-5,0
	1,5	0,366	0,20	15,0	5,00	1,068	2,071	1,0	-5,0
G4	0,5	0,380	0,30	45,0	3,33	1,022	2,022	2,585	0,5
O1	0,2	0,512	0,25	8,33	4,00	1,120	2,120	0,7	0,5
	0,5	0,515	0,25	20,0	4,00	1,050	2,037	0,7	0,5
	1,0	0,435	0,025	30,0	40,00	1,033	2,038	0,7	0,5
	1,5	0,470	0,05	47,36	20,00	1,023	2,023	0,7	0,5
O2	0,2	0,280	0,30	15,0	3,333	1,149	2,147	0,8	0,5
	0,5	0,362	0,30	15,0	3,333	1,067	2,067	0,8	0,5
	1,0	0,495	0,03	22,12	20,00	1,050	2,058	0,8	0,5
	1,5	0,385	0,05	50,0	15,44	1,020	2,020	0,8	0,5
O3	0,2	0,470	0,30	9,0	3,333	1,111	2,113	0,8	0,5
	0,5	0,500	0,28	15,0	3,571	1,067	2,065	0,8	0,5
	1,0	0,430	0,01	25,0	57,00	1,040	2,040	0,8	0,5
	1,5	0,470	0,01	55,0	57,00	1,020	2,020	0,8	0,5

S3 Soil water retention curves for each lysimeter at several depths

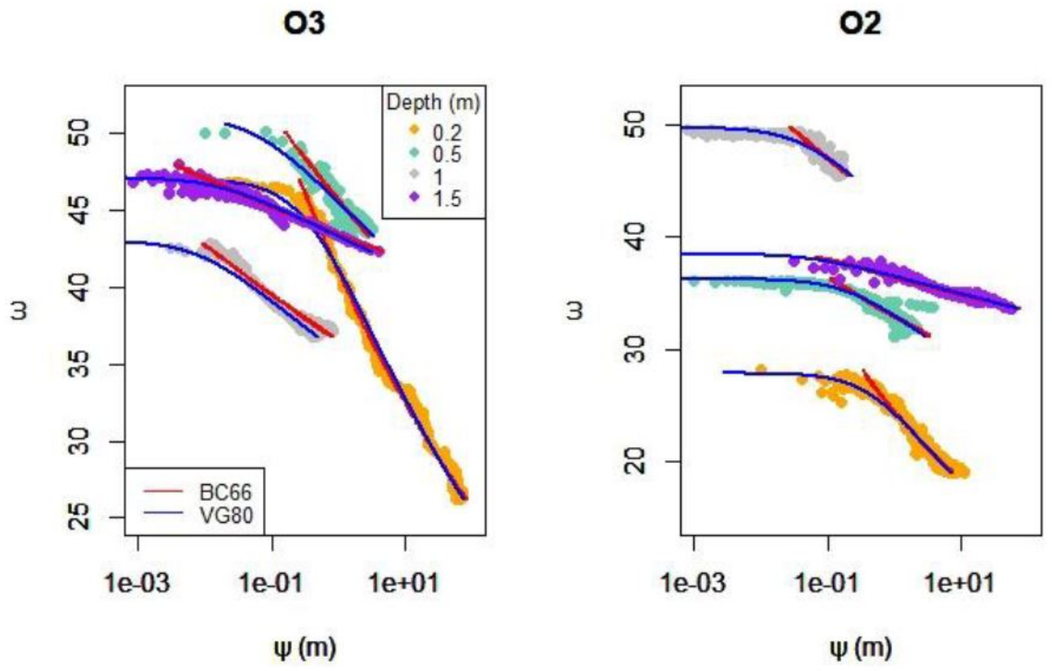

Figure S1. Soil water retention curves : volumetric water content (ω) and logarithm of the absolute value of the soil matric potential (ψ) for lysimeters O2 and O3. Observations at 0.2, 0.5, 1.0 and 1.5 m depth are in dot (orange, aquamarine, grey and purple respectively), estimations are in red and blue for BC66 and VG80, respectively. The dashed lines are the estimated values via observations for the water content at saturation and matric potential.

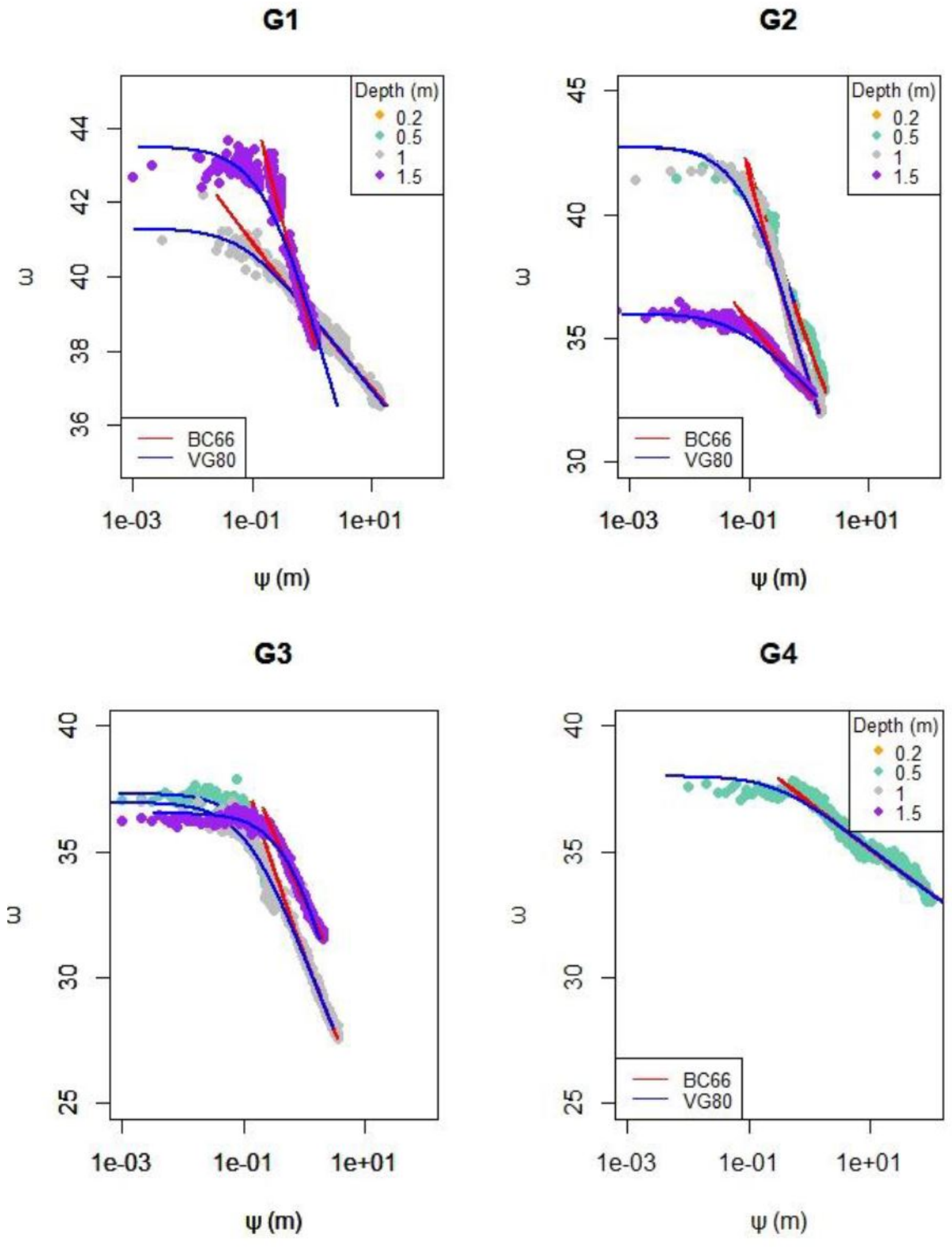

Figure S2. Same as S2 but for lysimeters G1, G2, G3 and G4.

S4 Hydraulic conductivity curves estimates near the base of each lysimeter

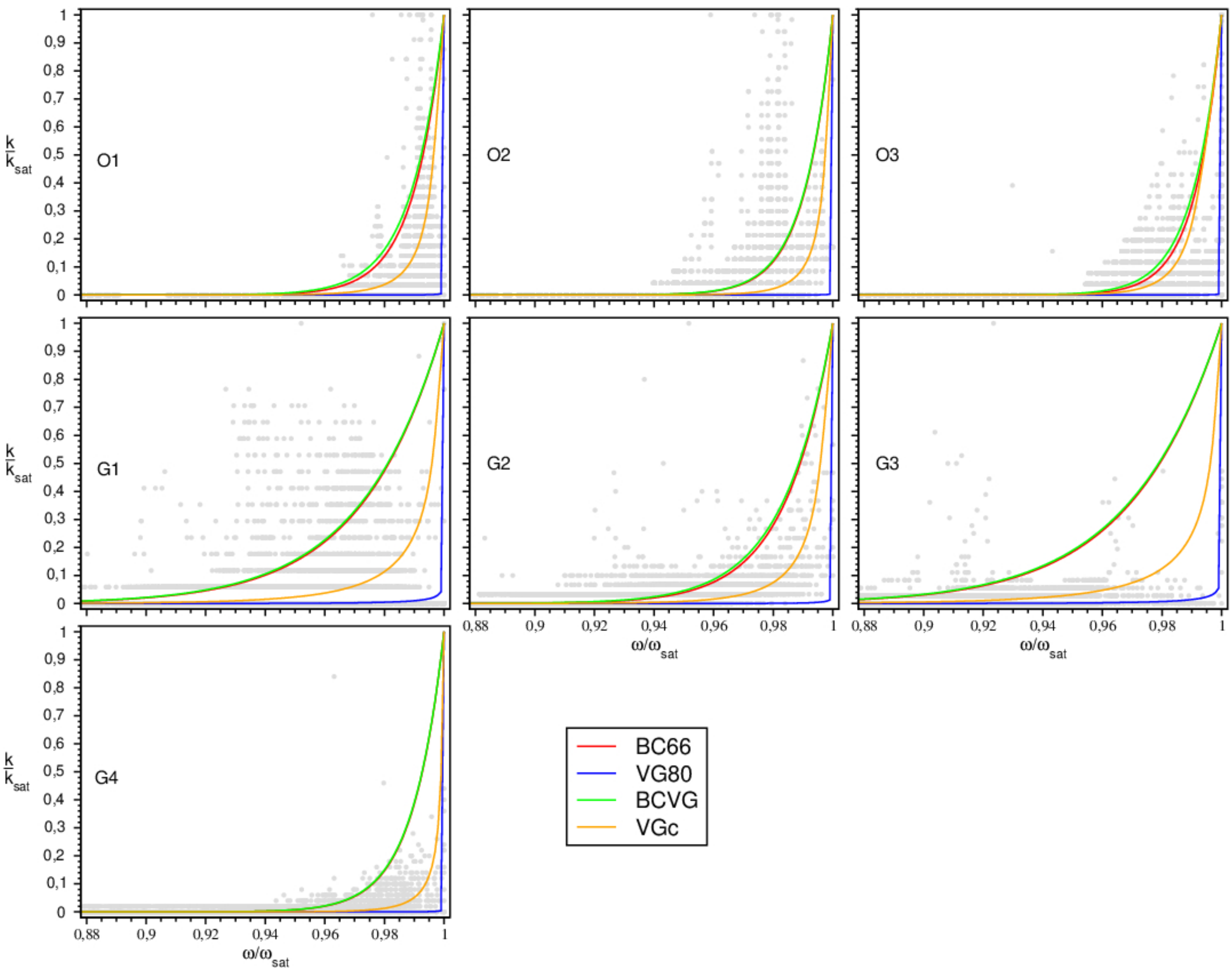

Figure S3. Near saturation estimates of the relative soil hydraulic conductivity, k/k_{sat}, as a function of the soil water content actual saturation, ω/ω_{sat}, near the base of all lysimeters. BC66, VG80, BCVG, VGc are given in red, blue, green and orange, respectively. The dots represent the observed hourly drainage water at 2 m depth (reduced to ksat) versus the actual saturation at 1.5 m depth (or 0.5m for G4).

S5 Simulated Leaf Area Index

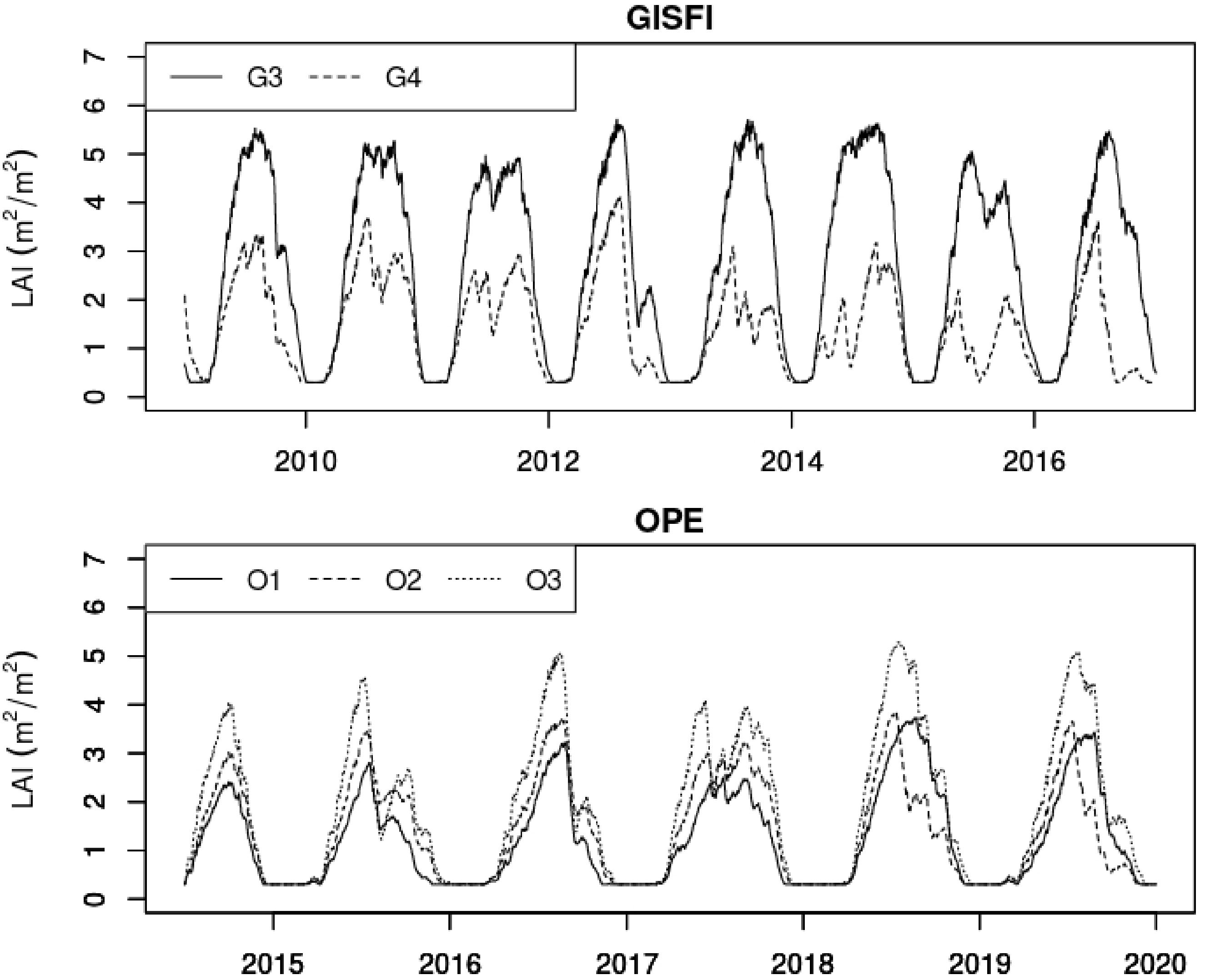

Figure S4. Hourly times series of LAI ($m^2.m^{-2}$) simulated for each lysimeter for BC66.

S6 Vgc model sensitivity to Homogeneous soil profile and usual PFT

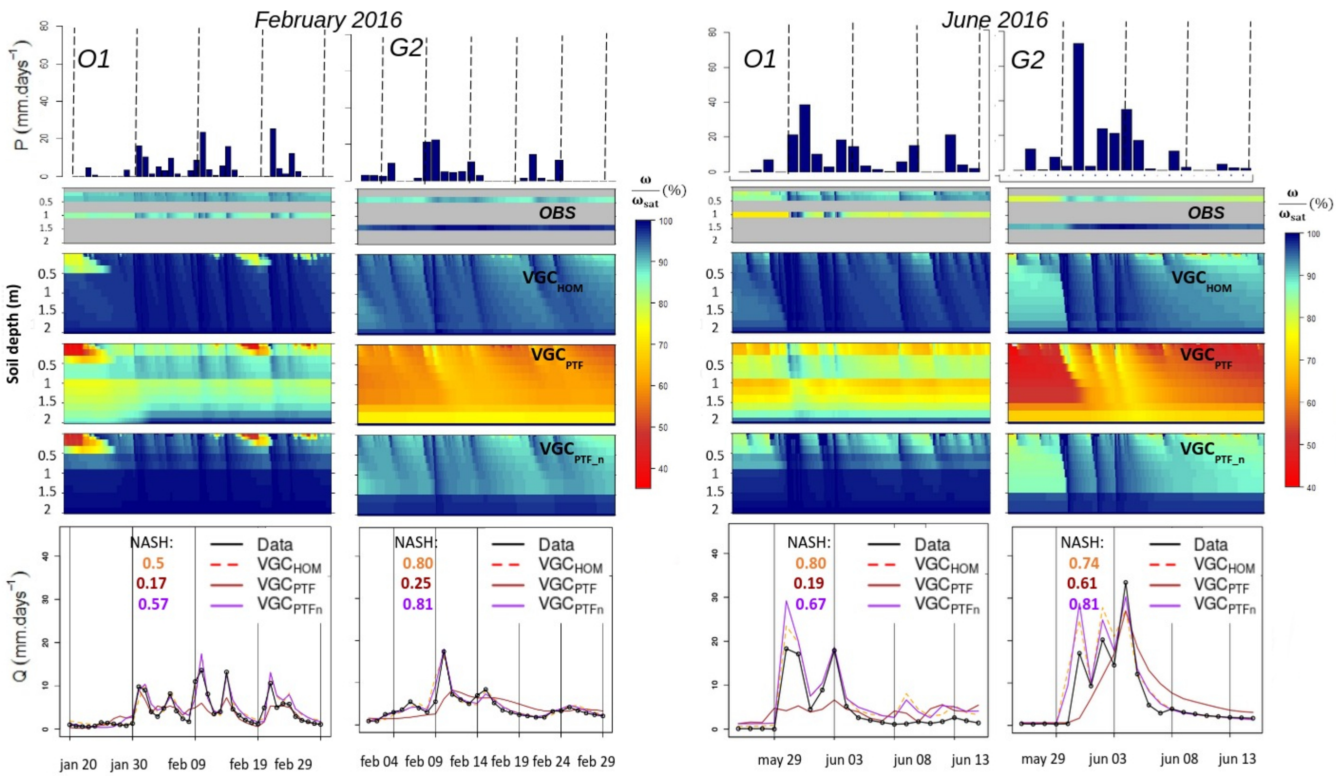

Figure S5. Same as Figure 13 but for the VGc model approach

S7 Lower Boundary Condition assessment

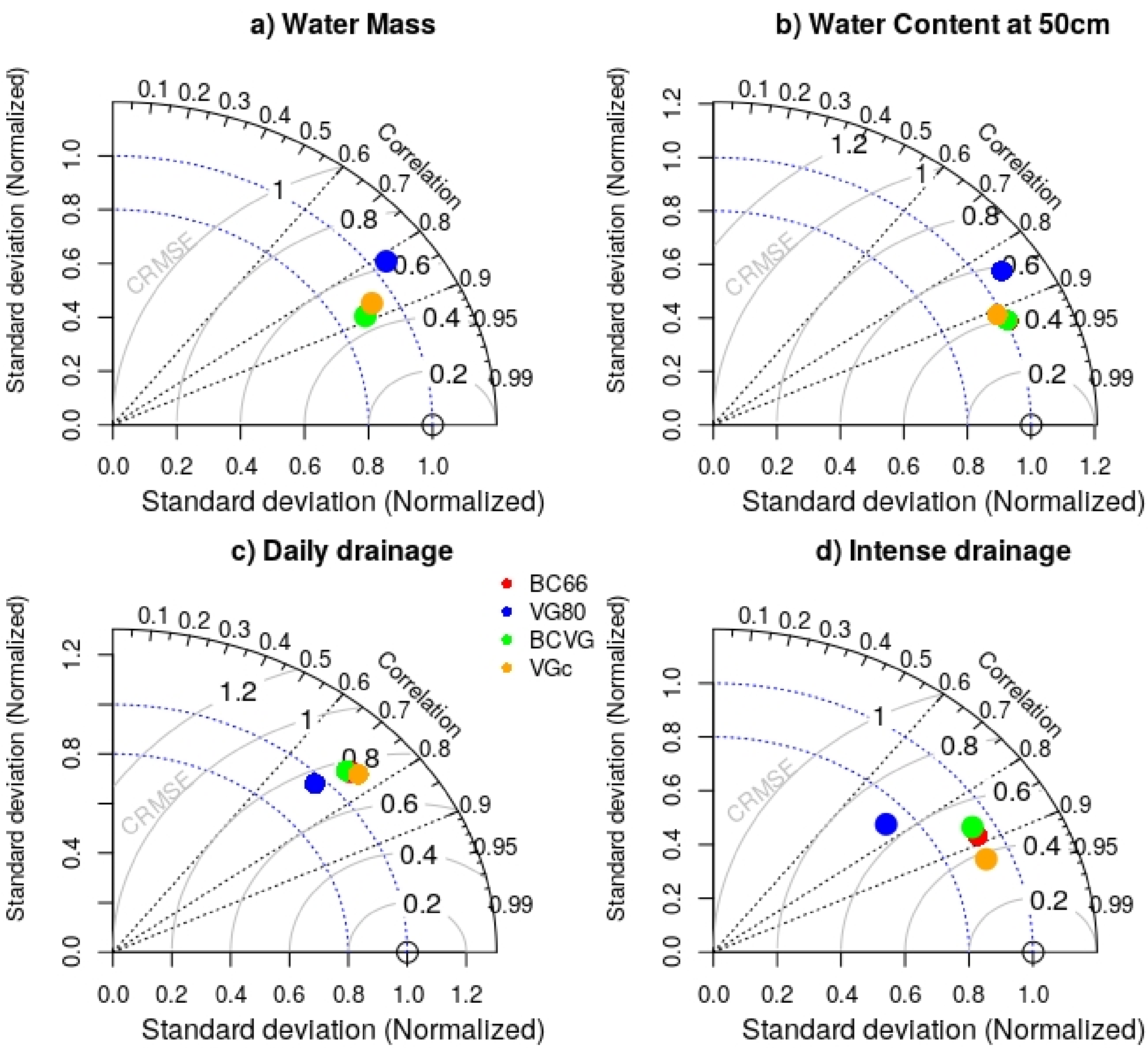

Figure S6. For free drainage : Taylor diagram on the masses, on the water contents at 50cm depth, on the drainages, and on the intense drainages, for the 4 experiments in free drainage on the lysimeters of GISFI and OPE: red for BC66, green for BCVGb, blue for VG80, and orange for VGc.

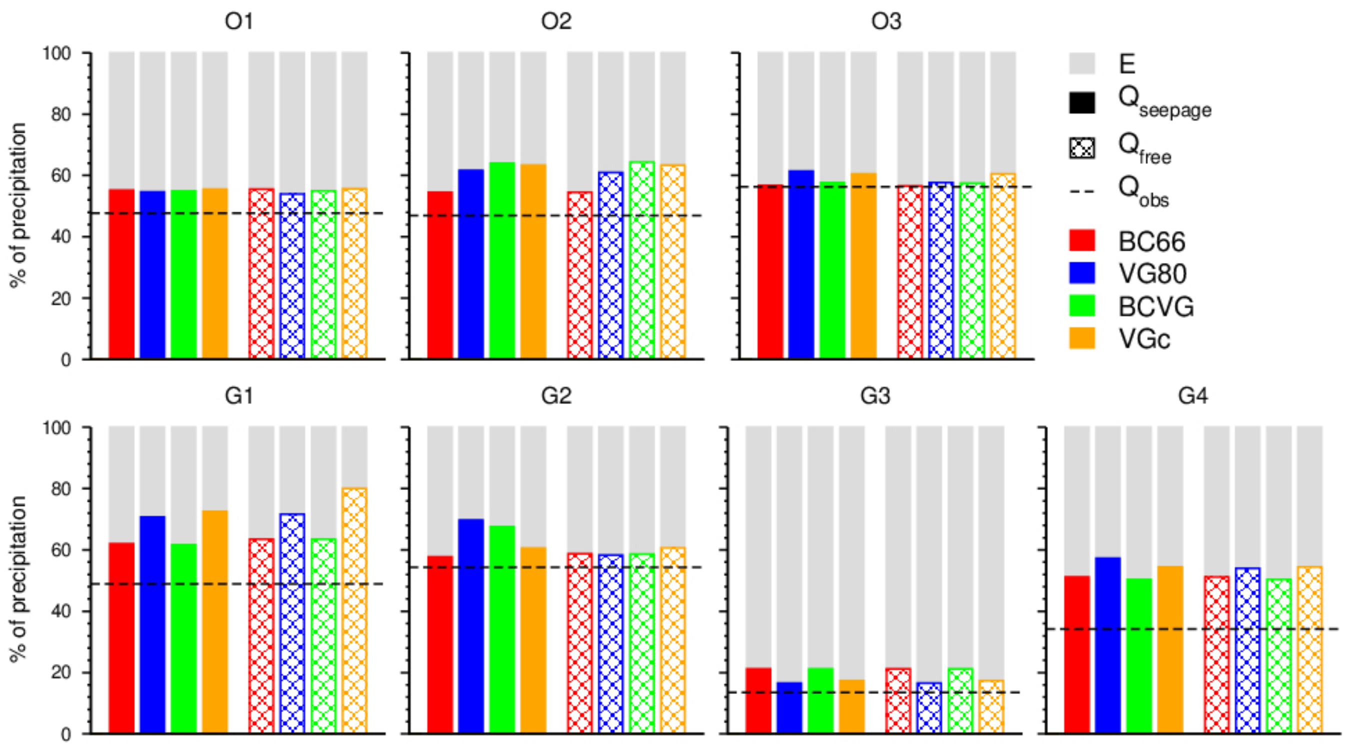

Figure S7. Comparison of the water budget partitioning of all model approaches (BC66, VG80, BCVG, and VGc) with a seepage face LBC ($Q_seepage$) as in Figure 9 and with a free drainage LBC (Q_free).