Empirical and optimal stomatal controls on leaf and ecosystem level CO₂ and H₂O exchange rates

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ABSTRACT

Linkage between the leaf-level stomatal conductance (gₛ) response to environmental stimuli and canopy-level mass exchange processes remains an important research problem to be confronted. How various formulations of gₛ influence canopy-scale mean scalar concentration and flux profiles of CO₂ and H₂O within the canopy and how to derive ‘effective’ properties of a ‘big-leaf’ that represents the eco-system mass exchange rates starting from leaf-level parameters were explored. Four widely used formulations for leaf-level gₛ were combined with a leaf-level photosynthetic demand function, a layer-resolving light attenuation model, and a turbulent closure scheme for scalar fluxes within the canopy air space. The four gₛ models were the widely used semi-empirical Ball-Berry approach, and its modification, and two solutions to the stomatal optimization theory for autonomous leaves. One of the two solutions to the optimization theory is based on a linearized CO₂-demand function while the other does not invoke such simplification. The four stomatal control models were then parameterized against the same shoot-scale gas exchange data collected in a Scots pine forest located at the SMEAR II-station in Hyytlä, Southern Finland. The predicted CO₂ (Fc) and H₂O fluxes (Fc) and mean concentration profiles were compared against multi-level eddy-covariance measurements and mean scalar concentration data within and above the canopy. It was shown that Fc comparisons agreed to within 10% and Fc comparisons to within 25%. The optimality approach derived from a linearized photosynthetic demand function predicted the largest CO₂ uptake and transpiration rates when compared to eddy-covariance measurements and the other three models. Moreover, within each gₛ model, the CO₂ fluxes were insensitive to gₛ model parameter variability whereas the transpiration rate estimates were notably more affected. Vertical integration of the layer-averaged results as derived from each gₛ model was carried out. The sensitivities of the up-scaled bulk canopy conductances were compared against the eddy-covariance derived canopy conductance counterpart. It was shown that canopy level gₛ appear more sensitive to vapor-pressure deficit than shoot-level gₛ. © 2011 Elsevier B.V. All rights reserved.

1. Introduction

The primary pathway by which gas molecules are exchanged between a leaf and the atmosphere was proposed to be through stomatal pores more than a century ago (e.g. Blackman, 1895). Since then, the precise regulatory mechanism controlling the opening and closure of a stoma continues to be the subject of intense research activity (Cardon et al., 1994; Parkhurst, 1994; Fan et al., 2004). Stomatal action is often studied with measurements of gas exchange conducted at a single leaf level. These measurements generally demonstrate that the response of stomatal conductance (gₛ) to environmental stimuli is well behaved when aggregated over numerous stoma (Schulze et al., 1972; Cowan and Farquhar, 1977). This finding invites the interpretation of gₛ in the context of an effective or ‘big stoma’ with an effective aperture (Mott and Peak, 2007). With conifers, a common practice is to use the shoot as the basic unit to determine the responses of stomatal conductance to microclimate (Gower and Norman, 1991), which involves aggregation of processes occurring at the needle surface elements. When aggregating to ecosystem level, the response of the canopy-scale conductance to environmental stimuli is more variable and not as well behaved as leaf- or shoot-level gₛ. However, clear deterministic trends do emerge also at such a scale (Jarvis and McNaughton, 1986) and these are commonly exploited in the so-called big-leaf representation. The aim of this work is to explore the connections...
between these deterministic trends at the canopy scale and the mechanisms governing the well-behaved leaf-level responses of \( g_s \) to variations in its local microenvironment.

The investigation of \( g_s \) responses to environmental stimuli at the leaf scale appeared to have followed one of two broad model classes. The first describes \( g_s \) as an empirical response to changes in photosynthetically active radiation, atmospheric vapor pressure deficit (\( D \)), air temperature, leaf water potential, and the rate of leaf carbon assimilation (Jarvis, 1976; Ball et al., 1987; Collatz et al., 1991; Leuning, 1995). These empirical and semi-empirical responses are often 'assigned' to a plant functional type thereby allowing their routine use in climate or hydrological models (Sellers et al., 1996; Lai et al., 2000). The second approach is based on the so-called 'economics of gas exchange' and assumes that the regulatory roles of the stomata are to autonomously maximize their carbon gains while minimizing water losses (Givnish and Vermeij, 1976; Cowan, 1977, 1982; Cowan and Farquhar, 1977; Hari et al., 1986; Berninger and Hari, 1993; Mäkelä et al., 1996). There are appealing attributes about this latter approach. First, the optimality hypothesis provides closed form analytical expressions for \( g_s \), assimilation rate and intercellular \( CO_2 \) concentration. Second, these expressions require only one physiological parameter – the marginal water use efficiency, \( \lambda \). Third, the derived \( g_s \) responses to several environmental stimuli can be viewed as an outcome of the optimization hypothesis thereby offering more transferability across plant functional types than empirical approaches, at least if the plant is operating its stomata optimally (Hari et al., 2000; Katul et al., 2009, 2010). Although the behavior of \( g_s \) to environmental stimuli are well described by both model classes, any general responses at the canopy scale can be obscured by highly inhomogeneous foliage distribution, complex wind and radiation fields, as well as the irregular variation in the mean atmospheric \( CO_2 \) concentration within the canopy volume.

The links between the responses of \( g_s \) to variations in its local environment as described by these two model classes and the canopy scale processes (including scalar fluxes and mean scalar concentration distribution within the canopy) is explored. Three inter-related questions, labeled Q.1–Q.3, frame the scope of this exploration:

(Q.1) How sensitive are the modeled vertical \( CO_2 \) and \( H_2O \) sink/source distributions, scalar fluxes, and mean ambient scalar concentrations within the canopy to the two commonly used model classes of \( g_s \)?

(Q.2) How well do the up-scaled scalar fluxes compare against measured whole-canopy fluxes if only shoot-scale measurements are available and, in particular, how do models based on the optimality principle contrast against semi-empirical descriptions?

(Q.3) What are the effective properties of a 'big-leaf' representation of this eco-system and how do they relate to the shoot-scale measurements?

Q.2 is a generalization of a recent effort by Schymanski et al. (2007, 2008), who explored it in the context of \( H_2O \) and \( CO_2 \) fluxes without considerations to predicted mean scalar concentration profiles – used here as additional independent measures to evaluate the skill of the model.

These three questions are addressed by combining a leaf photosynthesis model (Farquhar et al., 1980) and four commonly used descriptions of \( g_s \) at the leaf scale, as recently done in Katul et al. (2010). The up-scaling from leaf to canopy is carried out by incorporating a layer-resolving light attenuation model and a closure model for turbulent fluxes within the canopy air space, both dependent on the vertical leaf area density distribution. The parameters of the leaf-level photosynthesis and stomatal control models are independently inferred from leaf- and shoot-scale gas exchange measurements. The turbulent closure scheme and light attenuation model are tested against detailed velocity and radiation profiles collected in a Scots pine forest located at the SMEAR II-station in Southern Finland (Vesala et al., 2000; Hari and Kulmala, 2005; Launiainen et al., 2007). The novelty of the present approach is that it deconstructs the predictive skills within and between-model variability using two scalars (\( CO_2, H_2O \)) and turbulent scalar fluxes as well as mean scalar concentration profiles. The advantages of including the scalar concentration profiles in such comparisons are generally attributed to the high vertical resolution that far exceeds those of eddy-covariance (EC) measurements within canopies. Hence, these measurements do serve as independent checks on how well the \( CO_2 \) and \( H_2O \) source/sink distributions within the canopy are reproduced. The full scale-independency is retained by assessing the model predictions against independent EC and mean scalar concentration profile measurements noting that the physiological parameters are also independently inferred at the shoot-scale.

2. Theory

The up-scaling from leaf to canopy using the mean scalar continuity equation and physiological principles that include the four \( g_s \) models are considered next. The abbreviations used in the equations are listed in Table 1.

2.1. The \( CO_2 \) budget within a canopy layer

For a stationary and planar homogeneous high Péclet number flow in the absence of subsidence, the one-dimensional mean \( CO_2 \) continuity equation reduces to

\[
\frac{\partial \overline{wC} (z)}{\partial z} = S_c (z),
\]

(1)

where \( \overline{wC} \) is the turbulent flux of \( CO_2 \), overbar represents time and planar averaging (Raupach and Shaw, 1982; Finnigan, 2000), primed quantities represent excursions from this space-time average, \( \overline{wC} \) is the mean uptake or emission rate (sink or source strength) of \( CO_2 \) from the foliage at layer \( z \), and \( z \) is the vertical direction with \( z = 0 \) being at the forest floor.

Representing the turbulent flux by first order closure principles results in

\[
\overline{wC} (z) = -K_c (z) \frac{\partial c (z)}{\partial z},
\]

(2)

where \( K_c \) is the turbulent diffusivity for \( CO_2 \), and \( c \) is the mean atmospheric \( CO_2 \) concentration. The necessary conditions for the application of such closure scheme inside canopies are discussed within the context of predictions from second and third - order formulations in Juang et al. (2008) and Bash et al. (2010). Assuming Fickian diffusion from the atmosphere into the leaf intercellular pores results in an expression for \( S_c \) given by (Katul et al., 2000)

\[
S_c (z) = a(z)g_l(z)c_o(z) \left( \frac{c_l(z)}{c_o(z)} - 1 \right),
\]

(3)

where \( a(z) \) is the leaf area density, \( g_l \) is the total leaf conductance, which is dominated by stomatal regulation (vis-à-vis aerodynamic and mesophyll conductance), and \( c_l \) is the mean intercellular \( CO_2 \) concentration.

Defining \( R(z) = c_l(z)/c_o(z) - 1 \) so that \( S_c (z) = a(z) \left[ g_l(z) R(z) c_o(z) \right] \) and combining Eqs. (1) and (2) results in a homoge-
neous second-order ordinary differential equation for the mean CO₂ concentration given by (Siqueira and Katul, 2010)

\[
\frac{\partial^2 C_a}{\partial z^2} + \frac{1}{K_t} \left( \frac{\partial U}{\partial z} \frac{\partial C_a}{\partial z} + a(z) g_a R c_a \right) = 0
\]  

(4)

Invoking first-order closure principles for momentum transfer (see Appendix A) and using a mixing length hypothesis leads to (Harman and Finnigan, 2007),

\[
K_t = \left( \frac{1}{\nu_S} \right) L^2 \left| \frac{\partial U}{\partial z} \right|
\]  

(5)

where \(\nu_S\) is the turbulent Schmidt number defined as the ratio of momentum to scalar turbulent diffusivities (and need not be unity inside canopies), \(U\) is the mean velocity, and \(L\) is the effective mixing length. These first-order closure results link the mean momentum and mean scalar concentration budgets via

\[
\frac{\partial^2 C_a}{\partial z^2} + \left( \frac{\partial U}{\partial z} \frac{\partial C_a}{\partial z} \right) + \frac{a(z) g_a R c_a}{K_t} = 0
\]  

(6)

To solve Eq. (6) for \(c_a\) at a given layer inside the canopy, additional equations describing the vertical variations of \(g_a\) and \(R\) (or \(c_i/c_a\)) must be formulated from leaf-gas exchange principles considered next.

### 2.2. Leaf-gas exchange principles

As noted earlier, mass transfer of CO₂ and H₂O through leaves (i.e. expressed in m² of leaf area) occur via Fickian diffusion:

\[
f_c = g_a(c_a - c_i)
\]  

(7)

\[
f_c = a_1 g_1(c_1 - c_e) \approx a_2 g_2 D
\]  

(8)

where \(f_c\) and \(f_e\) are the CO₂ and H₂O fluxes from the leaf surface (i.e. \(S(z) = a(z) f_c\), \(a_i=1.6\) is the relative molecular diffusivity of water vapor with respect to carbon dioxide in air, \(e_i\) is the intercellular and \(e_e\) the ambient water vapor mixing ratio and \(D\) is the vapor pressure deficit representing \(e_i - e_e\) when the leaf is well- coupled to the atmosphere. Furthermore, when leaf respiration is small with respect to \(f_c\) and the mesophyll conductance is much larger than the stomatal conductance, the biochemical demand for CO₂ is described by the Farquhar photosynthesis model given by (Farquhar et al., 1980):

\[
f_c = \frac{a_1(c_1 - c_p)}{a_2 + c_1}
\]  

(8)

where \(c_p\) is the CO₂ compensation point, \(a_1\) and \(a_2\) are coefficients whose values depend on whether the photosynthetic rate is restricted by electron transport or Ribulose bisphosphate
(RuBP) carboxylase (or Rubisco). Under light-saturated conditions, \( a_1 = V_{c,\text{max}} \) (maximum carboxylation capacity) and \( a_2 = K_c \left( 1 + C_{\text{a}} / K_{\text{a}} \right) \), where \( K_c \) and \( K_{\text{a}} \) are the Michaelis constants for CO\(_2\) fixation and oxygen inhibition, and \( C_{\text{a}} \) is the oxygen concentration in air. When light is limiting, \( a_1 = a_0 \gamma n Q_\phi \) and \( a_2 = 2 c_p \), where \( a_0 \) is the leaf absorptivity of photosynthetically active radiation (Q\(_\phi\)), \( n \) is the maximum quantum efficiency of leaves and \( \gamma \) is the apparent quantum yield determined from empirical light-response curves. Hence, expressed in terms of leaf stomatal conductance, \( g_s \), Eqs. (7) and (8) can be combined to yield the following leaf-level expressions:

\[
\frac{c_i}{c_a} = \frac{1}{2} + \frac{-a_1 - a_2 g_s + \sqrt{(a_1 + (a_2 - c_0) g_s)^2 + 4g_s (a_1 c_p + a_2 c_p c_0)}}{2g_s c_a}
\]

(9)

and

\[
f_c = \frac{1}{2} \left( a_1 + (a_2 + c_p) g_s - \sqrt{(a_1 + g_s(a_2 - c_0))^2 + 4g_s (a_1 c_p + a_2 c_p c_0)} \right).
\]

(10)

These expressions do not assume any functional relationship for \( g_s \) with its local environment. They show how \( f_c \) and \( c_i \) can be predicted from \( g_s \) if \( c_a \) and the physiological attributes of the leaf \( (a_1, a_2, \text{ and } c_p) \) are known or can be inferred from the local light regime and temperature. Eq. (10) also shows that \( f_c \) is non-linearly related to \( g_s \), with a convexity that is necessary for optimality solutions to exist as discussed later.

2.3. The closure problem at the leaf scale – semi-empirical formulations for stomatal conductance

To mathematically ‘close’ Eqs. (9) and (10), an independent formulation for \( g_s \) is needed so that \( f_c \) and \( c_i \) can be computed. The so-called Ball–Berry (Ball et al., 1987) and the Leuning (1995) formulations can be used for such ‘closure’ schemes in multi-layer biosphere-atmosphere models (Baldocchi and Meyers, 1998; Lai et al., 2000; Siqueira and Katul, 2002; Juang et al., 2008). These formulations are, respectively:

\[
g_s = \frac{m_1}{c_a - c_p} f_c \frac{RH}{b_1}; \quad \text{(11a)}
\]

and

\[
g_s = \frac{m_2}{c_a - c_p} f_c l_{\text{EUV}}(D) + b_2; \quad \text{ l}_{\text{EUV}}(D) = \left( 1 + \frac{D}{D_0} \right)^{-1} \text{ (11b)}
\]

where \( RH \) is the mean air relative humidity, \( l_{\text{EUV}} \) reflects the sensitivity of the stomata to vapor pressure deficit, \( D_0 \) is a vapor pressure deficit constant, and \( m_1, m_2, b_1, \) and \( b_2 \) are empirical fitting parameters (slope and residual conductance, respectively). Eqs. (11a) and (11b) provide the necessary mathematical closure (i.e., three equations and three unknowns: \( f_c, c_i \), and \( g_s \)) if \( c_a, a_1, a_2 \), and \( c_p \) are known. The formulations in Eqs. (11a) and (11b) provide a posteriori that \( g_s \) is linearly related to \( f_c/(c_a - c_p) \), a result that is supported from a large number of experiments (e.g. Palmoth et al., 1999). However, Eq. (10) already suggests that a linear relationship between \( g_s \) and \( f_c \) can only be approximate.

2.4. An optimality model

An alternative formulation to Eqs. (11a) and (11b) can be derived from an optimality principle, originally proposed by Cowan (1977) and Givnish and Vermeij (1976) and retained in the work by Cowan and Farquhar (1977), Hari et al. (1986), Berninger and Hari (1993), and more recently by Konrad et al. (2008), and Katul et al. (2009, 2010). Assuming each leaf is autonomous, an objective function to be maximized at the leaf scale can be defined as

\[
f(g_s) = f_c - \lambda f_e = \frac{1}{2} \left( a_1 + (a_2 + c_0) g_s - \sqrt{(a_1 + a_2 - c_0)^2 + 4g_s (a_1 c_p + a_2 c_p c_0)} \right) - \lambda g_s D
\]

(12)

where Eq. (10) was used to determine \( f_e \) and Eq. (7) was used to determine \( f_c \). The premise here is that stomata regulate their aperture so as to maximize the carbon gain while minimizing water loss (in units of carbon) for a leaf specific cost parameter \( \lambda \) (note that the notation by Hari et al. (1986) is used here instead of the original notation proposed by Cowan and Farquhar, 1977). Provided \( \partial f_c / \partial f_e < | \partial f_e / \partial f_c | \), the \( g_s \) that maximizes this objective function can be determined from \( \partial f(g_s) / \partial g_s = 0 \) (i.e., \( f(g_s) \)) is an extremum guaranteed to be a maximum given the expected convexity of \( f(g_s) \) with respect to \( g_s \) in Eq. (12). The optimization problem framed in Eq. (12) does not a priori assume any functional response of \( g_s \) to \( D \) or \( RH \) nor does it assume a priori any linear dependence between \( g_s \) and \( f_c/(c_a - c_p) \) as in the case of Eqs. (11a) and (11b). Instead, it assumes that excessive water losses can induce stomatal closure, which is consistent with the experimental findings of Mott and Parkhurst (1991) who, using a ‘helox’ gas medium, demonstrated that stomata appear to respond to transpiration rates rather than measures of air humidity.

Differentiating Eq. (12) with respect to \( g_s \) results in (Katul et al., 2010)

\[
\frac{\partial f(g_s)}{\partial g_s} = \frac{1}{2} \left( a_2 + c_0 + \frac{a_1 (a_2 + c_0 - 2c_p) - g_s(a_2 + c_0)^2}{\sqrt{(a_1 + (a_2 - c_0) g_s)^2 + 4g_s (a_1 c_p + a_2 c_p c_0)}} \right) - 2\lambda a_D.
\]

(13)

When setting \( \partial f(g_s) / \partial g_s = 0 \) and solving for \( g_s \), we obtain:

\[
g_s = \frac{-a_1(a_2 - c_0 + 2c_p)}{(a_2 + c_0)^2} + \frac{\sqrt{a_D a^2 (c_a - c_p)^2 a_2 + c_0 (a_2 + c_0) - 2a_D a_2^2 (a_2 + c_0 - a_D a)^2}}{a_D a_2 (a_2 + c_0)^3 (a_2 + c_0 - a_D a)}.
\]

(14)

This \( g_s \) formulation is explicit in relating conductance to \( c_a \) and \( D \). However, unlike the empirical formulations in Eqs. (11a) and (11b), both relating \( g_s \) to the photosynthetic rate leaving two (Ball–Berry) or three (Leuning formulation) unknown parameters, this formulation relates conductance to the three parameters of the photosynthesis model and leaving only one unknown physiological parameter \( \lambda \) related to conductance. Moreover, the model formulation in Eq. (14) suggests that \( \lambda \) cannot be entirely ‘free’ and must be bounded to ensure real and positive conductance (Katul et al., 2010).

Linearizing the biochemical demand function in Eq. (8) results in a much simpler (and insightful) model for the optimal \( g_s, f_c \), and subsequently \( c_i \) given as (see Appendix B for discussion)

\[
g_s = \frac{a_1}{a_2 + sc_a} \left[ -\frac{c_a - c_p}{a_1 \lambda D} \right] - 1 + \sqrt{\frac{c_a - c_p}{a_1 \lambda D}}
\]

(15)

\[
f_c = \frac{a_1(c_a - c_p)}{a_2 + sc_a} \left[ 1 - \frac{a_1 \lambda D}{(c_a - c_p)} \right]
\]

\[
c_i = 1 - \sqrt{\frac{a_1 \lambda D}{c_a}} \left( \frac{c_a - c_p}{c_a} \right).
\]
Table 2
Photosynthesis model and stomatal control model parameters. All values are given per projected leaf area.

<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Variable</th>
<th>Value</th>
<th>Units</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>(V_{\text{max,25}})</td>
<td>Maximum carboxylation velocity at 25 °C</td>
<td>37 (pine), 31 (understory)</td>
<td>(\mu\text{mol m}^{-2}(\text{leaf})\text{s}^{-1})</td>
<td>Wang et al. (1996), Kolari et al. (2006)</td>
</tr>
<tr>
<td>(V_{\text{max}})</td>
<td>(V_{\text{max,25}}) (C = \frac{\exp[(S_{\text{T}0} - H_{\text{T}})/RT_0]}{1 + \exp[(S_{\text{T}0} - H_{\text{T}})/RT_0]})</td>
<td>(\mu\text{mol m}^{-2}(\text{leaf})\text{s}^{-1})</td>
<td>Wang et al. (1996)</td>
<td></td>
</tr>
<tr>
<td>(a_{\gamma})</td>
<td>Absorptivity of leaves for PAR</td>
<td>0.8</td>
<td>-</td>
<td>Campbell and Norman (1998)</td>
</tr>
<tr>
<td>(\gamma')</td>
<td>Apparent quantum yield</td>
<td>0.042 (pine), 0.055 (understory)</td>
<td>(\text{mol(CO}_2\text{)}\text{mol(PAR)}^{-1})</td>
<td>Cris-2 measurements (pine), Kolari et al. (2006)</td>
</tr>
<tr>
<td>(r_{d,25})</td>
<td>Dark respiration at 25 °C</td>
<td>(r_{d,25} = 0.015V_{\text{max,25}})</td>
<td>(\mu\text{mol m}^{-2}(\text{leaf})\text{s}^{-1})</td>
<td>Collatz et al. (1992)</td>
</tr>
<tr>
<td>(r_d)</td>
<td></td>
<td></td>
<td>(\mu\text{mol m}^{-2}(\text{leaf})\text{s}^{-1})</td>
<td>Wang et al. (1996)</td>
</tr>
<tr>
<td>(K_o)</td>
<td>Michaelis–Menten constant for CO2 fixation</td>
<td>460</td>
<td>ppm</td>
<td>Aalto (1998)</td>
</tr>
<tr>
<td>(K_o)</td>
<td>Michaelis–Menten constant for oxygen inhibition</td>
<td>330,000</td>
<td>ppm</td>
<td>Aalto (1998)</td>
</tr>
<tr>
<td>(C_{\text{cmax}})</td>
<td>Oxygen concentration in air</td>
<td>210,000</td>
<td>ppm</td>
<td>Aalto (1998)</td>
</tr>
<tr>
<td>(c_p)</td>
<td></td>
<td></td>
<td>ppm</td>
<td>Campbell and Norman (1998)</td>
</tr>
<tr>
<td>(D_o)</td>
<td>Vapor pressure deficit constant in Leuning model (Eq. (11b))</td>
<td>1.3</td>
<td>kPa</td>
<td>Shoot chambers</td>
</tr>
<tr>
<td>(\tau_0)</td>
<td>Scaling temperature</td>
<td>25</td>
<td>°C</td>
<td>Campbell and Norman (1998)</td>
</tr>
<tr>
<td>(m_1)</td>
<td>Slope in Ball–Berry model (Eq. (11a))</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>(m_2)</td>
<td>Slope in Leuning model (Eq. (11b))</td>
<td>0.001</td>
<td>(\text{mol m}^{-2}(\text{leaf})\text{s}^{-1})</td>
<td>Shoot chambers</td>
</tr>
<tr>
<td>(b_1, b_2)</td>
<td>Residual conductance for CO2 (Eqs. (11a) and (11b))</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>(\lambda, \lambda_{\text{eff}})</td>
<td>Marginal water use efficiency (cost parameter) for non-linear and linear optimality model, respectively</td>
<td>-</td>
<td>(\text{mol(CO}_2\text{)}\text{mol(H}_2\text{O)}^{-1})</td>
<td>Shoot chambers</td>
</tr>
<tr>
<td>(a_1)</td>
<td>Coefficient of Farquhar-model</td>
<td>-</td>
<td>(\mu\text{mol m}^{-2}(\text{leaf})\text{s}^{-1})</td>
<td>Eq. (8)</td>
</tr>
<tr>
<td>(a_2)</td>
<td>Coefficient of Farquhar-model</td>
<td>-</td>
<td>ppm</td>
<td>Eq. (8)</td>
</tr>
</tbody>
</table>

The \(g_s\) expression here is similar to the one in Hari et al. (1986). Hereafter, we refer to the solution in Eq. (14) as the ‘nonlinear model’ (denoted by Opti) and the result in Eq. (15) as the ‘linear model’ (Optil).

Eq. (15) reproduces a number of known stomatal responses documented across many species. For example, when expressed as \(g_{s, \text{ref}} = g_s / g_{s, \text{ref}}^\prime\) with \(g_{s, \text{ref}}^\prime\) defined as \(g_s\) for \(D = 1.0\) kPa, Oren et al. (1999) found that \(g_{s, \text{ref}} / g_{s, \text{ref}}^\prime = 1 - m_0 \log(D)\) with \(m_0 \in [0.5, 0.6]\). Katul et al. (2009) showed that Optil is mathematically equivalent to this empirical formulation across a wide range of \(D\) values. Moreover, when \(\lambda\) increases linearly with \(c_p\) (i.e. \(\lambda = \lambda_0 c_p / c_{\text{cmax}}\), where \(c_{\text{cmax}}\) is a reference CO2 concentration at which \(\lambda_0\) is known to have acclimated to), Eq. (15) can be re-arranged so that

\[
g_s = \frac{1}{\sqrt{a c_{\lambda_0} (f_c / c_p)}} \frac{1}{\sqrt{D}} \quad (16)
\]

This result shows that the assumed linear relationship between \(g_s\) and \(f_c / (c_p - c_{\text{cmax}})\) in Eq. (11a) and (11b) for the Ball–Berry or the Leuning models is an outcome of Optil. Moreover, it shows that there is a one-to-one mapping between Optil and the Leuning (1995) model of Eq. (11b) when \(I_{\text{EU}}(D) = D^{-1/2}\) and \(b_2 \approx 0\) resulting in \(m_2 = (g_s / \lambda)_{\text{ref}}^{-1/2}\). In other words we do expect \(m_0\) to be inversely correlated with \(\lambda_{\text{eff}}\) in the Optil framework.

For the calculation of \(a_1\), the vertical attenuation of photosynthetically active radiation and the estimation of the fraction of sun and shaded leaves at various depths within the canopy are needed and discussed in Appendix C. The gas-exchange calculations were performed separately for sunlit and shaded leaves to yield weighted averages at each layer. Hereafter, we refer to this combined radiative – turbulence closure – physiological–conductance biosphere–atmosphere transfer scheme as multi-layer model (MLM).

2.5. Effective ‘big-leaf’ representation using MLM

To derive the effective parameters of the ‘big-leaf’ representation of ecosystem level fluxes from MLM, an integrated big-leaf conductance (\(G_s\)) and \(c_{\text{cmax}} / c_p\) ratio are computed using the approach of Lai et al. (2000). We assume that \(D\) does not vary appreciably within the canopy volume when compared to the light environment and thus \(G_s\) for CO2 transport is

\[
G_s = h \int a(z) g_s(z) dz, \quad (17)
\]

where \(g_s\) is given by the leaf-level solution derived by coupling the Farquhar photosynthesis model, Fickian diffusion, and one of the four stomatal conductance models described in previous section.

Similarly, the net canopy assimilation (\(A_{\text{can}}\)) is

\[
A_{\text{can}} = G_c a h \left[ 1 - \left( \frac{c_{\text{cmax}}}{c_{\text{cmax}}} \right)_{\text{eff}} \right] = \int S_c(z) dz \quad (18)
\]

\[
= \int a(z) g_s(z) c_{\text{cmax}}(z) \left[ 1 - \left( \frac{c_{\text{cmax}}(z)}{c_{\text{cmax}}} \right) \right] dz,
\]
where \( c_a(h) \) is the ambient CO\(_2\) mixing ratio at canopy top (h). With \( G_c \) inferred from Eq. (17), the \( c_i/c_a \) ratio characteristic for the big-leaf canopy is

\[
\left( \frac{c_i}{c_a} \right)_{\text{eff}} = 1 - \frac{\int_0^h a(z)g_i(z)c_a(z)(1 - c_i(z)/c_a(z))dz}{G_c c_a(h)}.
\]  

(19)

How \( G_c \) and the big-leaf \( (c_i/c_a)_{\text{eff}} \) vary with environmental stimuli will be discussed using above formulations (in the context of Q.3).

3. Measurements and model parameterization

The leaf-photosynthetic and stomatal conductance model parameters required in the MLM were determined using shoot gas-exchange measurements conducted in a Scots pine (Pinus sylvestris L.) stand. This stand was sown in 1962 and is currently serving as one of the long-term flux-monitoring sites (SMEAR II station) in southern Finland (61° 51’ N, 24° 17’ E, 181 m above sea level). In 2006, the main canopy was characterized by the following: total leaf area index \((LAI) \sim 6.5 \text{m}^2 \text{m}^{-2}\), stand density 1400 ha\(^{-1}\), the mean tree height \((h) \sim 15\) m and the mean diameter at breast height ~16 cm. The forest floor vegetation is relatively low (mean height ~0.2–0.3 m) but dense (total LAI ~1.5 \text{m}^2 \text{m}^{-2}) and is dominated by dwarf shrubs, mainly lingonberry (Vaccinium vitis-idaea), Blueberry (V. myrtillus), and mosses (Kolari et al., 2006; Kulmala et al., 2008).

3.1. Leaf-level physiological measurements

**Photosynthetic parameters:** The parameters \( a_1, a_2, \) and \( \eta_p \) were taken either from the literature or defined using shoot-level gas-exchange measurements made at the site (Table 2). The photosynthetic light response of the Scots pine was estimated from needle gas-exchange measurements. In July 2006, shoot gas exchange measurements were made at different levels (shading conditions) in the canopy using a portable photosynthesis measuring device (CIRAS-2, PP Systems, Hitchin, UK). Apart from the irradiance, the conditions within the measuring cuvette were kept close to the ambient conditions. The quantum efficiency \((\gamma, \text{per-projected leaf area})\) was determined by a non-linear regression fitting of a rectangular hyperbola (Michaelis–Menten-equation) to each of the measurements and then averaged to represent a representative value to be used in computing \( a_1 \) from \( \gamma Q_p(z) \). The maximum carboxylation velocity \((V_{\text{max25}})\) and its temperature dependency is taken from Wang et al. (1996) (Table 2). The light response of the main forest floor species were measured in a previous study (Kolari et al., 2006). We use their biomass-weighted averages as an effective value in the MLM for ground vegetation. They reported values of the light-saturated assimilation rate \((a_{\max})\) instead of \(V_{\text{max25}}\), but we approximated the latter by \( 2 \times a_{\max}\) (Leuning, 1997).

**Stomatal conductance parameters:** The necessary parameters for the four leaf-scale \( g_b \) models were determined using continuous shoot gas exchange chamber measurements (Table 2). Two chambers, acrylic plastic boxes with a volume of 1 dm\(^3\), are located in the upper part of the canopy (~0.9 h) and open most of the time thereby exposing the shoot in the canopy to ambient conditions. To measure the gas exchange, the chambers were closed 70–100 times a day for 1 min. The details of chamber measurements are described in Hari et al. (1999) and are not repeated here. The shoot-level \( g_b \) parameters were estimated as follows: First, all the available chamber data in dry daytime conditions \((Q_a > 200 \text{mol} \text{m}^{-2} \text{s}^{-1} \text{and RH < 90\%})\) were pooled together and the Ball–Berry and Leuning model parameters (Eqs. (11a) and (11b), respectively) were determined using linear least square regression (i.e. regressing \( G_c \) against \( f_e/(c_a - c_p) \)). Then, the intercepts \((b_1, b_2)\) and \( D_a\) for Leuning-model were fixed to their long-term mean values and the slope estimation was done separately for each measurement solving \( m_2 \) and \( m_3 \) from Eq. (11). We further averaged these to obtain daily values. Similarly, the average cost parameter \( \lambda \) was estimated from measured shoot water use efficiency (WUE) by regressing WUE against \( D^{1/2} \) and solving for \( \lambda \) from the slope of the expression

\[
\text{WUE} = \frac{f_e}{f_e} = \frac{c_a}{a_e} \frac{1 - \frac{c_a}{c_p}}{a_e D} = \frac{a_e}{a_e D} \frac{\lambda D}{c_a} \frac{c_a - c_p}{c_a} = \left[ \frac{\lambda (c_a - c_p)}{a_e} \right] D^{1/2}.
\]

In this computation, \( c_a \) and \( c_p \) were taken equal to their mean values over the period. Several studies have indicated that \( \lambda \) is nearly constant during a day whereas optimality can be achieved at longer time scales only if \( \lambda \) varies as a response to changing environmental conditions, drought stress in particular (Mäkelä et al., 1996; Schymanski et al., 2008; Manzoni et al., 2011). Therefore, we determined the temporal variability of \( \lambda \) as in Katul et al. (2010, their Eqs. (17–20)), which included several approximations: First, in abundant light \((Q_p > 600 \text{mol} \text{m}^{-2} \text{s}^{-1})\) the photosynthesis is Rubisco-limited and the parameter \( a_1 \sim V_{\text{max}}\) in the Farquhar model (Eq. (8)). Second, we assumed that \( a_1 \) and \( a_2 \) follow their “generic” temperature dependencies, and \( c_p \) is only a function of temperature (Table 2). Using these simplifications, \( a_1 \) can be solved for each gas exchange measurement by inverting Eq. (8). Finally, inverting Eq. (14) (or Eq. (15) when determining \( \lambda \) from the linearized optimality model) provides instantaneous \( \lambda \). Also \( \lambda \) was further averaged to daily mean values to be used in MLM.
3.2. Boundary conditions for the MLM

The upper boundary conditions (values at the highest layer above the canopy) are based on time series of half-hourly averaged friction velocity \( u_\ast \) (m s\(^{-1}\), measured by EC at 23.3 m height), ambient CO\(_2\) mixing ratio \( C_a \) (ppm), atmospheric pressure \( P \) (kPa), air temperature \( T_a \) (°C), air relative humidity \( RH \) (%) and diffuse and direct PAR \( Q_{ph} \) (\( \mu \)mol m\(^{-2}\) s\(^{-1}\)) determined from measurements made above the canopy. Instruments and details of the data acquisition are described elsewhere (Hari and Kulmala, 2005; Vesala et al., 1998). During the model runs, \( T_a \) and ambient RH (and \( D \)) were assumed to be vertically uniform within the canopy each 1/2 h thereby eliminating the need for a full leaf energy balance. This assumption is justified for the range of air temperatures considered here. Moreover, in this geographic region, the leaf satisfies its carbon demand first thereby incurring a concomitant water loss, with leaf temperature being a "by-product" (via the leaf energy balance) of these carbon uptake priorities. In other words, we are assuming here that \( g_s \) is not operating to control the temperature status of the leaf. Moreover, measured mean air temperature and H\(_2\)O concentration profiles suggest that the vertical variability in \( D \) is about 0.05 kPa and hence does not exceed 5% in typical conditions within the stand.

The woody biomass \( R_{stem} \) and soil \( R_{soil} \) respiration, and soil evaporation \( (E_a) \) provide the necessary boundary conditions on the scalar budgets. The \( R_{soil} \) was taken from the automated soil chamber measurements (Pumpanen et al., 2001). The modeled stem respiration was computed as (Kolari et al., 2009):

\[
R = R_{10} Q_{ph}(10)^{T_a - 10}/10
\]

(21)

where \( R_{10} = 0.3 \) \( \mu \)mol m\(^{-2}\) s\(^{-1}\) is the base respiration rate at 10 °C per unit trunk area in July and \( Q_{ph} \) the temperature sensitivity (~2) during typical June–August. The stem temperature lags air temperature and was approximated as

\[
\frac{dT_{stem}}{dt} = \frac{T_a - T_{stem}}{\tau}
\]

(22)

where \( \tau \) is a time constant estimated to be 4h and discussed elsewhere (Kolari et al., 2009). The obtained \( R_{stem} \) per m\(^2\) of stem surface area was scaled to per m\(^2\) ground area by multiplying it by
the total stem and branch surface area (≈0.5 m² m⁻²). The vertical distribution of $R_{stem}$ was based on measurements reported by Hölttä and Kolari (2009). The CO₂ efflux from the stem roughly scales with $a(z)$ in the crown peaking where $a(z)$ is at its highest value. The $R_{stem}$ below the foliage layer is roughly 1/2 of the maximum value.

The $E_i$ was modeled assuming equilibrium evaporation (e.g. Jarvis and McNaughton, 1986) driven by radiation load computed at the forest floor. However, when the measured volumetric humus water content ($θ$) was below saturation, $E_i$ was reduced linearly with the decreasing water content.

3.3. Canopy-scale CO₂ flux and concentration measurements model evaluation data

The MLM fluxes and corresponding mean scalar concentration profiles are compared against fully independent canopy-scale measurements made at the site. Continuous EC measurements of CO₂...
(\(F_c\)) and latent heat (\(F_e\)) fluxes were carried out at 23.3, 11.7 and 3.0 m (1.55, 0.78 and 0.2 times \(h\), respectively) using closed-path analyzers (LI-6262 and LI-7000, LI-Cor Inc., Lincoln, NE, USA) and the 1/2h average fluxes were calculated according to the standard FluxNet methodology (Aubinet et al., 2000) and corrected for storage below the measurement height to allow comparison for nighttime conditions. The details of the EC-measurements both above and below the canopy can be found in Launiainen et al. (2005, 2007) and Launiainen (2010) and are not repeated here. The ambient mean concentrations of \(\text{CO}_2\) and \(\text{H}_2\text{O}\) were measured at 33.6, 16.8, 8.4 and 4.2 m heights and are described in Rannik et al. (2004).

### 3.4. Model calculations

The MLM was run for the period of 1st of June–20th of August, 2006. The results were derived as follows: The canopy was first divided into 200 horizontal layers and the radiative environment at each layer was solved. Second, initial guesses for the combined assimilation — stomatal conductance — transpiration were computed separately for sunlit and shaded leaves at each layer, assuming a constant \(c_a\) and \(D\) profile (values set to the measured ones above the canopy for each 1/2 h period). Then, the turbulent closure scheme was applied and the vertical \(c_a\) profile following...
from the sink/source distribution was calculated and then used to refine estimates on the $f_c$, $g_s$ and $f_r$ iteratively. The iterations were continued until the results converged. Convergence was defined as the maximum difference between two successive iterations to be within 0.1% for all the state variables and across all the layers. Within each iteration, the semi-empirical $g_s$ models (Eq. (11)) were also solved iteratively while the two optimality models do not require any further iterations given their analytical form (Eqs. (14) and (15)), a decisive advantage in such model applications. For consistency between $g_s$ predictions of the optimality models and Ball–Berry–Leuning, the dark respiration ($r_d$) was neglected when the $f_r$ to $g_s$-relationship was iteratively "optimized"; thus, $r_d$ was taken into account only in the sink/source profiles and neglected as the leaf’s internal CO$_2$ source.

4. Results and discussion

Prior to addressing Q.1–Q.3, the environmental conditions above the canopy during the experiment period are first discussed. Next, the shoot-scale parameters and their daily variation reflecting the physiological states as computed from the shoot-scale gas-exchange are presented. With these results, the predictions from the four leaf-level stomatal control models are integrated into MLM and compared against independently measured canopy-level mean scalar concentration and turbulent flux data. Note that the four versions of the $g_s$ models only differ in their canonical responses to humidity or vapor pressure deficit. Hence, differences among models in terms of canopy-scale predictions 'fingerprints' the role of stomatal controls and any concomitant two-way coupling between the leaf and its micro-environment. All model versions significantly overpredicted the canopy scale gas exchange in August when drought stress was strongest, which hints that down-regulation of the photosynthetic capacity had occurred. Therefore, the analysis of MLM results are restricted to period during which the photosynthetic machinery was not significantly mediated by drought (1st June–31st July).

4.1. Environmental conditions

The growing season of 2006 was very dry in Southern Finland; the cumulative precipitation from June to August was only about half of the typical 250 mm long-term value. Consequently, volumetric soil moisture content decreased from 0.4 m$^3$ m$^{-3}$ in early June to 0.1 m$^3$ m$^{-3}$ at end of July. The stand showed clear signs of drought stress in late July and during first half of August, manifested in leaf- and canopy scale reductions of photosynthesis, transpiration and also decreased rates of the decomposition of organic matter (Duursma et al., 2008; Kolari et al., 2009; Launiainen, 2010). The period of progressing drought provides a rather unique possibility to explore the stomatal control theories for a wide range of climatic conditions occurring in a boreal Pine forest. During the period of this study, air temperature varied between 10 and 28 °C and typical diurnal amplitude was ~8–10 °C. The first week of June was cooler and $T_a$ remained below 15 °C. The diurnal amplitude of $D$ was on the order of 1.5 kPa providing sufficient stimuli for stomatal opening and closure.

Fig. 5. Comparison of measured (abscissa) and modeled (ordinate) 1/2 h average net CO$_2$ exchange ($F_c$). The linear least-squares regression equation and proportion of explained variance ($R^2$) are given for comparison. The squares represent afternoon (13:00–17:00) values and the dashed line gives 1:1 relationship. Only periods when the canopy was dry are included.
4.2. Radiation attenuation and leaf-level parameters

Because within-canopy radiation is needed to infer $a_1$, a brief validation of the radiation attenuation model used is presented here. Fig. 1 shows the leaf area density profile and the light regime and demonstrates good agreement between measured and modeled $Q_0$ throughout the canopy. The measurements were conducted during one clear and one cloudy day (from 10:00 to 16:00) in late June of 1998 using a multi-point sensor system (20–48 sensors each level) described in Vesala et al. (2000). The measured $a(z)$ was not available for that 1998 period and in the model data comparison here, the shape function of $a(z)$ was assumed to be stationary and only $h$ was adjusted for the recorded changes from 13 (in 1998) to 15 m (in 2006). The stand was partly thinned in 2002 (Vesala et al., 2005) but in 2006 the leaf area index had recovered to its 1998 level.

The quantum yield estimated from shoot gas-exchange measurements was nearly constant ($0.042 \pm 0.012 \text{ mol mol}^{-1}$, mean $\pm$ Std) irrespective of the shading conditions the shoot had acclimatized to. The light-saturated assimilation ($A_{\text{max}}$) at the needle level showed marked difference between the brightshoots ($7.6 \pm 3.4 \text{ mol m}^{-2} \text{s}^{-1}$, mean $\pm$ Std) and shoots growing in shaded conditions ($4.7 \pm 2.1 \text{ mol m}^{-2} \text{s}^{-1}$) in the lower canopy (the degree of shading was determined from hemispherical photographs) but the difference was statistically non-significant ($p > 0.05$) justifying the use of uniform photosynthesis parameters for this Scots pine canopy. The average $\gamma$ matches the values in Palmroth and Hari (2001) measured in June. However, they found higher $\gamma$ (0.054) in July, a similar value to the one (0.057) reported in Leverenz (1987) for Scots pine.

The stomatal conductance parameters were determined from linear regression analysis for all models as described in Section 3.1 and the results are shown in Fig. 2. There was distinct temporal (Fig. 2d and e) and shoot-to-shoot variability both in $m_1$ and $m_2$. As a response to a progressive drying of the soil, $\lambda$ increased and $m_1$ and $m_2$ decreased significantly during the last weeks of the experiment when $\theta$ decreased below $0.12 \text{ m}^2 \text{m}^{-2}$ (not shown). The similarity in the temporal courses of $\lambda$ and $m_2$ is expected given their unambiguous dependency as earlier discussed (Eq. (16)). In contrast, there was no significant correlation between $m_1$ and $m_2$ for the same period. The marginal water use efficiency determined from Optil, $\lambda_{\text{opt}}$, was about 7% higher than the $\lambda$ obtained from the non-linear model ($R^2 = 0.98$), in qualitative agreement with Katul et al. (2010) in a Loblolly pine stand in the Southeastern U.S.

4.3. Addressing Q1

To address Q1, modeled scalar sources, fluxes and mean concentration profiles are considered in detail followed by a direct comparison between the aggregated and eddy-covariance measured canopy-level fluxes. In addition, differences between the models and the measurements are discussed. Fig. 3 shows the ensemble-averaged daytime canopy profiles between 8.00 and 18.00. The net leaf CO$_2$ exchange ($f_{c}$) profile (Fig. 3a) shows rapid
In contrast, the other formulations predict increased \( c_l/c_a \) when descending deeper into the canopy volume. Recall that the nonlinear model is the only model that does not assume (or produce) a linear dependence between \( g_s \) and \( f_c \). The increase in \( c_l/c_a \) with depth inside the canopy is however what can be expected based on carbon isotope data presented in the literature. For instance, Ellsworth (1999, 2000) explored \( c_l/c_a \) ratios in Loblolly pine (\textit{Pinus taeda}) and found that it varied between 0.66 and 0.75, the latter measured in the shaded shoots in the lower canopy.

Despite these differences, the flux profiles (i.e. scalar flux at each height represents the net effect of the sources and sinks per m\(^2\) ground below the height of interest) behave consistently and compare well with the EC data (Fig. 3e and f). The forest floor contributes, in an ensemble sense, about 12% of the canopy scale photosynthesis despite the fact that it represents some 20% of the total LAI. This MLM estimate is similar to what was reported by Kolari et al. (2006) who concluded that forest floor GPP was 13% of the stand GPP during the period from 20th of April to November 20th in 2003. All the models overpredicted the ensemble averaged canopy net CO\(_2\) exchange (\( F_c \)) by 0.5–1.9 \( \mu \text{mol m}^{-2} \text{s}^{-1} \) (~6–20% of the measured). The crown and trunk-space EC measurements were well matched (Fig. 3e). During nocturnal conditions, the ensembles of measured and modeled \( F_c \) were rather well balanced (average difference ~0.2 \( \mu \text{mol m}^{-2} \text{s}^{-1} \)) indicating that the respiratory components were adequately described in the model and thus the mismatch of daytime fluxes was mainly due to assimilation rates. Because of the assumptions of a depth-constant \( D \) (set to its value above the canopy), the water vapor sources are simply ‘slaved’ to the carbon fluxes and modeled as the leaf conductance profile multiplied by \( a(z) \) and \( D \). Hence, the models predicting highest \( g_s \) also resulted in highest water vapor fluxes, shown here in terms of latent heat flux (\( f_c \), Fig. 3f). In relative terms, the combined understory transpiration and soil evaporation was 17–19% of the stand-scale values, slightly less than the fraction (~23%) measured by the EC systems. The correspondence between the ensemble averaged EC-data and MLM results was encouraging considering that the models were only calibrated with the shoot chamber data independent of any canopy level mean concentration or EC flux measurements.

The water use efficiency profiles show highest WUE at the top, ranging from 4.8 \( \times 10^{-3} \) to 5.8 \( \times 10^{-3} \) mol CO\(_2\)/(mol H\(_2\)O)\(^{-1} \) followed by estimates of the order of ~5 \( \times 10^{-4} \) drop within the crown indicating that assimilating a unit of CO\(_2\) becomes more uneconomical in terms of water loss deeper in the canopy (Fig. 3g). Again, the non-linear optimum model is an exception and predicts strong WUE increase within these canopy layers. At the shaded forest floor, the higher quantum efficiency enhances \( f_c \) per leaf area and WUE becomes comparable to its upper canopy value except for Opti. The various stomatal closure schemes only resulted in minor differences for ambient mean scalar concentrations. The predicted \( c_a \) and H\(_2\)O profiles (Fig. 3h and g) show rather good agreement with the measured concentrations considering the small scalar gradients caused by strong mixing during daytime.

Although the MLM assumes the photosynthesis and stomatal conductance model parameters remain uniform with height within the canopy, the importance of stomatal control on regulating \( f_c \) diminishes deeper inside the canopy (Fig. 4). The fraction of sunlit foliage degreases rapidly in the crown and the transition from primarily temperature to light limited assimilation occurs accordingly. Thus, in the deeper layers, the diurnal pattern of \( g_s \) becomes more ‘symmetrical’ since any alteration in \( Q_b \) creates a linear change in \( f_c \), thereby explaining the lesser WUE in the lower canopy predicted by the majority of the \( g_s \)-schemes. Because of the compensating effects of \( c_l \), the diurnal patterns of \( f_c \) are more symmetrical during the day than those of \( g_s \). The fingerprint of stomatal regulation is hardly visible in \( g_s \) below ~0.6 h. A notable difference is that the non-linear optimality model predicts smaller \( g_s \) during the morning.
hours, when $D$ is typically low, than the other models. At the shaded portions of the crown, the $c_i/c_a$ ratio predicted by Opti remains low throughout the day (Fig. 4), while in the upper layers, the model predicts $g_s$, $F_c$ and thus $c_i/c_a$ similar to Optil.

4.4. Addressing Q.2

To address Q.2, ensemble averaged daytime flux profiles were computed from MLM and compared with the EC measurements above the canopy. This comparison indicated reasonably good comparison between the measured and modeled whole-canopy fluxes. The linear least squares regressions of modeled canopy scale CO$_2$ fluxes ($F_c$) on measured 1/2h fluxes yield regression slopes of 0.94–1.03 and intercepts from −0.87 to −0.39 (Fig. 5). The data-model agreement of latent heat flux ($F_l$) was marginally poorer and the scatter was larger; regression slopes were between 0.75 (Ball–Berry) and 1.01 (Optil) and intercepts between 12 and 17 W m$^{-2}$ (Fig. 6). The ensemble diurnal cycles indicate that the measured $F_c$ and $F_l$ are more asymmetric than their modeled counterparts (Fig. 7), also evident in Figs. 5 and 6. The measured canopy scale fluxes peak around noon and decline thereafter, indicative of stomatal closure as a response to changes in microclimate. The modeled $F_c$ and $F_l$ using Ball–Berry, Leuning and Optil follow closely the measured values during morning and evening hours but do not reproduce as strong reduction during the afternoon as recorded by the EC system. During this time of day, the difference between $D$ and the ‘true’ driving force ($D_T = e_a(T_s) - e_d$), where $T_s$ is needle surface temperature) are likely to be greatest. However, a separate analysis (not shown) indicated that this finding alone cannot explain the slower decrease of modeled canopy-scale fluxes, which partly has to be attributed to different $D$ sensitivities at canopy and shoot scale. Unlike the other models and measurements, the Optil predicts steeper flux increases during the morning and these predicted fluxes remain higher throughout the afternoon when compared to the EC measured values. The difference is because the Optil is based on linearized $f_c(c_i)$ response and thus the predictions are sensitive to the chosen value of the long-term mean $c_i/c_a$ ratio $s$ (Appendix B). Moreover, $s$ should equal the $c_i/c_a$ ratio which, on average, balances the $f_{c_l}/c_l$ ratio based on the full (Eq. (8)) and linearized CO$_2$ demand function (Appendix B). Here, $s$ was determined on this premise and was taken equal to 0.74 based on shoot gas-exchange measurements. The sensitivity of Optil predictions of $s$ are greater when the leaf operates in light-limited regime and also the difference between the linearized and full CO$_2$ demand function increases in
these conditions. Hypothesizing that $c_i/c_a$ exceeds $s$ in light limited conditions during morning and evening hours when $D$ and thereby the degree of stomatal closure are low, the linear optimality model provides higher $f_c$ and $g_i$ than the full optimality model. Unlike the other models, the Ball-Berry model predictions remain below the EC recorded midday maximum.

The MLM assumes space-time averaged canopy properties (e.g. Eq. (1)) while the EC measurements represent only time averages. According to Katul et al. (2004a), the time average inferred from the EC system may converge to a space-time average (computed from MLM) in the canopy sub-layer when ensemble-average over sufficiently long periods are employed to cover natural variations in wind direction (e.g. ergodicity in the flow statistics). Hence, the scatter in Figs. 5 and 6 is not surprising given that MLM results are for space-time averaged quantities while the EC measurements are for individual 1/2h periods. Moreover, the scatter in modeled versus measured canopy $F_c$ is, depending on the magnitude of $F_c$, of the same order or smaller than typical scatter ($\sim 100-50\text{ W m}^{-2}$) in the measured energy balance closure (i.e. whether $R_n - G = H + F_c$; $R_n$ is net radiation, $G$ ground heat flux and $H$ sensible heat flux) at the site. Thus, it can be argued that some of the scatter in Fig. 6 originates from uncertainties in the short term energy balance closure and measured $F_c$. However, the biases do not. The measured ensemble-averaged energy-balance was not closed (absolute bias $<50\text{ W m}^{-2}$) in the morning until noon but good ‘closure’ ($\sim 90\%$) was obtained in the early afternoon, where vapor pressure deficit is at its maximum (not shown).

4.5. Addressing Q.3

Thus far, the comparison between MLM-derived canopy level fluxes revealed that differences in the leaf-level stomatal control models alone can have as large as 10% influence on canopy scale CO$_2$ and 25% on water fluxes. Concurrently, the vertical mean concentration profiles indicated that the contribution of a single layer to the upscaled fluxes differs somewhat between models – spawning a question as to how these differences manifest themselves if leaf-level theories are used in a big-leaf framework, which is the basis of Q.3. The effective big-leaf conductance for CO$_2$ ($G_s$) and $(c_i/c_a)_{eff}$ are considered next to address this question. Fig. 8 shows the sensitivities of canopy conductance to $D$ in ample light ($Q_e > 600\text{ pmol m}^{-2}\text{s}^{-1}$). The ‘measured’ $G_s$ is inverted from EC data in two ways: The first assumes that the canopy is ‘well-coupled’ to the atmosphere (i.e. effective $T_e$ equals air temperature) so that

---

**Fig. 9.** Big-leaf $(c_i/c_a)_{eff}$ against $D^{1/2}$ in high light ($Q_e > 600\text{ pmol m}^{-2}\text{s}^{-1}$) conditions. In panel (a) the closed gray circles and dashed line show measured shoot-scale data.
$D$ approximates the driving force for transpiration. The second assumes the canopy is not entirely well-coupled to the atmosphere necessitating an estimate of ‘true’ vapor pressure gradient ($D_{T}$). Here, an approximation of ‘effective’ $T_e$ was inferred from the measured emitted upwelling long-wave radiation above the canopy (not shown). Roughly, the long-wave radiation measurements suggest that the difference between skin and air temperature measured near the canopy top ($T_{e} - T_{c}(h)$) are <1 °C during most of the daytime conditions. For direct comparison, the $G_{i}$ was normalized by its value at vapor pressure deficit of 1.0 kPa ($G_{1}$) and the slope $m_{o}$ of equation $G_{i}/G_{1} = -m_{o} \times ln(D) + 1$ is shown for reference (Oren et al., 1999). Recall that this formulation with $m_{o}$ ∈ [0.5 – 0.6] is consistent with predictions from Optil.(i.e. $D^{-1/2}$) as discussed in Katul et al. (2009). This logarithmic formulation was selected here because the sensitivity parameter $m_{o}$ can be compared across scales (and models) and was shown to be robust whether leaf, tree, or canopy scales were considered (Oren et al., 1999).

The canopy conductance $G_{i}$ scales well with $D^{-1/2}$, and results in $m_{o}$ ranging from 0.54 (Optil) to 0.71 (Ball–Berry). The sensitivity of measured $G_{i}$ is stronger than the modeled, while the shoot-scale $g_s$ appears least sensitive to $D(m_{o} = 0.48)$ (Fig. 8). The sensitivity of $G_{i}$ to $D$ varies by ~25% and the optimality models, where no a priori sensitivity to $D$ (or RH) was assumed, matched rather well other formulations and measurements. The $(c_{i}/c_{a})_{left}$ scales non-linearly with $D$ in high light ($Q_{0} > 600$ μmol m$^{-2}$ s$^{-1}$), particularly if Optil and Optil are considered (recall that the leaf-scale $c_{i}/c_{a}$ scale linearly in $D$ or RH in the Leuning and Ball- Berry models). Fig. 9 shows $(c_{i}/c_{a})_{left}$ as a function of $D^{1/2}$. The sensitivity to $D$ varies from ~0.14 (Optil) to ~0.22 (Ball–Berry, Optil) which closely resembles the behavior of measured shoot-scale $c_{i}/c_{a}$. This behavior is consistent with that observed by Katul et al. (2009) who showed that based on the optimization hypothesis $c_{i}/c_{a}$ should vary predictably with $D$, namely

$$c_{i}/c_{a} = 1 - (a \cdot \lambda / c_{a})^{1/2} \cdot D^{1/2}. \quad \text{(23)}$$

In further support of the conclusions in Katul et al. (2009), the restricted range in $c_{i}/c_{a}$ often masks such non-linearity, and linear fitting to the data is often no worse. In fact, it is this near-linear trend between $c_{i}/c_{a}$ and $D$ that was the basis of the Leuning (1995) $g_{s}$ model (Eq. (11b)).

5. Conclusions

We showed that the up-scaled canopy-level CO$_2$ and H$_2$O flux and concentration profiles compare well against the canopy level eddy-covariance measurements by predicting the variability within 6% ($F_{i}$) and 25% ($F_{c}$) (Figs. 5 and 6). The correspondence was remarkable considering that the models rely largely on the parameter values obtained from the literature and only few parameters were inferred using measurements collected at the shoot-scale being hence entirely independent of the canopy scale measurements. Thus, the model-data inter-comparison implies that the simplified MLM proposed here was sufficient to capture the essential interplay between the vertical variation of foliage distribution and its local microclimate and any resulting controls on the mean scalar concentration profiles and fluxes. The observed inter-model differences between Ball-Berry, Leuning and the two optimality formulations were on the order of 10% ($F_{i}$) and 25% ($F_{c}$). In addition, the sensitivity of each stomatal control scheme to their respective parameters was conservative and of similar magnitude in each of the models. The median and 25th/75th percentile values of daily stomatal sensitivities provide a legitimate estimate of the variability of these skewed distributions and were therefore used to examine the effect of parameter values on the up-scaled fluxes. Use of leaf-scale $g_{s}$ model parameter values corresponding to the 25th/75th percentiles lead to under- or overestimation of $F_{i}$ by 3%–5% and $F_{c}$ by 14%–16%. This implies that calibration errors or biased literature values of stomatal control parameters can significantly alter the predicted transpiration rates from a specific ecosystem. However, the photosynthesis remains less affected because of the compensating effect of $c_{i}/c_{a}$. The influence of varying stomatal control parameters is comparable to the effect of varying the quantum efficiency and maximum carboxylation capacity. The MLM predictions of canopy CO$_2$ uptake and transpiration are affected by ~5% when $\gamma$ is adjusted by 20% of the original value. For similar change in $V_{\text{max}_{25}}$, the MLM prediction change by ~10%; hence the up-scaled results are more sensitive to the exact value of $V_{\text{max}_{25}}$ rather than quantum efficiency. Nevertheless, the results of this study call for a thorough research of both within and across-species variability of stomatal control parameters. Moreover, operating in the Farquhar framework, the marginal water use efficiency ($\lambda$) required by the optimality models should be determined independently of photosynthesis parameters to allow transferability across sites. We also showed that the canopy scale bulk conductance appears more sensitive to variations in vapor pressure deficit than that of the uppermost shoots, even when ‘true driving force’ (D$_{T}$) is used in lieu of $D$ in the bulk canopy conductance computations. Moreover, the effective ‘big-leaf’ and the shoot-scale $c_{i}/c_{a}$ do scale well with $D^{1/2}$ as predicted by stomatal optimization theories. To summarize, the choice of a stomatal control scheme can have as large as ~25% impact on up-scaled canopy fluxes even when $g_{s}$ model parameterization is done against the same shoot-scale dataset.

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Appendix A. Generation of the mean flow and turbulent diffusivity

In a stationary and planar-homogeneous flow at high Reynolds number and with no subsidence, the mean momentum budget reduces to:

$$\frac{\partial \vec{u} \vec{w}}{\partial z} = C_d(\alpha(z))U^2 \quad \text{(A.1)}$$

where $C_d$ is the foliage drag coefficient (here 0.15), usually between 0.1 and 0.3 (Katul et al., 2004b). Using first order closure principles for simplicity,

$$\vec{u} \vec{w} = -K_{\text{end}} \frac{\partial U}{\partial z} \quad \text{(A.2)}$$

resulting in a second-order nonlinear ordinary differential equation, given as

$$K_{\text{end}} \frac{\partial^2 U}{\partial z^2} + \frac{\partial K_{\text{end}}}{\partial z} \frac{\partial U}{\partial z} - C_d(\alpha(z))U^2 = 0. \quad \text{(A.3)}$$
where the eddy diffusivity for momentum \( (K_m) \) is

\[
K_m = \bar{p} \left| \frac{\partial U}{\partial z} \right| \tag{4.4}
\]

The mixing length \( (l) \) is given as

\[
l = \begin{cases}
    k_s z, & z < \alpha h/k_s \\
    \alpha h/k_s, & \alpha h/k_s \leq z < h \\
    k_s (z - d), & z \geq h
\end{cases}
\tag{4.5}
\]

where the parameter \( \alpha' = k_s (1 - d/h) \) to ensure continuity (but not smoothness) in the mixing length, \( d \) is the zero-plane displacement height (here 0.7 h), \( k_s = 0.4 \) is the von Karman constant and \( h \) is the canopy height. This equation can be solved when two boundary conditions on the mean velocity are imposed (zero-stress at the ground given the density of the canopy, and measured mean velocity above the canopy). The eddy diffusivity of scalars may differ from \( K_m \) (the turbulent Schmidt number \( S_N = K_m/k_c \) does not have to be unity). In near-neutral surface layer, neglecting the roughness sub-layer effects (or assuming them similar for both scalars and momentum), setting \( K_m = k_s (z - d) u_w \), where \( u_w \) is the friction velocity, and applying the first-order closure gives

\[
\frac{\partial \bar{S}}{\partial z} = -k_s \frac{\partial \bar{s}}{\partial z} = -k_u \frac{\partial \bar{s}}{S_N \partial \ln z},
\tag{4.6}
\]

which allows estimation of \( S_N \) from the direct flux and concentration gradient measurements made above the forest. According to the analysis for the site of this study, \( S_N \) was around unity for the studied scalars with a median and 25th to 75th percentiles as follows: 0.92 (0.68/1.20) for CO\(_2\), 1.01 (0.77/1.33) for H\(_2\)O. Therefore, \( S_N \) was in this analysis set to 1 for both scalars considered.

**Appendix B. A linearized optimality model**

Linearizing the biochemical demand function in Eq. (8) results in a much simpler (and insightful) model for the optimal \( g_s \), which can be readily implemented as well. The linearization requires the assumption that the variability of \( c_i \) affects only marginally the denominator of Eq. (8), leading to an approximation \( a_2 + c_i = a_2 + (c_i/c_a) c_a = a_2 + sc_a \). As a result,

\[
f_c = \frac{a_1 (c_i - cp)}{a_2 + sc_a}
\tag{B.1}
\]

where \( s \) is treated as a constant set equal to the long-term mean of \( c_i/c_a \). It must be stressed here that only in the denominator of equation (8) \( s \) is treated as a model constant, while in Eq. (9) \( c_i/c_a \) is allowed to vary (and hence \( R \) does vary within the canopy). Note also that the geometric interpretation of the group of parameters \( a_1/(a_2 + sc_a) \) in Eq. (B.1) is simply the slope of the \( f_c(c_i) \) curve. Combining this linearized photosynthesis model with Eq. (7) results in an expression for \( f(g_c) = f_c - \lambda f_c = \frac{a_1(c_i - cp) cp}{a_1 + g_c(a_2 + sc_a)} - \lambda a_c g_c D \), and \( f_c \) given by

\[
c_i(g_c) = \frac{a_1 c_p + cp + c_p^2 g_c}{a_1 + g_c(a_2 + sc_a)} \tag{B.2}
\]

The objective function in Eq. (12) simplifies to

\[
f(g_c) = f_c - \lambda f_c = \frac{a_1 (c_i - cp) g_c}{a_1 + g_c(a_2 + sc_a)} - \lambda a_c g_c D, \tag{B.3}
\]

and upon differentiating this objective function with respect to \( g_c \) yields

\[
\frac{\partial f(g_c)}{\partial g_c} = -\lambda D + \frac{a_1 (c_i - cp)}{[a_1 + g_c(a_2 + sc_a)]^2} \tag{B.4}
\]

Note that the convexity of \( f(g_c) \) versus \( g_c \) ensures that a maximum exist and can be determined by setting \( \partial f(g_c)/\partial g_c = 0 \) (i.e. maximum carbon gain while minimizing water losses). Solving for \( g_c \) results in

\[
g_c = \frac{a_1}{a_2 + sc_a} \left( -1 + \sqrt{\frac{c_a - cp}{a_1 \lambda D}} \right) \tag{B.5}
\]

Apart from the compensation point \( (c_p) \), this expression is identical to the one derived in Hari et al. (1986). Replacing Eq. (B.5) into Eqs. (B.2) and (B.3) provides closed form of expressions for \( c_i \) and \( f_c \) given by

\[
f_c = \frac{a_1 (c_i - cp)}{a_2 + sc_a} \left[ 1 - \sqrt{\frac{c_a - cp}{c_a - c_p}} \right] \tag{B.6}
\]

and

\[
c_i = \frac{c_a - c_p}{c_a - c_p} \tag{B.7}
\]

Hereafter, we refer to the solution in Eq. (B.7) as the ‘linear model’ (denoted by Optil). The derivation of linearized optimality model here is identical to Katul et al. (2010) except that they assumed \( c_a \gg c_p \) and thus neglected the latter.

**Appendix C. Radiation attenuation within the foliage**

A simple horizontal slab model was used to provide the within-canopy light regime needed in gas-exchange calculations. The attenuation of the direct beam \( (r_d) \) and diffuse \( (r_d) \) radiation were modeled, respectively, as (Campbell and Norman, 1998)

\[
r_d(\psi) = \exp[-K_d(\psi)] L_d(z) \Pi \tag{C.1}
\]

\[
r_d = \exp[-K_d] L_d(z) \Pi \tag{C.2}
\]

where \( L_d(z) \) is the cumulative plant area density above \( z \) and \( \Pi \) is a clumping factor which accounts for the shading effect by other leaves (Stenberg, 1998). The extinction coefficient of direct PAR, defined here as \( K_d \), for an ellipsoidal leaf distribution can be determined as (Campbell and Norman, 1998):

\[
K_d(\psi) = \frac{(x^2 + \tan^2 \psi)^{0.5}}{x + 1.774(x + 1.182)^{-0.733}} \tag{C.3}
\]

where \( \psi \) is the solar zenith angle and \( x \) is the leaf angle distribution index. Here we assume \( x \) to be unity (spherical leaf angle distribution), which is reasonable for the coniferous foliage. The attenuation of diffuse PAR is independent of direction and we set \( K_d = 0.7 \) based on the measurements.

At each layer the fraction of sunlit leaves is given by Eq. (C.1) and PAR at sunlit \( (Q_{d1}) \) and shaded \( (Q_{d0}) \) leaves, respectively, by

\[
Q_{d1} = Q_{d0} + Q_{dc} + r_d Q_{d0} \tag{C.4}
\]

\[
Q_{d0} = r_d Q_{d0} + Q_{dc} \tag{C.5}
\]

where \( Q_{dc} \) and \( Q_{d0} \) are the beam and diffuse radiation above the canopy. \( Q_{dc} \) is the down-scattered beam radiation

\[
Q_{dc} = \exp[-\sqrt{\alpha K_d(\psi)} L_d(z) \Pi] Q_{d0} \tag{C.6}
\]

where \( \alpha \) is the PAR absorptivity of the leaf (0.8).

**References**


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