

Partitioning of total O₃ flux into stomatal uptake and non-stomatal deposition: calculation procedure

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Measured input parameters needed:

u_*	friction velocity ($\text{m}\cdot\text{s}^{-1}$)	Solent R2 (Gill Instruments)
H	sensible heat flux (W m^{-2})	Solent R2 (Gill Instruments)
E	water vapour flux ($\text{g m}^{-2}\cdot\text{s}^{-1}$)	EdiSol system (Moncrieff et al. 1997)
$F(\text{O}_3)$	ozone flux ($\text{g m}^{-2}\cdot\text{s}^{-1}$)	OS-G-2 (Güsten et al. 1992)
ρ_{O_3}	O ₃ concentration at a reference height $z_{\text{ref, O}_3}$ above ground ($\mu\text{g}\cdot\text{m}^{-3}$)	
$u(z)$	horizontal wind velocity at the height of the eddy systems $z_{\text{ref, eddy system}}$ ($\text{m}\cdot\text{s}^{-1}$)	
$T(z)$	absolute air temperature at the height of the eddy systems $z_{\text{ref, eddy system}}$ (K) ($T = t_a + 273.15$)	
p	air pressure (hPa)	
rH	air humidity (%)	
h	canopy height (m)	



CO₂/H₂O eddy system



O₃ eddy system

Total O₃ flux $F_{\text{total}}(\text{O}_3)$ can be partitioned into the flux absorbed by the plants through the stomata and the cuticle into the mesophyll tissue $F_{\text{absorbed}}(\text{O}_3)$ and into non-stomatal deposition $F_{\text{non-stomatal}}(\text{O}_3)$:

$$F_{\text{total}}(\text{O}_3) = F_{\text{absorbed}}(\text{O}_3) + F_{\text{non-stomatal}}(\text{O}_3),$$

with

$$F_{\text{absorbed}}(\text{O}_3) = F_{\text{stomatal}}(\text{O}_3) + F_{\text{cuticle}}(\text{O}_3)$$

and

$$F_{\text{non-stomatal}}(\text{O}_3) = F_{\text{external plant surfaces}}(\text{O}_3) + F_{\text{soil}}(\text{O}_3)$$

Investigations of cuticular permeability of O₃ and other trace gases show that penetration through the cuticle can be neglected in comparison to stomatal uptake (Kerstiens & Lenzian 1989a, b, Lenzian & Kerstiens 1991, Kerstiens et al. 1992). Therefore it can be presumed that $F_{\text{cuticle}}(\text{O}_3)$ is negligible compared to $F_{\text{stomatal}}(\text{O}_3)$ thus:

$$F_{\text{absorbed}}(\text{O}_3) \cong F_{\text{stomatal}}(\text{O}_3)$$

and

$$\begin{aligned} F_{\text{total}}(\text{O}_3) &= F_{\text{stomatal}}(\text{O}_3) + F_{\text{non-stomatal}}(\text{O}_3) \\ &= -\frac{\rho_{\text{O}_3}}{R_{\text{total}, \text{O}_3}} = -\frac{\rho_{\text{O}_3}}{R_{\text{ah}} + R_{\text{b}, \text{O}_3} + R_{\text{c}, \text{O}_3}} \\ &= -\frac{\rho_{\text{O}_3}}{R_{\text{ah}} + R_{\text{b}, \text{O}_3} + \left[\frac{1}{R_{\text{c}, \text{stomatal}, \text{O}_3}} + \frac{1}{R_{\text{c}, \text{non-stomatal}, \text{O}_3}} \right]^{-1}} \end{aligned}$$

where ρ_{O_3} is the O₃ concentration at a reference height $z_{\text{ref}, \text{O}_3}$. According to Laisk et al. (1989) and Wang et al. (1995) it is convenient to assume that there are sinks in the plant/canopy reducing the O₃ concentration ρ_{O_3} to zero.

R_{ah} is the turbulent atmospheric resistance ($\text{s}\cdot\text{m}^{-1}$)

describing the atmospheric transport properties for O₃ between a reference height $z_{\text{ref}, \text{O}_3}$ above the canopy and the conceptual height $z = d + z_{0\text{m}}$ which represents the sink for momentum (d = displacement height, $z_{0\text{m}}$ = roughness length for momentum),

R_{b, O_3} is the quasi-laminar layer resistance ($\text{s}\cdot\text{m}^{-1}$)

between momentum sink height $z = d + z_{0\text{m}}$ and the O₃ sink height $z = d + z_{0, \text{O}_3}$,

R_{c, O_3} is the bulk canopy or surface resistance ($\text{s}\cdot\text{m}^{-1}$)

describing the influences of the plant/soil system on the vertical exchange of O₃,

which can be partitioned into $R_{\text{c}, \text{stomatal}, \text{O}_3}$ and $R_{\text{c}, \text{non-stomatal}, \text{O}_3}$.

Taking into account Kirchhoff's Current Law $F_{\text{stomatal}}(\text{O}_3)$ and $F_{\text{non-stomatal}}(\text{O}_3)$ can be calculated as:

$\rho_A = 100$

$R_1 = 20$

$R_{2a} = 20$ $R_{2b} = 50$

F_1 F_2

$\rho_B = 0$

$F_{total} = -2.917$

$F_{total} = -\frac{\rho_A - \rho_B}{R_1 + (1/R_{2a} + 1/R_{2b})^{-1}}$

Kirchhoff's Current Law

$F_{total} = F_1 + F_2$

$$F_1 = -\frac{\rho_A}{R_1 + R_{2a}} = -2.5$$

$$F_2 = -\frac{\rho_A}{R_1 + R_{2b}} = -1.429$$

}

☹️

= -3.929

$$F_1 = -\frac{\rho_A}{R_1 + R_{2a} + (R_1 \cdot R_{2a} \cdot 1/R_{2b})}$$

$$F_2 = -\frac{\rho_A}{R_1 + R_{2b} + (R_1 \cdot R_{2b} \cdot 1/R_{2a})}$$

}

😊

= -2.083

= -0.833

Σ = -2.917

$F_1 = F_{stomatal}$ $F_2 = F_{non-stomatal}$

$R_1 = R_{ah} + R_b$ $R_{2a} = R_{stomatal}$ $R_{2b} = R_{non-stomatal}$

(units: ρ in μg·m⁻³, R in m·s⁻¹, F in μg·m⁻²·s⁻¹)

$$F_{stomatal}(O_3) = -\frac{\rho_{O_3}}{R_{ah} + R_{b,O_3} + R_{c,stomatal,O_3} + \left[[R_{ah} + R_{b,O_3}] \cdot R_{c,stomatal,O_3} \cdot \frac{1}{R_{c,non-stomatal,O_3}} \right]}$$

and

$$F_{non-stomatal}(O_3) = -\frac{\rho_{O_3}}{R_{ah} + R_{b,O_3} + R_{c,non-stomatal,O_3} + \left[[R_{ah} + R_{b,O_3}] \cdot R_{c,non-stomatal,O_3} \cdot \frac{1}{R_{c,stomatal,O_3}} \right]}$$

Bulk stomatal resistance for O₃ is given by

$$R_{c,stomatal,O_3} = R_{c,stom,H_2O} \cdot \frac{D_{H_2O}}{D_{O_3}}$$

taking into account the differences between the molecular diffusivity for water vapour D_{H_2O} and ozone D_{O_3} (ratio = 1.51; cf Grünhage & Haenel 1997).

If $F_{total}(O_3)$ and ρ_{O_3} are **measured** and R_{ah} , R_{b,O_3} and $R_{c,stomatal,O_3}$ are estimated (see below), non-stomatal O₃ resistance can be calculated as follows:

$$F_{total}(O_3) = -\frac{\rho_{O_3}}{R_{ah} + R_{b,O_3} + R_{c,O_3}} \Rightarrow R_{c,O_3} = -\frac{\rho_{O_3}}{F_{total}(O_3)} - (R_{ah} + R_{b,O_3})$$

with

$$R_{c,O_3} = \left[\frac{1}{R_{c,stomatal,O_3}} + \frac{1}{R_{c,non-stomatal,O_3}} \right]^{-1}$$

⇒

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$$R_{c, \text{non-stomatal}, O_3} = \left[\frac{1}{-\frac{\rho_{O_3}}{F_{\text{total}}(O_3)} - (R_{ah} + R_{b, O_3})} - \frac{1}{R_{c, \text{stomatal}, O_3}} \right]^{-1}$$

Estimation of R_{ah}

According to the Monin-Obukhov theory (Monin & Obukhov 1954), the turbulent atmospheric resistance R_{ah} between the heights z_1 and z_2 can be expressed by

$$R_{ah}(z_1, z_2) = \frac{\ln\left(\frac{z_2 - d}{z_{0m}}\right) - \Psi_h\left(\frac{z_2 - d}{L}\right) + \Psi_h\left(\frac{z_1 - d}{L}\right)}{\kappa \cdot u_*}$$

with $z_2 = z_{\text{ref}}$ of the respective parameter (ρ_{O_3} or T) and $z_1 = d + z_{0m}$
and

L is the Monin-Obukhov length [m], κ is the dimensionless von Kármán constant (= 0,41; cf Dyer 1974), u_* is the **measured friction velocity** and Ψ_h is the integrated atmospheric stability function for sensible heat.

The **MONIN-Obukhov LENGTH** is given by

$$L = - \rho_{\text{moist air}} \cdot c_{p, \text{moist air}} \cdot \frac{\bar{\theta} \cdot u_*^3}{\kappa \cdot g \cdot H}$$

$$\approx - \rho_{\text{moist air}} \cdot c_{p, \text{moist air}} \cdot \frac{T(z_{\text{ref}}) \cdot u_*^3}{\kappa \cdot g \cdot H}$$

with $\bar{\theta}$ average potential temperature of the air layer under consideration (K)
 T **measured air temperature** at the height of the eddy systems z_{ref} , eddy system
 g gravitational acceleration (= 9.81 m·s⁻²)
 H **measured turbulent vertical flux density of sensible heat**
 $\rho_{\text{moist air}}$ density of moist air (g·m⁻³)
 $c_{p, \text{moist air}}$ specific heat of moist air (m²·s⁻²·K⁻¹)

specific heat of moist air at constant pressure

$$c_{p, \text{moist air}} = c_{p, \text{dry air}} \cdot (1 + 0.84 \cdot q)$$

with $c_{p, \text{dry air}} = 1004.67 \text{ m}^2 \cdot \text{s}^{-2} \cdot \text{K}^{-1}$

and q specific air humidity [g·g⁻¹]

$$q = \frac{0.622 \cdot e_{\text{water vapor pressure}}}{p - 0.378 \cdot e_{\text{water vapor pressure}}}$$

density of moist air at temperature T

$$\rho_{\text{moist air}} = \rho_{\text{dry air}} \cdot \left(1 - 0.378 \cdot \frac{e_{\text{water vapor pressure}}}{p} \right)$$

with
$$\rho_{\text{dry air}} = \frac{p}{R_{\text{dry air}} \cdot (273.15 + t_a)} \cdot 100$$

and $R_{\text{dry air}}$ the gas constant for dry air (= 287.04 J·kg⁻¹·K⁻¹)

saturation water vapour pressure of the atmosphere e_{sat} (hPa; after Magnus)

actual air temperature $t_a \geq 0^\circ\text{C}$:
$$e_{\text{saturation water vapour pressure}} = 6.1078 \cdot e^{\frac{17.08085 \cdot t_a}{234.175 + t_a}}$$

actual air temperature $t_a < 0^\circ\text{C}$:
$$e_{\text{saturation water vapour pressure}} = 6.1078 \cdot e^{\frac{22.44294 \cdot t_a}{272.44 + t_a}}$$

actual water vapour pressure e (hPa)

$$e_{\text{water vapour pressure}} = e_{\text{saturation water vapour pressure}} \cdot \frac{rH}{100}$$

The **ATMOSPHERIC STABILITY FUNCTION** Ψ_h is calculated using the set of coefficients published by Dyer (1974) with $\kappa = 0,41$.

- *unstable atmospheric stratification* ($L < 0$ m)

$$\Psi_h(\zeta) = 2 \cdot \ln \left[\frac{1}{\phi_h(\zeta)} + 1 \right]$$

with
$$\phi_h(\zeta) = (1 - 16 \cdot \zeta)^{-0.5}$$

and
$$\zeta = \frac{z - d}{L} \quad \text{with} \quad z = z_2 = z_{\text{ref, T}} \quad \text{and} \quad z = z_1 = d + z_{0m}$$

- *stable atmospheric stratification* ($L > 0$ m)

$$\Psi_h(\zeta) = -5 \cdot \zeta$$

and
$$\zeta = \frac{z - d}{L} \quad \text{and} \quad z = z_2 = z_{\text{ref, T}} \quad \text{and} \quad z = z_1 = d + z_{0m}$$

- *neutral atmospheric stratification* ($|L| \rightarrow \infty$)

$$\Psi_h = 0$$

DISPLACEMENT HEIGHT d and **ROUGHNESS LENGTH** z_{0m} can be approximated for tall vegetation as follows:

$$\text{Brutsaert (1984): } d = 0.67 \cdot h \quad \text{and} \quad z_{0m} = 0.13 \cdot h$$

⇒

$$d = 5.154 \cdot z_{0m}$$

and

$$z_{0m} = 0.194 \cdot d$$

Measured friction velocity u_* and **measured horizontal wind velocity** $u(z)$ leads to:

$$u_* = \frac{\kappa \cdot u(z_2')}{\ln\left(\frac{z_2' - d}{z_{0m}}\right) - \Psi_m\left(\frac{z_2' - d}{L}\right) + \Psi_m\left(\frac{z_1 - d}{L}\right)}$$

with $z_2' = z_{\text{ref}, u}$ and $z_1 = d + z_{0m} = 0.194 \cdot d$

and Ψ_m the **ATMOSPHERIC STABILITY FUNCTION FOR MOMENTUM**, which is calculated using the set of coefficients published by Dyer (1974) with $\kappa = 0,41$.

• *unstable atmospheric stratification* ($L < 0$ m)

$$\Psi_m(\zeta) = 2 \cdot \ln\left[\frac{1}{\phi_m(\zeta)} + 1\right] + \ln\left[\frac{1}{\phi_m^2(\zeta)} + 1\right] - 2 \cdot \arctan\left[\frac{1}{\phi_m(\zeta)}\right]$$

with $\phi_m(\zeta) = (1 - 16 \cdot \zeta)^{-0.25}$

and $\zeta = \frac{z - d}{L}$ with $z = z_2' = z_{\text{ref}, u}$ and $z = z_1 = d + z_{0m}$

• *stable atmospheric stratification* ($L > 0$ m)

$$\Psi_m(\zeta) = -5 \cdot \zeta$$

and $\zeta = \frac{z - d}{L}$ and $z = z_2' = z_{\text{ref}, u}$

and $z = z_1 = d + z_{0m}$

• *neutral atmospheric stratification* ($|L| \rightarrow \infty$)

$$\Psi_m = 0$$

The displacement height can now estimated as:

• *neutral atmospheric stratification* ($L < 0$ m)

$$\Rightarrow d = \frac{z_2'}{\left(\exp\left[\frac{\kappa \cdot u(z_2')}{u_*}\right] \cdot 0.194\right) + 1}$$

• *unstable and stable atmospheric stratification* ($L < 0$ m)

⇒ the above mentioned equations are solved numerically

Estimation of R_{b, O_3} and $R_{b, heat}$

The quasi-laminar layer resistance for ozone R_{b, O_3} is estimated according to a simple approach by Hicks et al. (1987) taking into account the empirical results for permeable rough canopies described by Brutsaert (1984); for details see Grünhage et al. (2000):

$$R_{b, O_3} = R_{b, heat} \cdot \left(\frac{Sc}{Pr} \right)^{\frac{2}{3}} = \frac{\ln \left(\frac{z_{0m}}{z_{0h}} \right) - \Psi_h \left(\frac{z_{0m}}{L} \right) + \Psi_h \left(\frac{z_{0h}}{L} \right)}{\kappa \cdot u_*} \cdot \left(\frac{Sc}{Pr} \right)^{\frac{2}{3}}$$

$$= \frac{2 - \Psi_h \left(\frac{z_{0m}}{L} \right) + \Psi_h \left(\frac{z_{0h}}{L} \right)}{\kappa \cdot u_*} \cdot 1,18$$

with $\ln(z_{0m} / z_{0h}) = 2$, i.e. roughness length for sensible heat $z_{0h} = z_{0m} / \exp(2)$ where $R_{b, heat}$ is the quasi-laminar layer resistance for sensible heat, Sc is the Schmidt number (the ratio of the kinematic viscosity of dry air and the molecular diffusivity of the respective trace gas) und Pr is the Prandtl number (the ratio of the kinematic viscosity of dry air and the molecular diffusivity of heat). For water vapor $(Sc/Pr)^{2/3}$ is 0,90.

Estimation of $R_{c, stom, H_2O}$

BULK STOMATAL RESISTANCE TO WATER VAPOUR R_{c, H_2O} is given by:

$$R_{c, H_2O} = \frac{\rho_{air} \cdot 0.622}{p} \cdot \frac{e_{sat}(T_S) - e(T_S)}{E}$$

with

ρ_{air}	air density ($\text{g} \cdot \text{m}^{-3}$)
0.622	ratio of molecular weights of water vapour ($18.016 \text{ g} \cdot \text{mol}^{-1}$) and dry air ($28.9644 \text{ g} \cdot \text{mol}^{-1}$)
p	measured air pressure (hPa)
$e_{sat}(T_S)$	saturation water vapour pressure at $z = d + z_{0h}$
$e(T_S)$	actual water vapour pressure at $z = d + z_{0h}$
E	measured water vapour flux ($\text{g} \cdot \text{m}^{-2} \cdot \text{s}^{-1}$)

according to Thom (1975).

eq. (91) in Thom (1975)	$R_{c, H_2O} = \frac{\rho_{air} \cdot c_p}{\gamma} \cdot \frac{e_{sat}(T_S) - e(T_S)}{\lambda E}$
eq. (10.10) in Brutsaert (1984)	$\gamma = \frac{c_p \cdot p_{air}}{0.622 \cdot \lambda}$

$e_{\text{sat}}(T_S)$ and $e(T_S)$ can be calculated as mentioned above with the **SURFACE TEMPERATURE** T_S . This can be deduced from

$$H = \rho_{\text{air}} \cdot c_p \cdot \frac{T_S - T(z_{\text{ref}})}{R_{\text{ah}} + R_{\text{b,heat}}} \quad \text{resp.} \quad F_h = \frac{T_S - T(z_{\text{ref}})}{R_{\text{ah}} + R_{\text{b,heat}}}$$

⇒

$$T_S = T(z_{\text{ref}}) + [F_h \cdot (R_{\text{ah}} + R_{\text{b,heat}})]$$

BULK STOMATAL RESISTANCE FOR WATER VAPOUR $R_{\text{c, stom, H}_2\text{O}}$ can now be parameterised according to:

$$\frac{1}{R_{\text{c, H}_2\text{O}}} = \left[(1 - \beta^*) \cdot \left(\frac{1}{R_{\text{c, stom, H}_2\text{O}}} + \frac{1}{R_{\text{c, cut, H}_2\text{O}}} \right) + \frac{\beta}{R_{\text{soil, H}_2\text{O}}} \right]$$

⇒

$$R_{\text{c, stom, H}_2\text{O}} = (1 - \beta^*) \cdot \left[\frac{1}{R_{\text{c, H}_2\text{O}}} - \frac{1 - \beta^*}{R_{\text{c, cut, H}_2\text{O}}} - \frac{\beta}{R_{\text{soil, H}_2\text{O}}} \right]^{-1}$$

with the cuticular resistance for water vapour $R_{\text{leaf, cut, H}_2\text{O}} = 9 \cdot 10^{-4} \text{ s} \cdot \text{m}^{-1}$ (cf Grünhage & Haenel 1997). $R_{\text{leaf, cut, H}_2\text{O}}$ must be up-scaled to canopy level. Taking into account the more or less constant ratio of $R_{\text{leaf, stom, H}_2\text{O}} \cdot R_{\text{c, stom, H}_2\text{O}}^{-1} = 3$ as described by Kelliher et al. (1995), $R_{\text{c, cut, H}_2\text{O}}$ for a fully developed canopy can be approximated with $3 \cdot 10^{-4} \text{ s} \cdot \text{m}^{-1}$.

With β^* and β the actual canopy development stage (leaf area index LAI_{green} , LAI_{total}) is taken into account (cf Grünhage & Haenel 1997, Grünhage et al. 2000):

$$\beta = e^{-c_{\text{LAI}} \cdot LAI_{\text{total}}} \quad \text{and} \quad \beta^* = e^{-c_{\text{LAI}} \cdot LAI_{\text{green}}}$$

where c_{LAI} is the a vegetation type-specific attenuation coefficient (cf discussion in Grünhage et al. (2000).

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