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Supplementary Materials: A Critical Evaluation on the Role of Aerodynamic and Canopy–Surface Conductance Parameterization in SEB and SVAT Models for Simulating Evapotranspiration: A Case Study in the Upper Biebrza National Park Wetland in Poland

Kaniska Mallick [1,*], Loise Wandera [1,2,*], Nishan Bhattarai [3], Renaud Hostache [1], Malgorzata Kleniewska [4] and Jaroslaw Chormanski [4]

Description of the SEB and SVAT models

1.1. STIC1.2

STIC1.2 is the most recent version of the original STIC formulation [1–4] and it is a one-dimensional physically-based SEB model that treats the vegetation-substrate complex as a single unit (Figure 1 in [4]). The main features of STIC1.2 are the integration of infrared temperature (T_S) into the Penman-Monteith (PM) equation and finding analytical solutions of the surface and aerodynamic conductances. The intrinsic link between the PM model and T_S presumably exists due to the dependence of the aerodynamic conductance (g_A) on T_R through free convection and due to the dependence of canopy (surface) conductance (g_S) on soil moisture and g_A. A framework was conceptualized where 'state equations' (Equations 2 to 5 below) for the conductances were developed in such a way that there is a direct feedback of T_S on g_A and g_S through an aggregated surface moisture availability (M). Detail can be found in [1–3,5] and [4]. The expression of λE in the PM equation is,

$$\lambda E = \frac{s\phi + \rho_A c_P g_A D_A}{s + \gamma\left(1 + \frac{g_A}{g_S}\right)} \tag{1}$$

where ρ_A is the air density (kg m^{-3}), c_P is the specific heat of air (J kg^{-1} K^{-1}), γ is the psychrometric constant (hPa K^{-1}), s is the slope of the saturation vapour pressure versus T_A (hPa K^{-1}), D_A is the saturation deficit of the air (hPa) at the reference level, and ϕ is the net available energy (i.e., $R_N - G$). The units for all the surface fluxes and conductances are W m^{-2} and m s^{-1}, respectively.

In Equation 1, the two biophysical conductances (g_A and g_S) are unknown, and the STIC1.2 methodology is based on finding analytical solutions for the two unknown conductances to directly estimate λE [1,2,4,5]. The need for such analytical estimation of these conductances is motivated by the fact that g_A and g_S can neither be measured at the canopy or ecosystem scales, and there is not a universally-agreed model of g_A and g_S that currently exists [4,6,7]. By integrating T_S with standard SEB theory and vegetation biophysical principles, STIC1.2 formulates multiple state equations (Equations 2–5 below) that eliminates the need of empirical parameterization for g_A, g_S, and T_0. The state equations for the conductances and T_0 were expressed as a function of those variables that are available through direct measurements. The state equations of STIC1.2 are provided below and their detailed descriptions are available in [1–3].

$$g_A = \frac{\phi}{\rho_A c_P\left[(T_0 - T_A) + \left(\frac{e_0 - e_A}{\gamma}\right)\right]} \tag{2}$$

$$g_S = g_A \frac{(e_0 - e_A)}{(e_0^* - e_0)} \tag{3}$$

$$T_0 = T_A + \left(\frac{e_0 - e_A}{\gamma}\right)\left(\frac{1 - \Lambda}{\Lambda}\right) \tag{4}$$

$$\Lambda = \frac{2\alpha s}{2s + 2\gamma + \gamma \frac{g_A}{g_S}(1+M)} \tag{5}$$

Here α is the Priestley-Taylor coefficient (unitless) [8]. In Equation 5, α appeared due to using the Advection-Aridity (AA) hypothesis [9] for deriving the state equation of Λ [3,10]. However, instead of optimising it as a 'fixed parameter', α is dynamically estimated by constraining it as a function of M, conductances, source/sink height vapour pressure, and temperature [3]. The derivation of the equation for α is described in [3] and [4].

Given the values of M, R_N, G, T_A, and R_H or e_A, the four state equations (Equations 2–5) can be solved simultaneously to derive analytical solutions for the four unobserved state variables and to simultaneously produce a 'closure' of the PM model that is independent of empirical parameterizations for both g_A and g_S [1–4]. However, the analytical solutions to the four state equations contain three accompanying unknowns; e_0, e_0^*, and α, and as a result there are four equations with seven unknowns. Consequently, an iterative solution was found to determine the three unknown variables [3–5]. STIC1.2 consists of a feedback loop describing the relationship between T_R and λE, coupled with canopy-atmosphere components relating λE to T_0 and e_0 [3] . Upon finding analytical solution of g_A and g_S, both variables are returned into Equation 1 to directly estimate λE. Estimation of aggregated moisture availability (M) is described in detail in [3,5] and [4].

1.2. SEBS

The detailed equations of SEBS model are described in [11] (also [4,12,13]). To summarize, SEBS formulation uses the Bulk Atmospheric Similarity Theory for planetary boundary layer scaling, and the Monin-Obukhov atmospheric surface layer similarity for surface layer scaling for the estimation of surface fluxes from thermal remote sensing data, and empirical sub-models for estimating the roughness lengths for momentum and heat (z_{0M} and z_{0H}) [11,14] for estimating the sensible heat flux (H). To estimate H, SEBS solves the similarity relationships for the profile wind speed (u) and the mean difference between potential temperatures ($\Delta\theta$; K) at the surface and reference height (z). The latent heat flux is estimated as a residual component of surface energy balance.

$$u = \frac{u_*}{k}\left[\ln\left(\frac{z-d_0}{z_{0M}}\right) - \psi_M\left(\frac{z-d_0}{L}\right) + \psi_M\left(\frac{z_{0M}}{L}\right)\right] \tag{6}$$

$$\Delta\theta = \frac{H}{k u_* \rho c_p}\left[\ln\left(\frac{z-d_0}{z_{0H}}\right) - \psi_H\left(\frac{z-d_0}{L}\right) + \psi_H\left(\frac{z_{0H}}{L}\right)\right] \tag{7}$$

$$L = -\frac{\rho_A c_p u_*^3 T_{VP}}{kgH} \tag{8}$$

Here L is the Monin-Obukhov length (m), T_{VP} is virtual potential temperature (K) near the surface [9], k is the Von Karman Constant (0.41), u_* is the friction velocity (m s^{-1}), and g is the acceleration due to gravity (9.8 m s^{-2}). Ψ_M and Ψ_H are the stability corrections for momentum and heat transport, respectively.

One of the key characteristics of the SEBS model is the use of a semi-empirical adjustment factor (kB^{-1}) to compensate for the differences between the scalar roughness lengths for momentum and heat transfers (z_{0M} and z_{0H}) [14]. Such compensation is needed to tackle the difference between the radiometric and aerodynamic temperature that arises due to the different scalar roughness lengths of momentum and heat.

$$z_{0H} = z_{0M}/\exp(kB^{-1}) \tag{9}$$

Estimation of kB^{-1} is detailed in [15]. For every half-hourly temporal resolution, energy balance at driest limit (λE= 0 or H = ϕ) and wettest limit (potential ET, E_P, rate based on Penman equation) is used in SEBS to estimate relative evaporation (Λ_r, the ratio of actual to the maximum evaporation rates) to further compute Λ[11].

$$\Lambda_r = 1 - \frac{H - H_{wet}}{H_{dry} - H_{wet}} \tag{10}$$

$$\Lambda = \frac{\Lambda_r \times \lambda E_{wet}}{R_N - G} \tag{11}$$

where H_{wet} and H_{dry} are H under the wet and dry limiting conditions, respectively. λE_{wet} is the λE at the wet limit.

1.3. SCOPE model

Soil Canopy Observations, Photochemistry and Energy fluxes (SCOPE1.7) [16] is a multi-layer SVAT model designed with the intention to link top of canopy (TOC) observations of radiance with the land surface processes. SCOPE model has 4 modules all working in synergy. (1) A semi-analytical radiative transfer module (RTM_O) for incoming radiation, based on [17]. This calculates the TOC outgoing radiation spectrum (0.4 to 50 μm), as well as the net radiation (R_N) and absorbed photosynthetically active radiation (PAR) per surface element. (2) A numerical radiative transfer module (RTM_t) for thermal radiation generated internally by soil and vegetation, based on [17]. This calculates the TOC outgoing thermal radiation and net radiation per surface element, but for heterogeneous leaf and soil temperatures. (3) A surface energy balance (SEB) module for λE, H and G per surface element, as well as photosynthesis, chlorophyll fluorescence and skin temperature at the leaf level. (4) A radiative transfer module (RTM_f) for the chlorophyll fluorescence based on the Fluspect-B model [18], which calculates chlorophyll reflectance and transmittance spectra.

In SCOPE1.7, canopy is presumed to have a homogeneous structure, and is 1-D only. For the computation, SCOPE1.7 model defines 60 elementary layers, with a maximum LAI of 0.1 each, so that numerical approximations to the radiative transfer equations are still acceptable up to a total canopy LAI of 6. The elements of the model are defined as; 60 elements for shaded leaves (corresponding to the 60 leaf layers), while 60 × 13 × 36 elements (60 leaf layers, 13 leaf inclinations angles and 36 leaf azimuth angles) for sunlit leaves. The soil is divided into two shaded and a sunlit fraction. The canopy architecture is as described in SAIL models [19,20].

Iteration between the RTM_t and the surface energy balance module is carried out to match the input of the RTMo with the output of the energy balance model (skin temperatures), while the input of the energy balance model with the output of the RTM_O (net radiation). In SCOPE1.7 the feedback of chlorophyll fluorescence to the surface energy balance is neglected. The RTM_O role is to predict the TOC radiance spectrum in the observation direction, and to predict the distribution of irradiance and net radiation over surface elements (leaves and the soil). The latter is input for the surface energy balance module. The role of the surface energy balance module is to calculate the net radiation (i.e., the turbulent energy fluxes and photosynthesis) and surface temperature.

In SCOPE1.7, R_N is calculated per element with the energy balance model then partitioned into the respective terms of the energy budget Equation 1. First G_0 is computed based on [21]:

$$G_0 = \frac{\Gamma}{\sqrt{2\omega\Delta t}}\left(T_S(t+\Delta t) - T_S(t) + \omega\Delta t\left[T_S(t) - \overline{T_S}\right]\right) \tag{12}$$

where ω (radians s^{-1}) is the frequency of the diurnal cycle, Γ (J K^{-1} m^{-2} $s^{-1/2}$) the thermal inertia of the soil, and T_s average annual temperature. The λE is computed based on the bulk transfer Equation 13

$$\lambda E = \lambda \frac{q_S(T_S) - q_a}{r_a - r_s} \tag{13}$$

q_s and q_a (kg m^{-3}) are the humidity of stomata or soil pores and above canopy respectively, r_c and r_a (m s^{-2}) are stomatal (or soil surface resistance) and aerodynamic resistance respectively. For the r_a, the formulation by [22] is used. A two-source model was used with separate resistances for soil and canopy. Aerodynamic resistance in SCOPE1.7 is computed for 4 layers:

A) Inertial layer sublayer

$$r_a^I = \frac{1}{K_{u*}}\left[\ln\left(\frac{z-d_0}{z_{OH}-d_0}\right)\right] - \varphi_{h_{c,v}}(z_{OH}) + \varphi^*_{h_{c,v}\,(z_{OH})} \tag{14}$$

B) Roughness sublayer

$$r_a^R = \frac{Z_{OH} - h_c}{K_{u*}(z_{OH} - d_0)} - \varphi_{h_{c,v}}(Z_{OH}) + \varphi^*_{h_{c,v}\,(Z_{OH})} \quad (15)$$

C) Above the canopy at level (Z_{OM} + d_O)

$$r_a^c = \frac{h_c \sinh_c(n)}{nK_{v\,(h_c)}}\left[\ln\left(\frac{e^n - 1}{e^n + 1}\right) - \ln\left(\frac{e^{n\left(Z_{OM}+\frac{d_0}{h_c}\right)-1}}{e^{n\left(Z_{OM}+\frac{d_0}{h_c}\right)+1}}\right)\right] \quad (16)$$

D) Boundary layer resistance of leaves

$$r_c^c = \frac{70}{L}\sqrt{\frac{\omega_1}{u_{z_{OM}}}} \quad (17)$$

E) Within canopy resistance

$$r_w^c = \frac{h_c \sinh_c(n)}{nK_{v\,(h_c)}}\left[\ln\left(\frac{e^{n\left(Z_{OM}+\frac{d_0}{h_c}\right)-1}}{e^{n\left(Z_{OM}+\frac{d_0}{h_c}\right)+1}}\right) - \ln\left(\frac{\frac{e^{n.^{0.001}}}{h_c - 1}}{\frac{e^{n.^{0.001}}}{h_c + 1}}\right)\right] \quad (18)$$

where k is Von Karman's constant, u_* (m s^{-1}) is the friction velocity, z_{0H} (m) is the reference height of the roughness sublayer, d_0 (m) is the zero-plane displacement height, and $\psi_{h,v}$ a stability correction function , h_c (m) is the vegetation height, z_{0M} (m) is the roughness length for momentum, n is wind extinction coefficient, ω_l (m) is leaf width, u_{zom} is wind speed at (Z_{0M} + d_0). In the within-canopy resistance formulation, 0.01 represents roughness length of soil. In the case of soil and surface resistance, apriori values are used where $r_b^s = 150 sm^{-1}$ and $r_s^s = 150 sm^{-1}$ respectively. Surface resistance values could be a function of soil moisture. The u_* is computed by Equation 19.

$$u_* = K_u h_c\left[\ln\left(\frac{h_c - d_0}{Z_{OM}}\right) - \ln\varphi_m\left(\frac{h_c - d_0}{L}\right)\right] \quad (19)$$

L is Monin-Obukhov length (m). For the detailed formulation, refer to [16].

Table A1. Table of symbols, their description and units used in the study.

Symbol	Description
λ	Latent heat of vaporization of water (J kg^{-1})
λE	Evapotranspiration (evaporation + transpiration) as latent heat flux (W m^{-2})
λE_{wet}	λE at wet limits (W m^{-2})
H	Sensible heat flux (W m^{-2})
H_{wet}	H at wet limits (W m^{-2})
H_{dry}	H at dry limits (W m^{-2})
R_N	Net radiation (W m^{-2})
G	Ground heat flux (W m^{-2})
φ	Net available energy (W m^{-2})
T_A	Air temperature (◦C)
T_C	Vegetation temperature (◦C)
T_{Soil}	Soil temperature (◦C)
T_D	Dew-point temperature (◦C)
T_S	Radiometric surface temperature (◦C)
R_H	Relative humidity (%)
E_p	Potential evapotranspiration (W m^{-2})
P	Precipitation (mm d^{-1})
e_A	Atmospheric vapor pressure at the level of TA measurement (hPa)
D_A	Atmospheric vapor pressure deficit at the level of TA measurement (hPa)
u	Wind speed (m s^{-1})

u_*	Friction velocity (m s^{-1})
T_{SD}	Dew-point temperature at the source/sink height (◦C)
T_{OD}	Dew point temperature at evaporating front (◦C)
T_0	Aerodynamic temperature or source/sink height temperature (◦C)
e_S	"Effective" vapor pressure of evaporating front near the surface (hPa)
e^*_S	Saturation vapor pressure of the surface (hPa)
e^*_0	Saturation vapor pressure at the source/sink height (hPa)
e_0	Atmospheric vapor pressure at the source/sink height (hPa)
D_0	Atmospheric vapor pressure deficit at the source/sink height (hPa)
g_A	Aerodynamic conductance (m s^{-1})
g_S	Stomatal/surface conductance (m s^{-1})
Sc	Schmidt Number (-)
Pr	Prandtl Number (-)
M	Surface moisture availability (0–1)
s	Slope of saturation vapor pressure vs. temperature curve (hPa K^{-1})
s_1	Slope of the saturation vapor pressure and temperature between ($T_{SD} - T_D$) vs. ($e_0 - e_A$) (approximated at T_D) (hPa K^{-1})
s_2	Slope of the saturation vapor pressure and temperature between (T_S-T_D) vs. (e^*_S-e_A), estimated according to Mallick et al. (2015) (hPa K^{-1})
s_3	Slope of the saturation vapor pressure and temperature between ($T_S - T_{SD}$) vs. ($e_{*S} - e_S$) (approximated at T_S) (hPa K^{-1})
q_s, q_a	Absolute humidity of the surface and the air (kgm^{-3})
r_a	Aerodynamic resistance at inertial sublayer (r^I), roughness height (r^H) at the canopy (r^c) (m s^{-1})
r_b	Boundary layer resistance for soil (r^s) or for leaves (r^c) (m s^{-1})
r_s	Resistance at soil surface (m s^{-1})
m	Ball-Berry stomatal conductance parameter (-)
rwc	Within canopy layer resistance (m s^{-1})
u^*	Friction velocity (m s^{-1})
u_{ZOM}	Windspeed at $Z_{OM} + d_O$ (m s^{-1})
L	Monin-Obukhov length (m)
ψ	Stability correction function (-)
ψ_m	Stability correction function for momentum transfer (-)
ψ_H	Stability correction function for heat transfer (-)
Γ	thermal inertia of the soil (J K^{-1} m^{-2} $s^{-1/2}$)
ω	Frequency of the diurnal cycle rad s^{-1}
z	Reference height (m)
z_{0M}	Effective source–sink height of momentum (m)
z_{0H}	Roughness length (m)
d_O	Displacement height (m)
γ	Psychrometric constant (hPa K^{-1})
c_d	Drag coefficient (-)
c_p	Heat capacity of the air (J kg^{-1} K^{-1})
h_c	Vegetation height m
$K_{h,v}$	Eddy diffusivity (m^2 s^{-1})
Kr	von Kármán constant (0.4)
k	von Kármán constant (0.4)
n	Wind extinction coefficient
Λ	Evaporative fraction (-)

Λ_r	Relative evaporative fraction (-)
β	Bowen ratio (-)
α	Priestley–Taylor parameter (-)
Pr	Prandtl number (-)
LAI	Leaf area Index
NDVI	Normalized difference vegetation index (-)
LIDFa	Leaf distribution function parameter a controlling average leaf slope (-)
LIDFb	Leaf distribution function parameter b controlling distribution bimodality (-)
lw	Leaf width (m)
VZA	Viewing zenith angle (Degree)
RAA	Relative azimuth angle (Degree)
SZA	Sun zenith angle (Degree)
θ	Surface (0–5 cm) soil moisture (m^3 m^{-3})
T_{VP}	Virtual potential temperature near the surface(K)
Vcmax	Maximum carboxylation rate (μmolm^{-2} s^{-1})

Table A2. Input variables and parameters of the SCOPE1.7 model.

Parameter	Symbol	Spring/Summer	Units	Source
1.PROSPECT				
Chlorophyll AB content	Cab	1.5/40	μg cm^{-2}	Fitted
Carotenoid content.	Cca	0/8.7	μg cm^{-2}	Fitted
Dry matter content	Cdm	0.005/0.001	g cm^{-2}	Fitted
Leaf water equivalent layer	Cw	0.0001/0.022	cm	Fitted
Senescent material fraction	Cs	0.6/0	fraction	Fitted
Leaf thickness parameters	N	1.5/1.5	(-)	Fitted
BSM model parameter 'lat'	BSMlat	18.9		apriori
BSM model parameter 'long'	BSMlong	43.32		apriori
2.LEAF BIOCHEMICHAL				
Maximum carboxylation capacity	Vcmo	6.5/14	μmol m^{-2} s^{-1}	[23]
Ball-Berry stomatal conductance	m	12/8		Fitted
Photochemical pathway: 0 = C3, 1 = C4	Type	0		apriori
Extinction coefficient for Vcmax	kV	0.6396		apriori
Respiration = Rdparam*Vcmax	Rdparam	0.015		apriori
Temp response.	Tparam	0.2		apriori
3.MAGNANI MODEL				
4.FLOURESCENCE				
5.SOIL				
Soil resistance for evaporation	rss	800/1200	s m^{-1}	apriori
	rs_therma			apriori
Soil reflectance thermal range	l	0.06		
specific heat capacity of the soil	cs	3.65E + 03	J K^{-1}	[24]
specific mass of the soil	rhos	1.10E + 03	kg m^{-3}	[24]
Heat conductivity of the soil	lambdas	0.5	J m^{-1} K^{-1}	[24]
Volumetric soil moisture content	SMC	0.4/0.6		
6.CANOPY				
Leaf area index	LAI	1.6/3.2	m^2 m^{-2}	Fitted
Vegetation height	hc	0.3/0.6	m	Measured
Leaf inclination	LIDFa	−0.35		apriori
Variation in leaf inclination	LIDFb	−0.15		apriori

Leaf width	leaf width	0.03	m	apriori
7.METEO		EC tower		Measured
8.AERODYNAMIC				
Roughness length for momentum	Z_{0H}	0.13*hc	m	Computed
Displacement height	d_0	0.67*hc	m	Computed
leaf drag coefficient	Cd	0.3		apriori
leaf boundary resistance	rb	10	s m^{-1}	apriori
Drag coefficient [25]	CR	0.35		apriori
fitting parameter [25]	CD1	20.6		apriori
Roughness layer correction [25]	Psicor	0.2		apriori
Drag coefficient for soil [25]	CSSOIL	0.01		apriori
Soil boundary layer resistance	rbs	10	s m^{-1}	apriori
Within canopy layer resistance	rwc	0	s m^{-1}	
Geometry				
solar zenith angle	VZA		Degree	Computed
Observation zenith angle	VZA		Degree	Computed
Azimuth angle	RAA		Degree	Computed

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