PLATIN (PLant-ATmosphere INteraction) - a model of biosphere/atmosphere exchange of latent and sensible heat, trace gases and fine-particle constituents

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Abstract

The exchange of energy and matter between phytosphere and near-surface atmosphere is a complex process controlled by a number of influence factors. Modelling has not only to consider the state of the air above and within the plant canopy (temperature, humidity, flow velocity, gas or particle concentration in the air) and the air's transport capability, but also several physical, physiological, and chemical properties of the vegetation (plant architecture, vertically varying capability to receive or emit energy and gases, water budget, chemical reactions).

The SVAT model PLATIN (PLant-ATmosphere-INteraction) presented here is, like numerous other SVAT models, based on the *big-leaf* concept in order to reduce modeling complexity. The *big-leaf* approach replaces the vertical resolution of sources and sinks within the plant stand (including the soil surface beneath) by the idea of a single *big leaf* with overall properties equivalent to those of the complete plant/soil-surface system. The core module of PLATIN is based on the canopy energy budget and calculates the exchange of sensible and latent heat between phytosphere and near-surface atmosphere. Coupled to this the vertical exchange of matter is quantified.

In order to improve the treatment of the influence of the vertical light distribution within the canopy as well as to provide an additional way to validate the model, PLATIN has been extended by a submodule to estimate the stomatal uptake of trace gases (e.g. ozone) by the two different categories of sunlit and shaded leaves. This is achieved by extending the *big-leaf* concept by subdividing the *big-leaf* into a sunlit and a shaded fraction. One of the results obtained by this submodule is the stomatal conductance for sunlit leaves normalized by the leaf area index. This stomatal conductance represents an interface to measurements of trace gas exchange on leaf level.

Keywords: biosphere/atmosphere exchange, big leaf approach, latent and sensible heat, trace gas, fine particle, modelling

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Zusammenfassung

PLATIN (PLant-ATmosphere INteraction) - ein Modell zur Bestimmung des Austausches von latenter und fühlbarer Wärme, Spurengasen und Schwebstaubinhaltstoffen zwischen bodennaher Atmosphäre und Phytosphäre

Der Austausch von Energie und Luftbeimengungen zwischen Phytosphäre und bodennaher Atmosphäre wird durch eine Vielzahl von Faktoren bestimmt. Eine Modellierung muss den Zustand der Luft oberhalb und innerhalb des Pflanzenbestandes und ihr Transportvermögen sowie eine Reihe von physikalischen, physiologischen und chemischen Eigenschaften der Vegetation berücksichtigen.

Das hier beschriebene SVAT-Modell PLATIN (PLant-ATmosphere-INteraction) beruht wie viele andere SVAT-Modelle auf dem *big-leaf*-Konzept. Dieses ersetzt die vertikale Differenzierung des Bestandes bezüglich der Quellen- und Senkenverteilung sowie der Transportmechanismen durch die Modellvorstellung eines einzigen „großen Blattes", dessen Eigenschaften den des gesamten Bestandes und des darunter liegenden Bodens entsprechen. Das Kernmodul von PLATIN berechnet den Austausch von fühlbarer und latenter Wärme zwischen Phytosphäre und bodennaher Atmosphäre unter Berücksichtigung des Energiehaushaltes des Pflanzenbestandes. In Wechselwirkung damit wird der vertikale Austausch von Luftbeimengungen quantifiziert.

Zur Verbesserung der Beschreibung des Einflusses der Lichtverteilung im Pflanzenbestand auf den Energie- und Stoffaustausch sowie zur Erweiterung der Möglichkeit zur Validierung wurde PLATIN um ein Sub-Modul ergänzt, das die Abschätzung der für sonnenbeschienene und abgeschattete Blätter unterschiedlichen stomatären Aufnahme von Spurengasen (z. B. Ozon) erlaubt. Hierfür wurde das *big-leaf*-Konzept mit einer Aufteilung des Pflanzenbestandes in besonnte und abgeschattete Anteile unterlegt. Daraus ergibt sich u. A. der auf eine Blattflächeneinheit normiert stomatäre Leitwert für besonnte Bestandespartien, der als direkte Schnittstelle zu Messungen des Spurengasaustausches auf Blattebene dienen kann.

Schlüsselworte: Austausch zwischen Biosphäre und bodennnaher Atmosphäre, big-leaf-Konzept, latente und fühlbare Wärme, Spurengase, Schwebstaubinhaltsstoffe, Modellierung

1 Introduction

Classical air pollution problems caused by very high concentrations of sulphur dioxide (SO_2) and London-type smog have decreased to acceptable levels in most parts of Europe. Nevertheless, there are still a number of potential ecological threats such as acidification and eutrophication of terrestrial and aquatic ecosystems, increased tropospheric ozone (O_3) concentrations and stratospheric ozone depletion, as well as greenhouse effects and human health problems caused by suspended particulate matter. Reactive atmospheric nitrogen species contribute to all these phenomena (cf. Dämmgen and Sutton, 2001; Erisman et al., 1998; Graedel and Crutzen, 1995).

During the 1970s it was recognised that transboundary air pollution has ecological as well as economic consequences e.g. for the forest and fish industries (UNECE, 2004). As a consequence, the countries of the UNECE (UN Economic Commission for Europe) developed a legal, organisational and scientific framework to deal with these problems. In 1979 the UNECE Convention on Long-Range Transboundary Air Pollution (LRTAP) was signed; it entered into force in 1983 (UNECE, 1979). In this context, the so called multi-pollutant multi-effect or Gothenburg protocol (UNECE, 1999) requires the quantification - or at least estimation - of fluxes of atmospheric reactive nitrogen and sulphur species as well as of ozone and particulate matter between the ecosystems under consideration and the atmosphere near the ground.

Ideally, fluxes should be measured continuously and in an area-covering manner. Of course, this is not feasible. Another problem is that for some air constituents the toxicologically relevant flux is only a part of the total flux. Therefore modelling of fluxes has become a useful tool. Measurement and modelling techniques separate into two main categories, according to the type of species under consideration and their deposition properties: gases and fine particles (0.002 µm < d_p < 2.5 µm, with d_p the aerodynamic diameter of particles) on the one hand and coarse particles ($d_p \geq$ 2.5 µm; Finlayson-Pitts and Pitts, 1986; Gallagher et al., 1997) on the other hand. 'Particles' in this context may be solid or liquid (including rain and cloud drops). In general, fluxes of inert gases or fine particles are governed by turbulent diffusion in the atmosphere, by molecular diffusion within the (quasi-laminar) boundary layer adjacent to plant and soil surfaces, and by chemical reactions at the surfaces. In case of reactive gases or fine particles, also chemical reactions in the air have to be taken into account. Fluxes of very large particles (d_p > 100 µm) are predominantly controlled by gravitational forces whereas fluxes of smaller particles (d_p < 100 µm) are a result of diffusive, gravitational and inertial effects (interception, including impaction and turbulent inertial effects), depending on particle size and density (cf. Slinn 1982, Grünhage et al. 1998). Overviews on monitoring and modelling of biosphere/atmosphere exchange of gases, fine and coarse particles as well as of wet deposition are given in Dämmgen et al. (1997), Grünhage et al. (2000), Krupa (2002), Dämmgen et al. (2005) and Erisman et al. (2005).

Modelling of biosphere/atmosphere exchange of gases and fine-particle constituents also depends on the resolution in space and time needed. Whereas local scale Soil-Vegetation-Atmosphere-Transfer (SVAT) models rely on the detailed description of the canopy energy balance of the ecosystem under consideration, regional or national scale models make use of simplifying and integrating assumptions and make use of typical deposition velocities rather than site-specific driving forces (cf. Erisman et al., 2005). At the European scale, flux estimates are based on large-scale modelled meteorology and concentration fields; ecosystem properties are replaced by those of a vegetation type (cf. Grünhage et al., 2004). Necessarily, the complexity of details and processes considered in flux modelling decreases with increasing scale in space in time. This means that those generalized approaches must be carefully calibrated by well validated local scale models.

SVAT models serve two purposes: (1) In agricultural and forest meteorology they are used to calculate water dynamics e.g. to predict irrigation; (2) in the context of the ecotoxicology of air constituents they are needed to derive dose-response relationships (cf. Dämmgen and Grünhage, 1998).

Any perturbation on plant or ecosystem level is a function of the absorbed dose, i.e. the integral of the absorbed flux density $F_{c,\ absorbed}$ over time (cumulative flux density). In the context of acidification and eutrophication of terrestrial ecosystems, $F_{c,\ absorbed}$ is the overall input of acidifying or eutrophying species into the system as a whole ($F_{c,\ absorbed} = F_{c,\ total}$). On the other hand, for SO_2 or for O_3 (in particular as phytotoxic agents), $F_{c,\ absorbed}$ is only a part of the total flux: the total flux $F_{c,\ total}$ must then be partitioned into fluxes (1) absorbed by the plant through the stomata and the cuticle ($F_{c,\ stom\ \&\ cut}$), and (2) deposited on external plant surfaces and the soil ($F_{c,\ non\text{-}stomatal}$; combined non-stomatal deposition). Studies show that penetration through the cuticle can be neglected in comparison to stomatal uptake (cf. literature cited in Grünhage et al., 2000). For ammonia (NH_3) bi-directional fluxes have to be taken into account, because, dependent on the nitrogen status of the respective system, deposition or emission situations can occur.

Non-stomatal deposition of phytotoxic gases (O_3, SO_2) is toxicologically almost irrelevant under ambient conditions in Europe but nevertheless a considerable part of the total flux (Grünhage et al., 1998; Fowler et al., 2001; Gerosa et al., 2003, 2004). Modelling of stomatal behaviour is crucial for the establishment of dose-response relationships (cf. Dämmgen et al., 1997; Grünhage et al., 2004; Tuovinen et al., 2004). As illustrated by Grünhage et al. (2003), any parameterization of stomatal behaviour in SVAT models for this purpose has to be validated at least via measurements of canopy level water vapour exchange.

This paper, which is a contribution to the European BIAFLUX joint programme (Biosphere Atmosphere Exchange of Pollutants; http://www.accent-network.org), presents important new aspects of an extended version of the *big leaf* SVAT model PLATIN (PLant-ATmosphere INteraction) published by Grünhage and Haenel (1997) for the estimation of the exchange of latent and sensible heat, trace gases and fine-particle constituents between the plant/soil system and the atmosphere near the ground. Already the former PLATIN model had been published (in a simplified version) as an EXCEL version (named WINDEP for Worksheet-INtegrated Deposition Estimation Programme, cf. Grünhage and Haenel, 2000) in order to allow users to easily reflect model structure and equations and to adapt the model to their own requirements. The new PLATIN model will be available as 'PLATIN for Excel' via download from: http://www.uni-giessen.de/cms/ukl-en/PLATIN

PLATIN consists of several modules, as is illustrated in Figure 1.

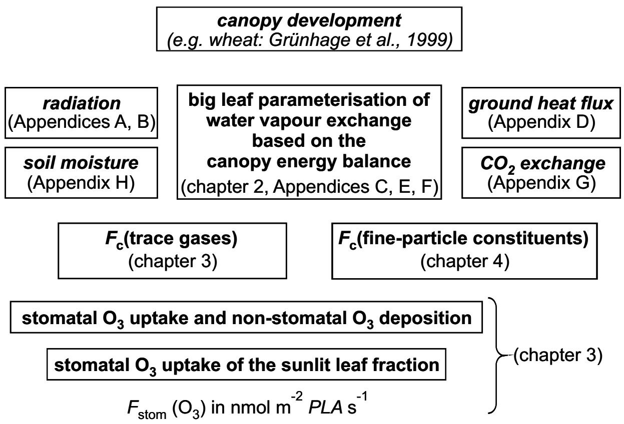

Figure 1:

Modular structure of the PLant-ATmosphere INteraction (PLATIN) model

The present paper restricts itself to the description of the updated versions of the core module, which solves the canopy energy balance (Chapter 2) and the module dealing with the biosphere/atmosphere exchange of trace gases (Chapter 3). Among other things, the processes described in these two chapters depend on the new radiation module, which is important not only for energy balance considerations but also to provide PLATIN with information to account for canopy development from sparse to dense canopy. Chapter 3 of this paper focuses on the partitioning of total atmosphere-canopy flux into stomatal uptake of the sunlit and shaded leaf fraction of the canopy, which provides an interface to measurements on gas exchange on leaf level.

Except for canopy development modelling (which is treated elsewhere, e.g. for wheat in Grünhage et al., 1999), all other modules and processes indicated in Figure 1 are presented in a full model description in the special issue 319 of this journal (Grünhage and Haenel, 2008). This special issue also comprises the modules quantifying biosphere/atmosphere exchange of O_3, SO_2, NH_3, nitric oxide (NO), nitrogen dioxide (NO_2), nitrous acid (HNO_2) and nitric acid (HNO_3) as well as of ammonium (NH_4), nitrate (NO_3) and sulphate (SO_4) in fine particles. The full model description is completed by a list of data needed to calibrate and run PLATIN.

A comparison of measured and modelled flux densities of trace gases will be published elsewhere.

2 Biosphere/atmosphere exchange of latent and sensible heat

Vertical flux densities of energy are part of the typical entities governing structure and function of ecotopes (Dämmgen et al., 1997). Energy fluxes must be known to establish the biosphere's energy budget, which, along with the budget of matter, is essential for the understanding of ecosystem behaviour. However, while energy fluxes between the near-surface atmosphere and the biosphere can be measured, it is far more difficult to derive the energy balance of the biosphere from measurements. Thus, a common approach has become to model the biosphere system. In general, this modelling is one-dimensional, i.e. based on the assumption that all properties be functions of height z only. A short description of model scheme principles is given in Grünhage et al. (2000).

The one-dimensional PLant-ATmosphere INteraction model (PLATIN) is based on the *big leaf* concept which assumes that the vertical distribution of sources and/or sinks of a scalar (sensible heat, latent heat, ozone or another trace gas) can be represented by a single source and/or sink at the *big leaf* surface located at the conceptual height $z = d + z_{0scalar}$. It is convenient to assume that the roughness length for gaseous species e.g. z_{0H2O} equals the roughness length for sensible heat z_{0h}.

The core module of PLATIN deals with the solution of the canopy energy balance defined for the *big leaf* surface by

$$R_{net} \quad H + \lambda E + G \tag{1}$$

with
R_{net} net radiation balance [$W \cdot m^{-2}$]
H turbulent vertical flux density of sensible heat [$W \cdot m^{-2}$]
λE turbulent vertical flux density of latent heat [$W \cdot m^{-2}$]
G ground heat flux density [$W \cdot m^{-2}$]

Net radiation balance R_{net} [$W \cdot m^{-2}$] is preferably provided by measurements. Otherwise it can be estimated in parts or completely as discussed in Appendix A (cf. Grünhage and Haenel, 2008). The same holds for the ground heat flux density G [$W \cdot m^{-2}$] the approximation of which is described in Appendix D (cf. Grünhage and Haenel, 2008).

The calculation of the fluxes of sensible and latent heat, H and λE, (and of gas fluxes) is based on Ohm's law making use of a resistance network as illustrated in Figure 2.

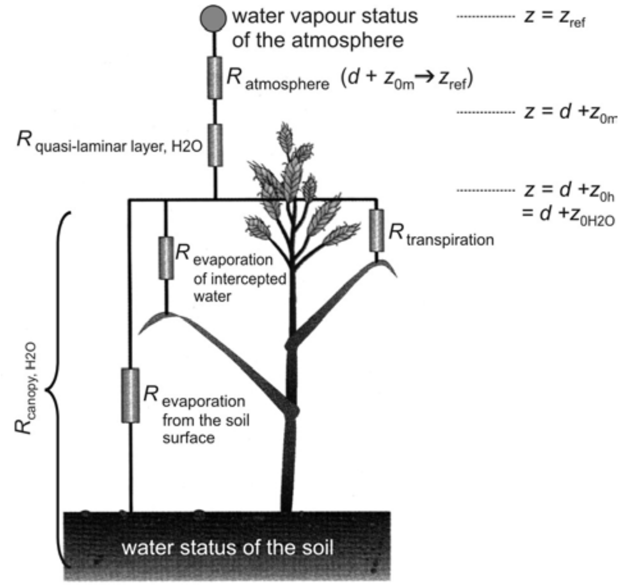

Figure 2:

A resistance analogue for water vapour (modified from PORG, 1997)

There are three major resistance components (which will be discussed in more detail in subsequent chapters):

(1) the atmospheric resistance $R_{atmosphere}(d+z_{0m}, z_{ref})$ [$s \cdot m^{-1}$], representing the atmospheric transport properties between the conceptual height of the momentum sink near the *big leaf* surface $z = d + z_{0m}$ and a reference height z_{ref} above the canopy, where d is the displacement height and z_{0m} is the roughness length for momentum. (Atmospheric turbulence is driven both by mechanical and thermal forces. The latter intensifies the mechanically induced turbulence within periods of atmospheric heating during daylight hours (unstable atmospheric stratification), whereas it weakens mechanically induced turbulence during cooling periods especially in the night (stable atmospheric stratification). Atmospheric transport by molecular diffusion can be neglected under turbulent conditions. Therefore $R_{atmosphere}$ can be approximated by $R_{atmosphere} \cong R_{ah}$, where R_{ah} is the turbulent atmospheric resistance for sensible heat transfer including a correction for non-neutral atmospheric stability conditions.);

(2) the quasi-laminar layer resistance $R_{quasi\text{-}laminar\ layer}$ or R_b [$s \cdot m^{-1}$] between momentum sink height $z = d + z_{0m}$ and the conceptual sink/source height for sensible heat and trace gases (including H_2O) at $z = d + z_{0h}$; and

(3) the bulk canopy or surface resistance R_{canopy} or R_c [$s \cdot m^{-1}$], describing the influence of the plant/soil system on the vertical exchange of trace gases (including H_2O).

2.1 Turbulent atmospheric resistance

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

$$R_{ah}(z_1, z_2) = \frac{\ln\left(\frac{z_2 - d}{z_1 - d}\right) - \Psi_h\left(\frac{z_2 - d}{L}\right) + \Psi_h\left(\frac{z_1 - d}{L}\right)}{\kappa \cdot u_*} \qquad (2)$$

with z_1 e.g. momentum sink height $d+z_{0m}$ [m]

z_2 e.g. reference height $z_{ref,\,T}$ for actual air temperature t_a [°C] or reference height $z_{ref,\,A}$ for a trace gas or fine-particle constituent

and L Monin-Obukhov length [m]

- κ dimensionless von Kármán constant ($\kappa = 0.41$; cf. Dyer, 1974)

u_* friction velocity [$m \cdot s^{-1}$]

Ψ_h atmospheric stability function for sensible heat

For vegetation like wheat or forests the displacement height and the roughness length are usually approximated by $d = 0.67 \cdot h$ and $z_{0m} = 0.13 \cdot h$, respectively, with h the canopy height (Brutsaert, 1984). A parameterization of canopy height h for spring and winter wheat as a function of phenological development is given in Grünhage et al. (1999).

Calculation of energy balance time series for growing agricultural crops requires also the definition of the roughness length for bare agricultural soil. There is no unique value for all types of soils and their possible surface states. Table 2.2 in Oke (1978) gives a range of 0.001 – 0.01 m (along with displacement height $d = 0$ m).

The roughness length for sensible heat z_{0h} is smaller than z_{0m}. According to Figure 4.24 in Brutsaert (1984) a typical value of $\ln(z_{0m}/z_{0h})$ is 2 for grass and corn so that we assume a value of 2 to be representative also for agricultural crops. For forests $\ln(z_{0h}/z_{0m}) = 1$ seems to be an acceptable value. Note that we use $\ln(z_{0m}/z_{0h}) = 2$ also for bare soil.

Eq. (2) is based on Monin-Obukhov theory. Strictly, this theory is valid only above the roughness sublayer which may range up to 2 or 2.5 times the vegetation height over tall and very rough canopies. For discussion see e.g. Cellier and Brunet (1992). Except for maize it seems tolerable to use eq. (2) for agricultural crops without further correction, because the height of the roughness sublayer is generally smaller than the typical agrometeorological reference height of 2 m (for e.g. air temperature measurements). Over forests, however, most often the reference height is located within or at least at the upper boundary of the roughness sublayer. For this case, PLATIN makes use of a modified resistance equation (see e.g. Sellers et al., 1986):

$$R_{\mathrm{ah,\,forests}}(z_1, z_2) = \frac{R_{\mathrm{ah}}(z_1, z_2)}{2} \tag{3}$$

The friction velocity is given by:

$$u_* = \frac{\kappa \cdot u(z_{\mathrm{ref}})}{\ln\left(\frac{z_{\mathrm{ref,u}} - d}{z_{0\mathrm{m}}}\right) - \Psi_{\mathrm{m}}\left(\frac{z_{\mathrm{ref,u}} - d}{L}\right) + \Psi_{\mathrm{m}}\left(\frac{z_{0\mathrm{m}}}{L}\right)} \tag{4}$$

with $u(z_{ref})$ horizontal wind velocity at reference height $z_{ref,\,u}$ [$m \cdot s^{-1}$]

Ψ_m atmospheric stability function for momentum

The Monin-Obukhov length L (Monin and Obukhov, 1954) is defined as:

$$\begin{aligned} L &= -\rho_{\mathrm{moist\,air}} \cdot c_{\mathrm{p,\,moist\,air}} \cdot \frac{\overline{\overline{\theta}} \cdot u_*^3}{\kappa \cdot g \cdot H} \\ &\approx -\rho_{\mathrm{moist\,air}} \cdot c_{\mathrm{p,\,moist\,air}} \cdot \frac{\theta(z_{\mathrm{ref}}) \cdot u_*^3}{\kappa \cdot g \cdot H} \end{aligned} \tag{5}$$

with $\overline{\overline{\theta}}$ average potential temperature of the air layer under consideration [K]

g gravitational acceleration (g = 9.81 $m \cdot s^{-2}$)

$\rho_{moist\ air}$ density of moist air [$kg \cdot m^{-3}$] at absolute temperature T [$T = t_a + 273.15$ K] with t_a the actual air temperature (°C) measured at reference height $z_{ref,\,T}$ (see Appendix F, eq. (F7) in Grünhage and Haenel (2008))

$c_{p,\ moist\ air}$ specific heat of moist air at a constant pressure [$m^2 \cdot s^{-2} \cdot K^{-1}$] (see Appendix F, eq. (F9) in Grünhage and Haenel (2008))

It is sufficient to approximate the layer-average potential temperature by the potential temperature at reference height, $\theta(z_{ref})$, which is estimated from the actual air temperature $T(z_{ref})$ according to (cf. Stull, 1988):

$$\theta(z_{\mathrm{ref}}) = T(z_{\mathrm{ref}}) + (z_{\mathrm{ref}} \cdot \Gamma_{\mathrm{d}}) \tag{6}$$

with Γ_d dry adiabatic lapse rate [$\Gamma_d = -9.76\ K \cdot km^{-1}$]

The atmospheric stability functions for momentum Ψ_m and sensible heat Ψ_h are given in Appendix C in Grünhage and Haenel (2008).

2.2 Quasi-laminar layer resistance for sensible heat and water vapour

The quasi-laminar layer resistance for water vapour $R_{b,\,H2O}$ is estimated according to the 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):

$$\begin{aligned} R_{\mathrm{b,\,H2O}} &= R_{\mathrm{b,\,heat}} \cdot \left(\frac{\mathrm{Sc_{H2O}}}{\mathrm{Pr}}\right)^{\frac{2}{3}} \\ &= \frac{\ln\left(\frac{z_{0\mathrm{m}}}{z_{0\mathrm{h}}}\right) - \Psi_{\mathrm{h}}\left(\frac{z_{0\mathrm{m}}}{L}\right) + \Psi_{\mathrm{h}}\left(\frac{z_{0\mathrm{h}}}{L}\right)}{\kappa \cdot u_*} \cdot \left(\frac{\mathrm{Sc_{H2O}}}{\mathrm{Pr}}\right)^{\frac{2}{3}} \end{aligned} \tag{7}$$

with $R_{b,\,heat}$ quasi-laminar layer resistance for sensible heat

Sc_{H2O} Schmidt number for water vapour (the ratio of the kinematic viscosity of dry air and the molecular diffusivity of the respective trace gas)

Pr Prandtl number (the ratio of the kinematic viscosity of dry air and the molecular diffusivity of heat)

For water vapour, $(Sc/Pr)^{2/3}$ is 0.90 (cf. Table 2 in Grünhage and Haenel (2008)).

2.3 Bulk canopy resistance for water vapour

The bulk canopy resistance $R_{c,\,H2O}$ is a composite resistance describing stomatal and cuticular transpiration and evaporation. $R_{c,\,H2O}$ can be approximated by a weighted combination of soil resistance R_{soil}, bulk stomatal resistance $R_{c,\,stom}$ and bulk cuticle resistance $R_{c,\,cut}$ known for a fully developed canopy (without senescent leaves) under optimum conditions for maximal transpiration. The weights depend on the actual canopy development stage taking into account the transition from a dense canopy (one-sided leaf area index $LAI = LAI_{max}$ [$m^2 \cdot m^{-2}$]) to a sparse canopy:

$$\frac{1}{R_{\mathrm{c,H2O}}} = \left[(1 - \beta^*) \cdot \left(\frac{1}{R_{\mathrm{c,\,stom,\,H2O}}} + \frac{1}{R_{\mathrm{c,\,cut,\,H2O}}}\right) + \frac{\beta}{R_{\mathrm{soil,\,H2O}}}\right] \tag{8}$$

In order to keep as close as possible to the single-leaf representation of the biosphere in PLATIN, eq. (8) makes use of a weighted R_{soil} (cf. Grünhage et al., 2000) instead of an additional in-canopy scalar transport resistance, where the coefficient β must be unity for bare soil and approaches zero for a fully developed dense canopy. If all leaves could contribute to the energy and water exchange between canopy and atmosphere, the weight of the reciprocal sum of $R_{c,\,stom,\,H2O}$ and bulk cuticle resistance $R_{c,\,cut,\,H2O}$ would be (1 – β). However, as only non-senescent leaves are relevant, a modified weight (1 – β*) is introduced.

Grünhage and Haenel (1997) presented a plausible ad-hoc approach to estimate (1 – β*) and β. It was based on the fact that the vertical distribution of incoming radiation energy within the canopy is one of the main limiting factors for the total canopy energy and water budget. Grünhage and Haenel (1997) simply assumed the available radiation energy to decrease exponentially with increasing distance from the top of the canopy and introduced a vegetation-type specific coefficient c_{LAI} to describe the attenuation effect. They defined:

$$1-\beta^* = 1 - e^{-c_{LAI} \cdot LAI_{non\text{-}senescent}} \tag{9}$$

and

$$\beta = e^{-c_{LAI} \cdot LAI_{total}} \tag{10}$$

The expression (1 – β*) may be interpreted as the fraction of radiation intercepted by non-senescent (green) leaves which is given by $LAI_{non\text{-}senescent}$ (= one-sided leaf area index of non-senescent leaves; = projected leaf area *PLA* according to UNECE (2004, 2007)). The weight β estimates the fraction of radiation reaching the ground depending on one-sided total leaf area index LAI_{total} (= non-senescent plus senescent leaves). For spring and winter wheat a parameterization to calculate LAI_{total} and $LAI_{non\text{-}senescent}$ as a function of phenological stages is given in Grünhage et al. (1999).

As radiation distribution within the canopy is (at least) a function of the solar elevation angle ϕ and of leaf angle distribution, the same should hold for c_{LAI}. However, Grünhage and Haenel (1997) made successfully use of a constant value for c_{LAI}, only dependent on vegetation type. This constant value may be interpreted as an effective mean value. Coefficients averaged over all solar elevations are summarized for different vegetation types e.g. in Monteith and Unsworth (1990). For most vegetation types c_{LAI} is in the range of 0.3 to 0.6 (Ross, 1981). This includes $c_{LAI} \approx 0.4$ for crops as described by Ritchie (1972) as well as 0.5 for spring wheat (Choudhury et al., 1987) and a maritime pine canopy (Granier and Lousteau, 1994). On the other hand, for canopies with predominantly horizontally arranged leaves (e.g. cabbage, clover) c_{LAI} approaches 1.8 as can be deduced from Monteith (1965).

PLATIN now incorporates a canopy radiation submodel (see Appendix B in Grünhage and Haenel (2008)), which allows to calculate the vertical radiation energy distribution and related entities within the canopy. Therefore, the parameterizations of the weights (1 – β*) and β, i.e. eqs. (9) and (10) had to be reconsidered in so far, as it could be possible and reasonable to replace the externally given coefficient c_{LAI} by an entity calculated by the canopy radiation model. However, as radiation distribution is only a predictor for the weights (1 – β*) and β, care had to be taken when adopting results from the new radiation model.

The canopy radiation model allows to calculate an attenuation coefficient k_b similar to c_{LAI}, but dependent on solar height:

$$k_b = \frac{k_{b,90°}}{\sin\phi} \tag{11}$$

with $k_{b,90°}$ k_b value for solar elevations of 90°

According to eq. (13) in Sellers (1985), $k_{b,90°}$ is 0.5 for spherically arranged leaves, 0.27 for vertical and 1.23 for horizontal leaves. However, there is no use to replace c_{LAI} in (10) by k_b according to (11), because (11) is valid only for daylight hours while the weight β is needed also during night. Therefore it was decided to replace c_{LAI} in the calculation of β by $k_{b,max}$ rather than k_b:

$$\beta = e^{-k_{b,max} \cdot SAI} \tag{12}$$

with *SAI* total surface area of the vegetation [$m^2 \cdot m^{-2}$]

and

$$k_{b,max} = \frac{k_{b,90°}}{\sin\phi_{max}} \tag{13}$$

where ϕ_{max} solar elevation at 12 h TST (true solar time)

A minor adjustment is the formal replacement of LAI_{total} in eq. (10) by *SAI*, the total surface area of the vegetation. *SAI* is set equal to LAI_{total} + 1 for forests (Tuovinen et al., 2004) and to LAI_{total} for short vegetation (crops, grassland).

The advantage of eq. (12) over (10) is that the annual course of solar height is now accounted for. The switch from c_{LAI} to $k_{b,max}$ does not change the results significantly.

Stomatal behaviour of the plants strongly depends on irradiance absorption. This means that, when simulating stomata-related processes, the fraction of radiation intercepted by the non-senescent leaves should be taken into account explicitly within the parameterization of (1 – β*). With entities calculated by the canopy radiation submodel, (1 – β*) has been redefined for the current PLATIN version as follows:

$$1-\beta^{*} = \frac{I_{\mathrm{c,\,sunlit}} + I_{\mathrm{c,\,shaded}}}{PAR} \qquad (14)$$

with $I_{\mathrm{c,\,sunlit}}$ irradiance absorbed by the sunlit fraction of non-senescent leaves of the canopy [µmol·m^{-2}·s^{-1}]
$I_{\mathrm{c,\,shaded}}$ irradiance absorbed by the shaded fraction of non-senescent leaves of the canopy [µmol·m^{-2}·s^{-1}]
PAR photosynthetically active radiation measured above the canopy [µmol·m^{-2}·s^{-1}]

Eq. (14) is needed as base for other calculations like the fractioning of the total ozone stomatal uptake into stomatal uptake by the sunlit and shaded leaf fraction of the canopy during daylight hours. Clearly, eq. (14) is meaningless during night time. But as the nocturnal stomatal uptake is of inferior importance, β* can then simply be replaced by β according to eq. (12), but calculated with the non-senescent *LAI*.

Soil resistance for water vapour

$R_{\mathrm{soil,\,H2O}}$ is a complex function of vertical soil water distribution. An important feature of evaporation from bare soil is a fast reduction due to the drying of the uppermost soil layer after rainfall. Therefore, $R_{\mathrm{soil,\,H2O}}$ is parameterized in the following manner:

(a) For a fully wet soil, $R_{\mathrm{soil,\,H2O}}$ equals $R_{\mathrm{soil,\,H2O,\,min}}$ (= 100 s·m^{-1}).

(b) For daylight hours (i.e. time intervals with global radiation $S_t \geq 50$ W·m^{-2}), $R_{\mathrm{soil,\,H2O}}$ is increased by a given fraction of $R_{\mathrm{soil,\,H2O,\,min}}$ if there is no precipitation:

$$(R_{\mathrm{soil,H2O}})_{\mathrm{n}} = (R_{\mathrm{soil,\,H2O}})_{\mathrm{n-1}} + \mathrm{RX}\cdot R_{\mathrm{soil,\,H2O,\,min}} \qquad (15)$$

where n is the index of the data set under consideration and n−1 denotes the previous data set. RX is chosen to be 0.05 for half-hourly data sets and 0.1 for hourly data sets. $R_{\mathrm{soil,\,H2O}}$ is bound by the upper limit of 4000 s·m^{-1}, the choice of which is based on the results of Daamen and Simmonds (1996).

(c) At night $R_{\mathrm{soil,\,H2O}}$ stays constant at the value calculated for the last late-afternoon daylight hour, i.e. $(R_{\mathrm{soil,\,H2O}})_{\mathrm{n}} = (R_{\mathrm{soil,\,H2O}})_{\mathrm{n-1}}$.

(d) At any time interval with precipitation not reaching the ground, $R_{\mathrm{soil,\,H2O}}$ stays constant at the value calculated before, i.e. $(R_{\mathrm{soil,\,H2O}})_{\mathrm{n}} = (R_{\mathrm{soil,\,H2O}})_{\mathrm{n-1}}$.

(e) At any time interval with precipitation and/or dew reaching the ground, $R_{\mathrm{soil,\,H2O}}$ is decreased by a fraction RY = $a_{\mathrm{soil}} \cdot W_{\mathrm{in}}$ of $R_{\mathrm{soil,\,H2O,\,min}}$:

$$(R_{\mathrm{soil,H2O}})_{\mathrm{n}} = (R_{\mathrm{soil,\,H2O}})_{\mathrm{n-1}} - a_{\mathrm{soil}}\cdot W_{\mathrm{in}}\cdot R_{\mathrm{soil,\,H2O,\,min}} \qquad (16)$$

with W_{in} amount of precipitation and/or dew reaching the ground (water input) [mm]

For short vegetation (crops, grassland), the empirical constant a_{soil} is set to 10 mm^{-1} for half-hourly and 20 mm^{-1} for hourly data sets.

The amount of precipitation and/or dew reaching the ground depends on the interception reservoir capacity of the canopy. In PLATIN, this capacity INT_{max} [mm] is assumed to be proportional to total *LAI*:

$$INT_{\mathrm{max}} = b_{\mathrm{INT}}\cdot LAI_{\mathrm{total}} \qquad (17)$$

The constant b_{INT} is chosen as 0.2 mm according to Dickinson (1984), neglecting the fact that leaves become able to intercept more precipitation during senescence (cf. Braden, 1995).

The interception reservoir is filled by precipitation *Precip* and dew and depleted by evaporation. Dew formation and depletion of the reservoir is estimated due to potential evapotranspiration rate E_{pot} [mm] applying the Penman-Monteith approach (see Chapter 2.4) with $R_{\mathrm{c,\,H2O}}$ = 0 s·m^{-1} assuming neutral atmospheric stratification. The interception *INT* [mm] is parameterized according to

$$INT_{\mathrm{n}} = Precip_{\mathrm{n}} + INT_{\mathrm{n-1}} - E_{\mathrm{pot,\,n}} \qquad (18)$$

with $0 \leq INT_{\mathrm{n}} \leq INT_{\mathrm{max}}$. The precipitation and dew reaching the ground W_{in} is than given by:

$$W_{\mathrm{in,\,n}} = Precip_{\mathrm{n}} + (INT_{\mathrm{n-1}} - E_{\mathrm{pot,\,n}}) - INT_{\mathrm{max}} \qquad (19)$$

with $W_{\mathrm{in}} \geq 0$ mm.

For forests, the coefficients RX and a_{soil} have not yet been properly adjusted. As a plausible working model, applicable to forests in Central Europe with generally non-drying soil, $R_{\mathrm{soil,\,H2O}}$ can be set to $R_{\mathrm{soil,\,H2O,\,min}}$.

Note: $R_{\mathrm{c,\,H2O}}$ is set to zero if the interception reservoir is not empty. Comparisons of modelled evapotranspiration rates with measured fluxes show that setting $R_{\mathrm{c,\,H2O}}$ to zero overestimates the real fluxes. Therefore, interception is not taken into account in latent heat flux modelling at present (see Chapter 2.4).

Bulk cuticle resistance for water vapour

Investigations of cuticular permeability of water vapour and other trace gases show that penetration through the cuticle can be neglected in comparison to stomatal exchange (Kerstiens and Lendzian, 1989a, b; Lendzian and Kerstiens, 1991; Kerstiens et al., 1992). According to the aforementioned authors $R_{cut, H2O}$ on leaf basis is $9 \cdot 10^4$ s·m^{-1} (cf. Table 3 in Grünhage and Haenel (2008)). According to Grünhage et al. (1999) resistances derived on leaf basis are upscaled to canopy level taking into account the PLATIN formulation of canopy architecture and radiation distribution within the canopy. Similar to the minimum value of the bulk stomatal resistance $R_{c, stom, min, H2O}$, which is representative for a fully developed canopy (without senescent leaves) under optimum conditions for maximal transpiration, upscaling from leaf to canopy level is performed applying $k_{b,max}$ at maximum solar elevation of the year (summer solstice):

$$R_{canopy} \quad R_{leaf, literature} \cdot \left(1 - e^{-k_{b,max, summer\ solstice} \cdot LAI_{leaf, literature}}\right) \tag{20}$$

Bulk stomatal resistance for water vapour

The gas transfer through the stomata is by molecular diffusion. An inverse dependence of stomatal resistance on molecular diffusivity is generally accepted. In PLATIN, the dependence of stomatal resistance on radiation, temperature and the water budgets of atmosphere and soil as well as on modifying influence of time of day, phenology, ozone and CO_2 is described according to the Jarvis-Stewart approach (Jarvis, 1976; Stewart, 1988):

$$R_{c, stom, H2O} = \left[\frac{1}{R_{c, stom, min, H2O}} \cdot f_1(S_t) \cdot f_2(t_a) \cdot f_{3/4}(VPD, SM) \cdot f_5(\mathrm{time}) \cdot f_6(\mathrm{PHEN}) \cdot f_7(\mathrm{O_3}) \cdot f_8(\mathrm{CO_2})\right]^{-1} \tag{21}$$

or

$$R_{c, stom, H2O} = \left[\frac{1}{R_{c, stom, min, H2O}} \cdot f_1(S_t) \cdot f_2(t_a) \cdot f_3(VPD) \cdot f_4(SM) \cdot f_5(\mathrm{time}) \cdot f_6(\mathrm{PHEN}) \cdot f_7(\mathrm{O_3}) \cdot f_8(\mathrm{CO_2})\right]^{-1} \tag{22}$$

where $R_{c, stom, min, H2O}$ represents the minimum value of the stomatal resistance for water vapour of the respective ecosystem. Functions $f_1(S_t)$, $f_2(t_a)$, $f_3(VPD)$ and $f_4(SM)$ account for the effects of solar radiation S_t [W·m^{-2}], air temperature t_a [°C], water vapour pressure deficit of the atmosphere *VPD* [hPa] and soil moisture *SM* [m^3·m^{-3}] on stomatal aperture ($0 \le f_i \le 1$). While eq. (22) is based on a multiplicative dependence of stomatal resistance on *VPD* and *SM* in PLATIN, a combined function $f_{3/4}(VPD, SM)$ is preferred for biological reasons. A combined function $f_{3/4}(VPD, SM)$ reflects the observation that increasing soil moisture deficits strongly influence stomatal closure due to *VPD*. It is recommended to use measured soil moisture content *SM* for $f_{3/4}(VPD, SM)$ or $f_4(SM)$. If no *SM* data are available they must be simulated by a soil water model, a simple one is described in Appendix H in Grünhage and Haenel (2008). With f_5(time) a time-dependent impact on stomatal resistance can be taken into account (cf. Körner, 1994). f_6(PHEN) and $f_7(O_3)$ represent the influence of phenology and ozone on stomatal resistance: both senescence due to natural ageing and premature senescence induced by ozone are limiting factors for stomatal aperture. The Jarvis-Stewart functions used are described in Appendix E in Grünhage and Haenel (2008). For $S_t = 0$, $R_{c, stom, H2O}$ is set to 20000 s·m^{-1}. Under ambient conditions with elevated CO_2 the influence of elevated CO_2 on stomatal aperture must be taken into account by an additional Jarvis-Stewart function $f_8(CO_2)$.

2.4 Latent and sensible heat flux densities

It is straightforward to formulate H and λE as analogs of Ohm's law and to use them to operate a SVAT model like PLATIN. However, for PLATIN another way has been chosen. Inserting the resulting resistance-based formula for H in eq. (1) and solving for λE yields the well-known Penman-Monteith equation (Monteith, 1965):

Once R_{net}, G, and λE are known (λE according to eq. (23)), their values are inserted into eq. (1) to obtain the sensible heat flux H as residual. This procedure exactly yields the same results as if both λE and H had been estimated by the simple Ohm's-law formulation. In any case the solution of the energy balance can be achieved only iteratively, because the real unknown in eq. (1) is the surface temperature T_s which is involved in a non-linear way in the set of equations described above to solve eq. (1). However, the method used in PLATIN offers the option to get rid of iterations by replacing eq. (24) by the slope of water vapour saturation pressure at reference-height air temperature (see eqs. (F5) or (F6) in Appendix F in Grünhage and Haenel (2008)). This is the way the Penman-Monteith equation is often used as a kind of stand-alone model to estimate evapotranspiration, because it yields results only slightly different from eq. (23), cf. discussion in McArthur (1990). Another advantage of the method used in PLATIN is that any kind of λE estimate can be entered instead of eq. (23). This may be of interest e.g. in the case that measured values of λE are available and shall be tested within the modelling frame, or that not all relevant data are available to use eq. (23) so that a less data-demanding approach must be taken to obtain λE. However, as far as not mentioned otherwise, PLATIN makes use only of eq. (23).

$$\lambda E = \frac{s_c \cdot (R_{net} - G) + \rho_{moist\,air} \cdot c_{p,\,moist\,air} \cdot \dfrac{VPD}{R_{ah}(d + z_{0m}, z_{ref,T}) + R_{b,\,heat}}}{s_c + \gamma \cdot \dfrac{R_{ah}(d + z_{0m}, z_{ref,T}) + R_{b,\,H2O} + R_{c,\,H2O}}{R_{ah}(d + z_{0m}, z_{ref,T}) + R_{b,\,heat}}} \tag{23}$$

with γ psychrometric constant (= 0.655 hPa·K^{-1})
VPD water vapour pressure deficit of the at mosphere [hPa] (see Appendix F, eq. (F1) in Grünhage and Haenel (2008))

and

$$s_c = \frac{e_{sat}(T_s) - e_{sat}(T(z_{ref}))}{T_s - T(z_{ref})} \tag{24}$$

with e_{sat} saturation water vapour pressure of the atmosphere [hPa] (see Appendix F, eqs. (F2) and (F3) in Grünhage and Haenel (2008))

and T_s absolute canopy surface temperature at conceptual height $z = d + z_{0h}$ [K]

$$\theta_s = \theta(z_{ref,T}) + \frac{H \cdot \left(R_{ah}(d + z_{0m}, z_{ref,T}) + R_{b,heat}\right)}{\rho_{moist\,air} \cdot c_{p,\,moist\,air}} \tag{25}$$

The surface temperature T_s is related to potential canopy surface temperature θ_s [K] by eq. (6). As eq. (25) is part of the set of model equations needed to solve iteratively the energy balance (eq. (1)), a starting value of θ_s is needed which is assigned the value of the air temperature at reference height minus 0.1 K.

2.5 Comparison of measured and modelled latent and sensible heat flux densities

At the Linden grassland site, friction velocity, latent heat, as well as sensible heat are measured using the eddy covariance method by means of a Solent R3 research ultrasonic anemometer (Gill Instruments Ltd, Hampshire, UK) in combination with a LI-7500 open path CO_2/H_2O gas analyzer (Li-COR Environmental, Lincoln, Nebraska, USA). To guarantee data sets of high accuracy several corrections and quality tests are applied (WPL correction, Schotanus/Liu correction, coordinate rotation, footprint analysis, test to check the fulfilment of stationarity and of well developed turbulence conditions; cf. Grünhage and Gerosa, 2008).

Model adjustment is based on data sets for which the energy balance residual is less then 30 W·m^{-2}. A descrip tion how to estimate displacement height d, roughness length for momentum z_{0m} and bulk canopy resistance for water vapour $R_{c,\,H2O}$ can be found in Appendices I and J in Grünhage and Haenel (2008).

Figure 3 clearly illustrates that PLATIN is able to simulate measured fluxes adequately.

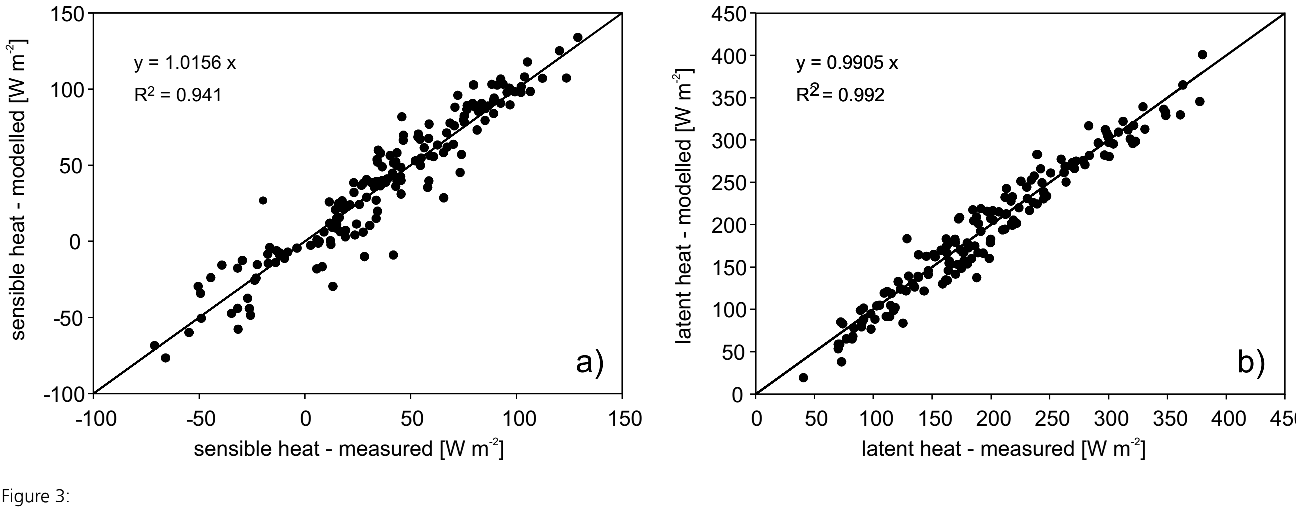

Figure 3:

Comparison of measured and modelled sensible heat (a) and latent heat (b) for daylight hours in June 2004 over a semi-natural grassland at the Linden field site (for details see Grünhage et al., 1996; Jäger et al., 2003)

3 Biosphere/atmosphere exchange of trace gases

The exchange of trace gas species A, F_c(A), between the phytosphere and the atmosphere near the surface can be modelled by:

$$F_{c}(\mathrm{A}) = \frac{\rho_{\mathrm{A}}(z_{\mathrm{ref,A}}) - \rho_{\mathrm{A}}(d + z_{0\mathrm{m}})}{R_{\mathrm{ah}}(d + z_{0\mathrm{m}}, z_{\mathrm{ref,A}})} \tag{26}$$

$$= \frac{\rho_{\mathrm{A}}(z_{\mathrm{ref,A}}) - \rho_{\mathrm{A}}(d + z_{0\mathrm{c}})}{R_{\mathrm{ah}}(d + z_{0\mathrm{m}}, z_{\mathrm{ref,A}}) + R_{\mathrm{b,A}}} \tag{27}$$

$$= \frac{\rho_{\mathrm{A}}(z_{\mathrm{ref,A}}) - \rho_{\mathrm{A,comp}}}{R_{\mathrm{ah}}(d + z_{0\mathrm{m}}, z_{\mathrm{ref,A}}) + R_{\mathrm{b,A}} + R_{\mathrm{c,A}}} \tag{28}$$

with
- F_c(A) total vertical atmosphere-canopy flux of trace gas A [$\mu g \cdot m^{-2} \cdot s^{-1}$]
- $\rho_A(z_{ref})$ measured concentration (potential) of trace gas A at height $z = z_{ref,\,A}$ [$\mu g \cdot m^{-3}$]
- $\rho_A(d+z_{0m})$ concentration of trace gas A at the conceptual height $z = d+z_{0m}$ [$\mu g \cdot m^{-3}$]
- $\rho_A(d+z_{0c})$ concentration of trace gas A at the conceptual height $z = d+z_{0c} = d+z_{0h}$ [$\mu g \cdot m^{-3}$]
- $\rho_{A,\,comp}$ canopy compensation concentration of trace gas A [$\mu g \cdot m^{-3}$]

Modelling details are given in Grünhage and Haenel (2008). In case of deposition, the resistance network allows to partition the total atmosphere-canopy flux $F_{c,\,total}$(A) into (1) fluxes absorbed by the plant through the stomata and the cuticle $F_{c,\,stom\,\&\,cut} = F_{c,\,stom}$(A) + $F_{c,\,cut}$(A), and (2) fluxes down to external plant surfaces $F_{c,\,ext}$(A) and the soil beneath the canopy F_{soil}(A). Studies show that penetration of gases through the cuticle $F_{c,\,cut}$(A) can be neglected in comparison to stomatal uptake $F_{c,\,stom}$(A) (cf. Chapter 2.3).

Combining $F_{c,\,ext}$ and F_{soil} to $F_{c,\,non\text{-}stomatal}$ and neglecting cuticular fluxes (i.e. approximating $F_{c,\,stom\,\&\,cut} \approx F_{c,\,stom}$) one obtains:

$$\begin{aligned} F_{\mathrm{c,total}}(\mathrm{A}) &= F_{\mathrm{c,stom\,\&\,cut}}(\mathrm{A}) + F_{\mathrm{c,ext}}(\mathrm{A}) + F_{\mathrm{soil}}(\mathrm{A}) \\ &\cong F_{\mathrm{c,stom}}(\mathrm{A}) + F_{\mathrm{c,non\text{-}stomatal}}(\mathrm{A}) \end{aligned} \tag{29}$$

The integral of $F_{c,\,stom\,\&\,cut} \cong F_{c,\,stomatal}$ over time t is the ***p**ollutant **a**bsorbed **d**ose*, *PAD*(A) [$\mu g \cdot m^{-2}$] (Fowler and Cape, 1982):

$$\begin{aligned} PAD(\mathrm{A}) &= \int_{t_1}^{t_2} \left| F_{\mathrm{c,stom\,\&\,cut}}(\mathrm{A}) \right| \cdot \mathrm{d}t \\ &\cong \int_{t_1}^{t_2} \left| F_{\mathrm{c,stom}}(\mathrm{A}) \right| \cdot \mathrm{d}t \end{aligned} \tag{30}$$

For O_3 the integral of $F_{c,\,stom\,\&\,cut} \cong F_{c,\,stom}$ over time t is called *accumulated stomatal flux of ozone, AF_{st}* (UNECE, 2004, 2007).

Applying concentration- or flux-based critical levels of O_3 (UNECE, 2004, 2007) or the maximum-permissible O_3 concentration concept (Grünhage et al., 2001) requires O_3 concentration measured at reference height above the canopy $\rho_{O3}(z_{ref})$ to be transformed to concentration at the upper surface of the laminar boundary layer of the uppermost sunlit leaves. According to the single-leaf concept, PLATIN disposes only of one single canopy-representative laminar boundary layer the surface of which is located at $d + z_{0m}$. The concentration at this height is calculated from:

$$\rho_{\mathrm{O3}}(d + z_{0\mathrm{m}}) = \rho_{\mathrm{O3}}(z_{\mathrm{ref,O3}}) + \left[F_{\mathrm{c,total}}(\mathrm{O_3}) \cdot R_{\mathrm{ah}}(d + z_{0\mathrm{m}}, z_{\mathrm{ref,O3}}) \right] \tag{31}$$

This is contrasted by the UNECE (2004, 2007) approach that the concentration at the upper surface of the laminar boundary layer of the sunlit upper canopy leaves be represented by the O_3 concentration at the top of the canopy $z = h$. Within the M-O framework, this concentration is given by:

$$\rho_{\mathrm{O3}}(h) = \rho_{\mathrm{O3}}(z_{\mathrm{ref,O3}}) + \left[F_{\mathrm{c,total}}(\mathrm{O_3}) \cdot R_{\mathrm{ah}}(h, z_{\mathrm{ref,O3}}) \right] \tag{32}$$

Besides the fact that the effective upper surface of all the laminar boundary layers existing within the canopy is probably represented better by $d + z_{0m}$ than by h, application of eq. (32) is prone to proper definition of h. Does h e.g. represent the maximum or the average height of canopy elements above ground? Due to numerous irregularities in canopy architecture as well as wind-driven bending of the upper parts of a canopy it may be difficult to find a robust estimate of canopy height. Therefore it seems worthwhile to demonstrate the differences in stomatal uptake calculated according to eq. (33; see below) with O_3 concentrations from eq. (32) for varying h. This is done exemplarily using the daylight-hour data sets from June 2004 at Linden. Except for h, all data needed to evaluate eq. (32) were determined by precedent PLATIN runs using the aforementioned data sets.

In order to obtain a reasonable measure for h, we inverted the usual relations between displacement height and roughness length for momentum on one hand and the canopy height on the other hand, which allows to calculate h from given displacement height d and roughness length z_{0m} by $h = (d + z_{0m}) \cdot 0.8^{-1}$ according to Brutsaert (1984). In order to reveal the influence of the differing heights in eqs. (31) and (32), the stomatal uptake as calculated with O_3 concentrations from eq. (32) has then been normalised by the one obtained with O_3 concentrations from eq. (31). As stomatal uptake is proportional to O_3 concentration, this ratio of stomatal uptake turns out to be identical to the ratio of the respective O_3 concentrations. This concentration ratio is displayed in Figure 4. Estimating stomatal uptake from h rather than $d + z_{0m}$ generally leads to overestimation of stomatal uptake which may not be negligible. This overestimation clearly depends on how much h differs from $d + z_{0m}$, which is demonstrated by varying h by plus 0.05 m and $d + z_{0m}$ by a factor of 1.1. (Diminishing h, on the other hand, would mean to approach $d + z_{0m}$ and therefore reduce overestimation. However, h should never reach $d + z_{0m}$, because then h would not be representative for canopy height any longer.)

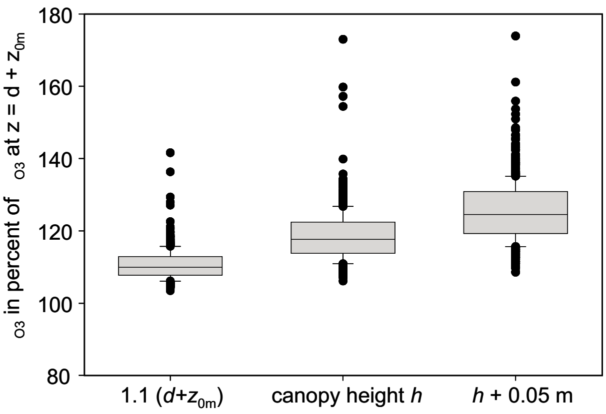

Figure 4:

Box-and-whisker plot of O_3 concentrations at $z = (d + z_{0m}) \cdot 1.1$, $z = h$ and $z = h + 0.05$ m in percent of O_3 concentrations at $z = d + z_{0m}$ during daylight hours in June 2004

Even if a stomatal uptake approach as given by UNECE (2004, 2007) could be combined with guidance how to properly estimate canopy height h, the problem still remains that h is not the best measure of the effective height of the canopy's laminar boundary layer. Therefore we recommend to calculate stomatal uptake by a model like PLATIN which is calibrated by a number of water and energy balance quantities and which, therefore, is much less sensitive to the correct estimation of canopy height.

Because stomatal uptake of O_3, $F_{c,\,stom}(O_3)$ is the toxicologically effective share of $F_{c,\,total}(O_3)$, flux-effect relationships should be based on that component which is given by:

$$F_{c,\,stom}(O_3) = -\frac{\rho_{O3}(z_{ref,\,O3})}{R_{ah} + R_{b,\,O3} + \frac{R_{c,\,stom+mes,\,O3}}{1-\beta^*} + \left([R_{ah} + R_{b,\,O3}] \cdot \frac{R_{c,\,stom+mes,\,O3}}{1-\beta^*} \cdot \left[\frac{1-\beta^*}{R_{c,\,cut,\,O3}} + \frac{1-\beta}{R_{c,\,ext,\,O3}} + \frac{\beta}{R_{soil,\,O3}} \right] \right)} \tag{33}$$

with $R_{ah} = R_{ah}(d + z_{0m}, z_{ref,\,O3})$

$$R_{c,\,stom+mes,\,O3} = R_{c,\,stom,\,O3} + R_{c,\,mes,\,O3} \tag{34}$$

$F_{c,\,stom}(O_3)$ can further be subdivided into the flux entering the compartment of sunlit leaves, $F_{c,\,stom,\,sunlit}(O_3)$, and the flux taken up by the shaded-leaves compartment, $F_{c,\,stom,\,shaded}(O_3)$:

$$F_{c,\,stom}(O_3) = F_{c,\,stom,\,sunlit}(O_3) + F_{c,\,stom,\,shaded}(O_3) \tag{35}$$

The estimation of $F_{c,\,stom,\,sunlit}(O_3)$ and $F_{c,\,stom,\,shaded}(O_3)$ is controlled by the O_3 bulk resistances assigned to the two compartments and their relation to the bulk canopy resistance $R^*_{c,\,stom,\,O3}$. The latter is proportional to the H_2O bulk canopy resistance $R^*_{c,\,stom,\,H2O}$, cf. eq. (37 in Grünhage and Haenel, 2008):

$$R^*_{c,\,stom,\,O3} = R^*_{c,\,stom,\,H2O} \cdot \frac{D_{H2O}}{D_{O3}} \tag{36}$$

$R^*_{c,\,stom,\,H2O}$ is obtained from

$$R^*_{c,\,stom,\,H2O} = \frac{R_{c,\,stom,\,H2O}}{1-\beta^*} \tag{37}$$

where $R_{c,\,stom,\,H2O}$ is given by eqs. (21) or (22) as the bulk resistance one obtains under neglection of the vertical distribution of within-canopy radiation extinction. In eq. (37), this extinction is accounted for by the correction term $1 - \beta^*$ (eq. (14)).

Similarly the resistances for the two compartments "sunlit leaves" and "shaded leaves", are defined by

$$R^*_{c,\,stom,\,sunlit,\,O3} = \frac{R_{c,\,stom,\,H2O}}{1-\beta^*_{sunlit}} \cdot \frac{D_{H2O}}{D_{O3}} \tag{38}$$

and

$$R^*_{c,\,stom,\,shaded,\,O3} = \frac{R_{c,\,stom,\,H2O}}{1-\beta^*_{shaded}} \cdot \frac{D_{H2O}}{D_{O3}} \tag{39}$$

where $1 - \beta^*_x$ (with x = sunlit, shaded) is given by (cf. Eq. (14)):

$$1-\beta^*_x = \frac{I_{c,\,x}}{PAR} \tag{40}$$

As the O_3 concentration within the plant can be assumed to be zero, the relations of fluxes are simply given by the inverse ratio of the resistances involved which turns out to be a function of β^*_x and β^*_{sunlit} or β^*_{shaded}, respectively:

$$\frac{F_{\mathrm{c,\,stom,\,sunlit}}(\mathrm{O_3})}{F_{\mathrm{c,\,stom}}(\mathrm{O_3})} = \frac{R^*_{\mathrm{c,\,stom,\,O3}}}{R^*_{\mathrm{c,\,stom,\,sunlit,\,O3}}} = \frac{1-\beta^*_{\mathrm{sunlit}}}{1-\beta^*} \tag{41}$$

$$\frac{F_{\mathrm{c,\,stom,\,shaded}}(\mathrm{O_3})}{F_{\mathrm{c,\,stom}}(\mathrm{O_3})} = \frac{R^*_{\mathrm{c,\,stom,\,O3}}}{R^*_{\mathrm{c,\,stom,\,shaded,\,O3}}} = \frac{1-\beta^*_{\mathrm{shaded}}}{1-\beta^*} \tag{42}$$

Dividing $F_{c,\,stom,\,sunlit}(O_3)$ by LAI_{sunlit} (see Appendix B in Grünhage and Haenel (2008)) yields the flux of O_3 through the stomatal pores per unit projected leaf area (*PLA*)

$$F_{\mathrm{leaf,\,stom,\,sunlit}}(\mathrm{O_3}) = \frac{F_{\mathrm{c,\,stom,\,sunlit}}(\mathrm{O_3})}{LAI_{\mathrm{sunlit}}} \tag{43}$$

as required by the UNECE Mapping Manual 2004 (UNECE, 2004, 2007). The re-calculation of stomatal conductance of sunlit leaves $g_{leaf,\,stom,\,sunlit,\,O3}$ from bulk stomatal resistance $R_{c,\,stom,\,O3}$ according to eq. (44)

$$g_{\mathrm{leaf,\,stom,\,sunlit,\,O3}} = \frac{1-\beta^*_{\mathrm{sunlit}}}{R_{\mathrm{c,\,stom,\,O3}}} \cdot \frac{1}{LAI_{\mathrm{sunlit}}} \tag{44}$$

provides a direct interface between canopy scale and leaf scale measurements as well as between micromet and impact research. Besides verification of the parameterization of stomatal conductance via measurements of canopy level water vapour exchange, *big leaf* stomatal conductance parameterization and water vapour fluxes can now be compared directly with porometer measurements on the leaf level. Upscaling algorithms from leaf to canopy level can be verified or adjusted.

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