# Supplement to "Global isoprene emissions calculated based on MEGAN, ECMWF analyses and a detailed canopy environment model"

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# Supplement to "Global isoprene emissions calculated based on MEGAN, ECMWF analyses and a detailed canopy environment model"

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**Abstract.** This supplement provides a detailed description of the model parameterizations for (1) radiative transfer in the canopy, (2) the leaf energy budget (including the determination of resistances for the exchange of heat and water vapor between leaves and the air), and (3) the vertical profile of windspeed in the canopy.

## 1 Radiative transfer

The model values for the PFT-dependent parameters influencing radiative transfer and the estimation of leaf temperature are given in Table 1.

Radiative transfer in the canopy follows Goudriaan and van Laar (1994). The radiation absorbed by shaded leaves,  $Q_{dif}$ , may be written as

$$Q_{dif}(L_c) = Q_{dif,atm}(L_c) + Q_{scat,leaf}(L_c)$$
 (1)

where  $L_c$  is the cumulative LAI measured downwards from the top of the canopy.  $Q_{dif,atm}$  and  $Q_{scat,leaf}$  are the contributions from the diffuse solar radiation and from the scattering of direct radiation by leaves, estimated using

$$Q_{dif,atm} (L_c) = (2)$$

$$\kappa_{dif} \cdot Q_{dif0} \cdot (1 - \rho_{can,dif}) \cdot \exp(-\kappa_{dif} L_c)$$

and

$$Q_{scat,leaf}(L_c) = \kappa_{dir} \cdot Q_{dir0} \cdot (1 - \rho_{can,dir})$$

$$\cdot \exp(-\kappa_{dir} L_c) - f_{sunlit} \cdot Q_{dir0} \cdot (1 - \sigma_l) \cdot \kappa_{bl,dir}$$
(3)

where  $Q_{dif0}$  and  $Q_{dir0}$  are the incoming diffuse and beam (direct) radiation, and  $\kappa_{dif}$ ,  $\kappa_{dir}$  and  $\kappa_{bl,dir}$  are extinction coefficients for diffuse radiation, for scattered beam radiation and for a theoretical canopy with black leaves (no reflection and no transmission),  $\sigma_l$  is the scattering coefficient (reflection plus transmission), and  $\rho_{can,dif}$  and  $\rho_{can,dir}$  are canopy

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reflection coefficients for diffuse and direct radiation, respectively. The scattered beam radiation is calculated in Eq. (4) as the difference between total absorbed beam radiation including scattering (first term) and the absorbed direct beam radiation alone (second term).

The absorption of the direct beam radiation by sunlit leaves is given by

$$Q_{dir} = \kappa_{bl,dir} \cdot Q_{dir0} \cdot (1 - \sigma_l) \tag{4}$$

multiplied by the fraction of sunlit leaves,  $f_{sun}$ , which is determined by using the extinction coefficient for black leaves  $(\kappa_{bl,dir})$ :

$$f_{sun} = \exp\left(-\kappa_{bl,dir} \cdot L_c\right) \tag{5}$$

The PPFD fluxes entering in the emission algorithm (i.e. in  $\gamma_P$ ) are obtained by dividing the absorbed radiation ( $Q_{dif}$  and  $Q_{dir}$ ) by  $(1 - \sigma_l)$ .

The fraction of radiation intercepted by a layer is equal to the surface of the layer multiplied by the extinction coefficient  $\kappa$ , which depends on the direction of radiation and on the orientation of the leaves. Its value for direct radiation is given by

$$\kappa_{bl,dir} = \frac{G(\beta_s)}{\sin \beta_s} \tag{6}$$

where  $G(\beta_s)$  is the mean projected leaf area in the direction of the solar beam, and  $\beta_s$  is the solar elevation. For a spherical distribution of the leaves,  $G(\beta_s)=0.5$ . For diffuse radiation, each light direction is intercepted at a different rate. The resulting radiation profile in the canopy consists of many subprofiles, each being an exponential with a specific coefficient  $\kappa$ . The combination of these subprofiles can be approached by a single exponential form with an extinction coefficient  $\kappa$ . For a spherical distribution of the leaves, it may be approximated (Goudriaan and van Laar, 1994) by

$$\kappa_{bl,dif} = 0.8 \tag{7}$$

These coefficients are representative for black leaves. In order to take reflection and transmission into account, these

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**Table 1.** Leaf- and canopy-related parameters in the canopy model. The plant functional types are 1: Needleleaf evergreen, 2: needleleaf deciduous, 3: broadleaf evergreen, 4: broadleaf deciduous, 5: shrubs, 6: grass, 7: crops.

Parameter			Plant functional types						
		1	2	3	4	5	6	7	
Leaf length <sup>a</sup> (m)	$L_l$	0.1	0.1	0.1	0.1	0.1	0.15	0.15	
Leaf width <sup>a</sup> (m)	$l_l$	0.005	0.005	0.05	0.05	0.01	0.01	0.02	
Cluster factor <sup>a</sup>	$f_c$	0.85	0.85	0.9	0.65	0.85	0.7	0.7	
Leaf side factor <sup>b</sup>	$f_l$	1.25	1.25	1.25	1.25	1	1.25	1.25	
Cuticular resistance $^{c,d}$ (s m $^{-1}$ )	$r_c$	$10^{4}$	$10^{4}$	$10^{4}$	$10^{4}$	$2 \cdot 10^{4}$	$5 \cdot 10^{3}$	$5 \cdot 10^{3}$	
Stomatal resistance parameters:									
Coeffi cien $\ell^{f,f,g}$ (J m <sup>-3</sup> )	$a_s$	2870	2870	2336	9802	52847	2582	7459	
Coeffi cien $f^{f,f,g}$ (W m <sup>-2</sup> )	$b_s$	3.70	3.70	0.0145	10.06	4.50	1.09	5.70	
Coeffi cien $\ell^{f,g}$ (s m <sup>-1</sup> )	$c_s$	233	233	154	180	447	110	25	
Lowest temperature $^{e,f}$ (K)	$T_l$	268	268	273	268	268	268	268	
Optimum temperature $^{e,f}$ (K)	$T_o$	283	283	303	290	290	290	300	
Highest temperature $^{e,f}$ (K)	$T_h$	316	316	318	316	315	315	315	
Coeffi cient $^{f,g}$ (mbar $^{-1}$ )	$d_s$	0.031	0.031	0.0273	0.0357	0.0308	0.0238	0	
Canopy height (m)	$h_c$	24	24	32	24	1	0.5	1	
Mean attenuation of windspeed $h,i,j,k$	$\overline{at_u}$	1.0	1.0	1.5	1.5	1.0	2.0	2.5	

<sup>a</sup> adapted from Lamb et al. (1993), <sup>b</sup>Campbell (1981), <sup>c</sup>Nobel (1983), <sup>d</sup>Larcher (1995), <sup>e</sup>Sellers and Dorman (1987), <sup>f</sup>Sellers et al. (1989), <sup>g</sup>Dorman and Sellers (1989), <sup>h</sup>Cionco (1978), <sup>i</sup>Wilson et al. (1982), <sup>f</sup>Raupach (1988), <sup>k</sup>Baldocchi (1997).

coefficients should be corrected following

$$\kappa_{dir(dif)} = f_c \cdot \kappa_{bl,dir(dif)} \cdot \sqrt{(1 - \sigma_l)}$$
 (8)

where  $f_c$  if the cluster factor (see Table 1),  $\kappa_{bl,dir(dif)}$  are provided by Eqs. (6) and (7) and  $\sigma_l$  is the scattering coefficient assumed equal to 0.2 for visible radiation and 0.8 for NIR (Goudriaan and van Laar, 1994; Leuning et al., 1995).

The canopy reflection coefficient  $\rho_{can}$  depends on the angle of incidence of the incoming radiation. A reasonable approximation, for a spherical distribution and for direct beam radiation, is given by Leuning et al. (1995):

$$\rho_{can,dir} = 1 - \exp\left[\frac{-2 \cdot \rho_{can,horiz} \cdot \kappa_{bl,dir}}{(1 + \kappa_{bl,dir})}\right]$$
(9)

where  $\kappa_{bl,dir}$  is given by Eq. (6) and  $\rho_{can,horiz}$  is the canopy reflection coefficient for horizontal leaves:

$$\rho_{can,horiz} = \frac{(1 - \sqrt{1 - \sigma_l})}{(1 + \sqrt{1 - \sigma_l})} \tag{10}$$

For the diffuse radiation and a spherical distribution, the canopy reflection coefficient is approximated by

$$\rho_{can,dif} = \rho_{can,horiz} \cdot \frac{2}{1 + 1.6 \sin \beta_s} \tag{11}$$

Typical values for  $\rho_{can,dif}$  are 0.057 for visible light and 0.389 for NIR (Goudriaan and van Laar, 1994; Leuning et al., 1995).

## 2 Calculation of the leaf energy budget

 $Q_{LW}$ , the net longwave radiation received by the leaf, results from a balance between thermal radiation emitted by

the leaf and thermal radiation emitted by the surrounding environment and absorbed by the leaf. Neglecting thermal exchanges with surrounding leaves, and using the the extinction coefficient for black leaves and diffuse radiation  $(\kappa_{bl,dif})$  to characterize the attenuation of thermal radiation by the canopy,  $Q_{LW}$  is written as

$$Q_{LW} = (-\varepsilon_l \sigma T_l^4 + \varepsilon_{atm} \sigma T_{eff,atm}^4) \cdot \kappa_{bl,dif}$$

$$\cdot \exp(-\kappa_{bl,dif} L_c)$$
(12)

 $\sigma$  is the Stefan-Boltzmann's constant (=5.67051·10<sup>-8</sup> W m<sup>-2</sup> K<sup>-4</sup>),  $T_l$  is leaf temperature and  $\varepsilon_l$  is the leaf emissivity, taken to be 0.96 for all plant functional types (Campbell, 1981).  $\varepsilon_{atm}$  and  $T_{eff,atm}$  are the emissivity and the effective temperature of the atmosphere. For a clear sky,  $\varepsilon_{atm}$  is given by (Brunt, 1932):

$$\varepsilon_{atm} = 0.52 + 0.065\sqrt{e_{air}} \tag{13}$$

where  $e_{air}$  is the water vapor pressure (hPa) of the air above the canopy. In this case,  $T_{eff,atm}$  is the air temperature above the canopy. For a cloudy sky, the net deficit  $Q_{LW}$  is taken as 10% of the clear-sky value obtained using Eq. (13).

The sensible heat flux,  $Q_{SH}$  is written as (Nobel, 1983; Goudriaan and van Laar, 1994)

$$Q_{SH} = \rho \cdot c_p \cdot \frac{\Delta T}{r_{b,h}} \tag{14}$$

where  $\rho$  is air density (kg m<sup>-3</sup>),  $c_p$  is the heat capacity of air (J kg<sup>-1</sup> K<sup>-1</sup>) at constant pressure,  $\Delta T$  is the difference of temperature between the leaf and the air and  $r_{b,h}$  is the boundary layer resistance for heat (s m<sup>-1</sup>).

The latent heat flux is

$$Q_{LH} = \frac{(e_l - e_{air}) \cdot \rho \cdot c_p}{\gamma_{ps} \cdot (r_{b,v} + r_{ep})}$$
(15)

where  $e_l$  is the water vapor pressure (Pa) in the leaf. Relative humidity is equal to 100% in the intercellular space in the leaf and in the substomatal cavities.  $e_l$  is therefore equal to the saturation vapor pressure at the leaf temperature.  $e_{air}$  is the water vapor pressure in the air,  $\gamma_{ps}$  is the adiabatic psychrometric coefficient, equal to 67 Pa K $^{-1}$  at 293 K (Goudriaan and van Laar, 1994).  $r_{b,v}$  and  $r_{ep}$  are the resistances of the air boundary layer and the leaf epidermis (the outermost layer of cells covering the leaves) to the exchange of water vapor, respectively.

#### 3 Determination of the resistances

#### 3.1 Leaf boundary layer

Frictional interactions between the leaf and the air lead to the presence of a boundary layer of air adhering to the leaf and across which heat and mass are exchanged. The average thickness  $\delta_b$  is affected by several factors such as windspeed (u) and leaf dimension  $(d_l)$  (Nobel, 1983):

$$\delta_b = 4.0 \cdot 10^{-3} \sqrt{\frac{d_l}{u}} \tag{16}$$

$$d_l = 0.6 \cdot L_l + 0.4 \cdot l_l \tag{17}$$

where  $L_l$  and  $l_l$  are the leaf length and leaf width, respectively (Table 1).

#### 3.2 Boundary layer resistance to heat

The resistance  $r_{b,h}$  depends on the ratio of the leaf dimension to the product of the thermal diffusivity of air  $D_{th}$  and the Nusselt number Nu:

$$r_{b,h} = \frac{1}{2} \cdot \frac{d_l}{(D_{th} \cdot Nu)}$$
 [s m<sup>-1</sup>] (18)

Thermal diffusivity depends on air temperature (Monteith and Unsworth, 1990):

$$D_{th} = \frac{C_{th}}{\rho c_p} \qquad [\text{m}^2 \, \text{s}^{-1}]$$
 (19)

with the coefficient of thermal conductivity of air:

$$C_{th} = \frac{2.64638 \cdot 10^{-3} T_{air}^{3/2}}{T_{air} + (245.4 \cdot 10^{-12} / T_{air})} \quad [\text{W m}^{-1} \text{ K}^{-1}] \quad (20)$$

## 3.3 Boundary layer resistance to water vapor

The resistance  $r_{b,v}$  is given by (Nobel, 1983; Monteith and Unsworth, 1990)

$$r_{b,v} = \frac{1}{f_l} \cdot \frac{d_l}{D_{uv} \cdot Sh_{uv}}$$
 [s m<sup>-1</sup>] (21)

where  $f_l$  is the effective number of sides of the leaf (Table 1).  $D_{wv}$  is the diffusivity coefficient of water vapor in air (Fuller

et al., 1966):

$$D_{wv} = b_1 \cdot \frac{10^{-11} \cdot T_{air}^{1.75} \cdot \sqrt{\frac{1}{M_{air}} + \frac{1}{M_{wv}}}}{p_{tot} \cdot (D_{air,v}^{1/3} + D_{wv,v}^{1/3})^2}$$
 [m<sup>2</sup> s<sup>-1</sup>]

where  $M_{air} = 28.9644 \text{ g mol}^{-1}$ ,  $M_{wv} = 18.0153 \text{ g mol}^{-1}$ ,  $p_{tot}$  is total pressure (Pa),  $D_{air,v} = 20.1 \cdot 10^{-6} \text{ m}^3$ ,  $D_{wv,v} = 12.7 \cdot 10^{-6} \text{ m}^3$ , and  $b_1 = 101325 \text{ Pa m}^4 \text{ g}^{0.5} \text{ mol}^{-0.5} \text{ s}^{-1} \text{ K}^{-1.75}$ .

 $Sh_{wv}$  is the Sherwood number. It depends on the Nusselt number which depends on nature of the convection (see next Section) (Monteith and Unsworth, 1990; Leuning et al., 1995):

$$Sh_{wv} = Nu \cdot (\frac{D_{th}}{D_{wv}})^{0.33} \tag{23}$$

where Nu is the Nusselt number (Eq. (24)),  $D_{th}$  is the thermal diffusivity of air (Eq. (19)) and  $D_{wv}$  is the diffusivity of the water vapor in the air (Eq. (22)).

# 3.4 Determination of the nature of convection in leaf-air exchanges

The Nusselt number depends on the nature of convection (forced, free or mixed). The analysis is facilitated by the use of the Grashof number and the Reynolds number.  $Re^2/Gr$  is the ratio of inertial forces to buoyant forces, which determines the relative importance of forced and free convection (Nobel, 1983; Monteith and Unsworth, 1990; Leuning et al., 1995). In the case of free convection  $(Re^2/Gr < 0.1)$ , Nu is proportional to the Grashof number (Gr), whereas in case of forced convection  $(Re^2/Gr > 10)$ , Nu depends on windspeed. In the case of mixed convection  $(0.1 < Re^2/Gr < 10)$ ), the Nusselt number is interpolated logarithmically between the following functions:

$$Nu = \begin{cases} 0.5 \cdot Gr^{0.25} & \text{if } Re^2/Gr < 0.1 \text{ free convection} \\ \frac{d_l}{\delta_b} & \text{if } Re^2/Gr > 10 \text{ forced convection} \end{cases}$$
(24)

The Grashof number is

$$Gr = \frac{g \cdot \beta_{th} \cdot \Delta T \cdot d_l^3}{\nu^2} \tag{25}$$

where g is the gravitational acceleration, and  $\beta_{th}=1/T_{air}$  is the coefficient of volumetric thermal expansion.  $\Delta T$  is the difference between leaf temperature and air temperature.  $\nu$  is the kinematic viscosity (Nobel, 1983):

$$\nu = \frac{\nu_d}{\rho} \qquad [\text{m}^2 \, \text{s}^{-1}] \tag{26}$$

where  $\nu_d$  is the dynamic viscosity given by:

$$\nu_d = \frac{a_1 \cdot T_{air}^{3/2}}{T_{air} + Su} \qquad [\text{kg m}^{-1} \text{ s}^{-1}] \qquad (27)$$

 $a_1 = 1.458 \cdot 10^{-6} \text{ kg m}^{-1} \text{ s}^{-1} \text{ K}^{-1/2}$ ) and Su is the Sutherland's constant (= 110.4 K).

The Reynolds number is given by

$$Re = \frac{ud_l}{\nu} \tag{28}$$

where u is windspeed and  $\nu$  is the kinematic viscosity (Eq. (26)).

#### 3.5 Stomatal resistance

To regulate  $CO_2$  assimilation and water vapor exchange, the epidermis has actively regulated openings, the stomata, and a waxy layer, the cuticle, which prevents evaporation when the stomata are closed. This cuticular resistance  $(r_c)$  is on the order of 2000 s m<sup>-1</sup> or more (see Table 1). The stomatal resistance vary from 50 to 10000 s m<sup>-1</sup>, depending on meteorological conditions, the  $CO_2$  level, and the leaf water potential.  $r_s$  is parameterized according to the SiB model (Sellers et al., 1986) based on previous work of Jarvis (1976); Sellers (1985):

$$r_s = r_{s,VIS} \cdot [f(T_l) \cdot f(\delta e) \cdot f(\psi_l)]^{-1}$$
 (29)

where  $r_{s,VIS}$  represents the dependence to light, and  $f(T_l), f(\delta e)$  and  $f(\psi_l)$  are stress factors for temperature, water vapor pressure deficit and leaf water potential, respectively. These factors vary from unity, under optimal conditions, to zero when transpiration is totally suppressed by adverse environmental condition. The different terms of the stomatal resistance relationship are given by

$$r_{s,VIS} = \frac{a_s}{b_s + Q_{PPFD}} + c_s \tag{30}$$

where  $a_s$  (J m<sup>-3</sup>),  $b_s$  (W m<sup>-2</sup>) and  $c_s$  (s m<sup>-1</sup>) are PFT-dependent constants (see Table 1) and  $Q_{PPFD}$  is the PPFD (in W m<sup>-2</sup>). The stress factors  $f(T_l)$ ,  $f(\delta e)$  and  $f(\psi_l)$  are given by

$$f(T_l) = T_1 \cdot (T_l - T_{low}) \cdot (T_{high} - T_l)^{T_2}$$
 (31)

with

$$T_1 = \frac{1}{(T_{opt} - T_{low})(T_{high} - T_{opt})^{T_2}}$$
(32)

$$T_2 = \frac{(T_{high} - T_{opt})}{(T_{opt} - T_{low})} \tag{33}$$

 $T_{high}$ ,  $T_{low}$  et  $T_{opt}$  are the highest, lowest and optimum temperatures for transpiration (Table 1);

$$f(\delta e) = 1 - d_s \, \delta e \cdot \tag{34}$$

where  $\delta e$  is the water vapor pressure deficit (hPa) and  $d_s$  is given in Table 1,

$$\delta e = e_{sat}(T_{air}) - e_{air} \tag{35}$$

where  $e_{air}$  is the water vapor pressure in the air, and  $e_{sat}(T_{air})$  is the vapor pressure at saturation parameterized as

$$e_{sat} = 6.107 \exp \frac{17.4 \, T_{air}}{239 + T_{air}}$$
 [hPa] (36)

 $f(\psi_l)$ , the dependence on the leaf water potential, is estimated from the volumetric soil water content,

$$\frac{1}{f(\psi_l)} = \max(0, \min(1, \frac{\theta_{av} - \theta_w}{\theta_{cap} - \theta_w}))$$
(37)

where  $\theta_w$  and  $\theta_{cap}$  are the soil moisture at the wilting point and at field capacity, respectively, and  $\theta_{av}$  is a weighted average of soil water

$$\theta_{av} = \sum_{l} [f_{root}^{l} \cdot \theta^{l}] \tag{38}$$

where  $f_{root}^l$  is the fraction of roots within the soil layer l Zeng (2001), and  $\theta^l$  is the volumetric soil water content in this layer (m³ m⁻³). Since our study uses soil moisture data from ECMWF analyses, the ECMWF model values for  $\theta_w$  (=0.171 m³ m⁻³) and  $\theta_{cap}$  (=0.323m³ m⁻³) are used in Eq. (37) as well as in the parameterization of the soil moisture dependence of the emissions.

#### 4 Windspeed profile in the canopy

The attenuation of windspeed by foliage follows an approximately exponential law (Cionco, 1978):

$$u(z) = u(h_c) \cdot \exp\left(\overline{at_u} \cdot \left(\frac{z}{h_c} - 1\right)\right) \tag{39}$$

where u(z) et  $u(h_c)$  are the windspeed values at altitude z and at canopy top, respectively, and  $\overline{at_u}$  is the mean attenuation coefficient (Table 1). The variation of windspeed between adjacent layers is modulated by the LAI profile and the layer thicknesses, i.e. (Businger, 1975; Raupach, 1988):

$$at_{u,j} = \alpha_u \left[ \Delta LAI_j \cdot (\Delta z_j)^2 \right]^{1/3}$$
 with  $\overline{at_u} = \sum_{j=1}^n at_{u,j}$  (40)

where  $at_{u,j}$  is the windspeed attenuation coefficient in the layer j,  $\Delta LAI_j$  is the LAI of layer j and  $\Delta z_j$  is the j layer thickness. The  $\alpha_u$  coefficient is determined as

$$\alpha_u = \frac{\overline{at_u}}{\sum_{j=1}^n \Delta LAI_j^{1/3} \cdot (\Delta z_j)^{2/3}}$$
(41)

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