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Comparison of different stomatal conductance algorithms for ozone flux modelling

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A comparison of an empirical and a semi-mechanistic stomatal conductance algorithm for European crop and forest species reveals a similar predictive capability.

Abstract

A multiplicative and a semi-mechanistic, BWB-type [Ball, J.T., Woodrow, I.E., Berry, J.A., 1987. A model predicting stomatal conductance and its contribution to the control of photosynthesis under different environmental conditions. In: Biggens, J. (Ed.), Progress in Photosynthesis Research, vol. IV. Martinus Nijhoff, Dordrecht, pp. 221–224.] algorithm for calculating stomatal conductance (g_s) at the leaf level have been parameterised for two crop and two tree species to test their use in regional scale ozone deposition modelling. The algorithms were tested against measured, site-specific data for durum wheat, grapevine, beech and birch of different European provenances. A direct comparison of both algorithms showed a similar performance in predicting hourly means and daily time-courses of g_s, whereas the multiplicative algorithm outperformed the BWB-type algorithm in modelling seasonal time-courses due to the inclusion of a phenology function. The re-parameterisation of the algorithms for local conditions in order to validate ozone deposition modelling on a European scale reveals the higher input requirements of the BWB-type algorithm as compared to the multiplicative algorithm because of the need of the former to model net photosynthesis (A_n).

Keywords: Stomatal conductance; Photosynthesis; Modelling; Parameterisation

1. Introduction

Tropospheric or ground level ozone is a phytotoxic pollutant causing serious damage to agricultural productivity, forest health and semi-natural ecosystems (e.g. Ashmore, 2005). The extensive body of evidence, both observational and experimental, that has been collated since the first observations of ozone injury has provided the impetus to develop air quality management strategies and formulate emission reduction policies to limit the negative effects of this pollutant. During this time, an effect based approach, introduced by the United Nations Economic Commission for Europe Convention on Long-range Transboundary Air Pollution (CLRTAP) (Working Group on Effects, 2004), have provided the basis to characterise ozone

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concentrations so as to enable prediction of ozone levels above which significants effects may be discernable on vegetation. Initial attempts to characterise ozone concentrations led to the development of a number of different concentration based indices (e.g. Mauzerall and Wang, 2001) that attempt to relate ozone impacts to the measured or modelled ambient ozone concentrations. However, there is general consensus that ozone-induced phytotoxic effects such as foliar injury, premature senescence and reduced biomass are more closely related to the cumulative ozone uptake than to external ozone exposure (Fuhrer and Achermann, 1999; Massman et al., 2000; Wieser et al., 2000). This finding highlights the importance of the behaviour of the stomates, the main regulator of the gas exchange of plants, as being crucial in determining the potential damage caused by ozone. In order to perform pan European risk assessments, as are required to meet the needs of the UNECE CLRTAP, there is a need to be able to accurately model stomatal conductance (and hence ozone flux) for key species representing different vegetation types namely crops, forests and semi-natural vegetation. A combination of such a model, that also incorporates non-stomatal ozone deposition, with a regional scale photo-oxidant model provides estimates of total ozone flux or ozone deposition (e.g. Emberson et al., 2001; Simpson et al., 2003) and hence risk across broad geographical regions.

Despite evidence of stomatal behaviour being driven by environmental parameters such as photosynthetic photon flux density (PPFD), vapour pressure deficit (VPD), air temperature and soil water potential (SWP) (e.g. Jones, 1992), mechanistic models of stomatal conductance (g_s) do not yet exist due to incomplete understanding of the complex physiological mechanisms of stomatal response to combinations of these parameters. Instead, (semi-)empirical approaches have been developed and proved successful in modelling stomatal conductance. Two types of algorithms have been widely used to predict stomatal conductance. The first is the multiplicative algorithm developed by Jarvis (1976) and further developed specifically to model ozone uptake to plants (e.g. Emberson et al., 2000; Grünhage et al., 2000) that calculates g_s as a function of phenology, PPFD, temperature, VPD and soil moisture related parameters. The second type of algorithm is the semi-mechanistic type of model that was initially developed by Ball et al. (1987), hereafter referred to as the BWB-algorithm. It is based on the evidence of a close relationship between g_s and net photosynthetic rate (A_n), which provides the link between the exchange of gases (e.g. CO_2, H_2O, O_3) and the prevailing climatic conditions. The BWB-algorithm calculates g_s as a function of A_n, CO_2 concentration and relative humidity, the two latter referring to the leaf surface. Stomatal responses to CO_2, PPFD and temperature are included by means of an A_n model. In contrast with the multiplicative algorithm, these responses act synergistically.

Currently, the UNECE CLRTAP uses the EMEP photo-oxidant model (Simpson et al., 2003) to estimate ozone concentration profiles across Europe, in order to compare a range of different ozone precursor emission scenarios for policy evaluation. To assess ozone loss from the atmosphere to the ground surface the model employs an ozone deposition module referred to as DO_3SE (Deposition of Ozone for Stomatal Exchange) that has been developed and applied specifically for use within the EMEP photo-oxidant model (Emberson et al., 2000; Simpson et al., 2003). DO_3SE models both non-stomatal (e.g. leaf and soil surfaces) and stomatal deposition, the latter currently estimating stomatal conductance (for stomatal ozone flux) using a multiplicative based g_s algorithm as described in Emberson et al. (2000) and Simpson et al. (2003).

The BWB-algorithm has become increasingly popular in combination with photosynthesis models (e.g. Farquhar et al., 1980) for plant growth simulations at different spatial scales (Nikolov and Zeller, 2003; Baldocchi, 1997; Arora, 2003). Since the BWB-algorithm offers the capability to model ozone-induced changes of the photosynthetic rate, it is of interest for ozone impact assessment (e.g. Weinstein et al., 1998).

However, few comparisons, all concentrating on tree species, of the performance of the two modelling approaches against measured stomatal conductance data have been presented so far (Van Wijk et al., 2000; Misson et al., 2004; Uddling et al., 2005). This paper reports a comparison of the ability of these two modelling approaches, represented by the DO_3SE (multiplicative) and the LEAFC3 (BWB-algorithm) models to predict g_s for a range of species located across Europe. Nikolov et al. (1995) developed the generic leaf-level photosynthesis model LEAFC3 which implements a BWB-algorithm for the calculation of g_s. The main aim of this study is to test how appropriate the two different g_s algorithms are for use in regional scale ozone deposition models. Therefore, both g_s modelling approaches have been evaluated focussing on (i) the model (input) requirements, (ii) the parameterisation requirements and (iii) the performance of the models in predicting g_s against site-specific data. The models were parameterised for two crop (grapevine (*Vitis vinifera*) and durum wheat (*Triticum durum*)) and two tree (beech (*Fagus sylvatica*) and birch (*Betula pendula*)) species and have been applied using data sets that have been collected from sites across Europe encompassing different European regions (North, Central and South Europe). The data sets each comprised the necessary environmental variables that are required as inputs to both models along with corresponding g_s observations.

2. Data

Four European data sets were identified to evaluate g_s predicted using the algorithms described above: (i) a Mediterranean grapevine data set from Spain (Jacobs et al., 1996), (ii) a boreal birch data set from Finland (Oksanen, 2003), (iii) a temperate beech data set from Switzerland (Novak, pers. comm.) and (iv) a Mediterranean wheat data set from Spain (de la Torre, 2004).

Tables 1 and 2 describe the four data sets, listing the range of the key meteorological, physiological and phenological variables. The model runs were performed using minute-by-minute (i.e. initial time steps of measurements) input data, however,

Table 1
Description of locations, species, experiments and instruments used to provide stomatal conductance data

Country	Site	Latitude	Longitude	Experimental set-up	g_s-instrument	Species
Spain	Tomelloso	39° 10′ N	3° 1′ W	Field	IRGA	Grapevine
Spain	Alcalá de Henares	40° 31′ N	3° 22′ W	Field	IRGA	Durum wheat
Switzerland	Lattecaldo	45° 51′ N	9° 3′ E	OTC	IRGA	Beech
Finland	Kuopio	62° 13′ N	27° 35′ E	Field	Porometer	Birch

the results are presented as hourly means. The conversion to hourly means ensures that g_s measurements reflect the prevailing meteorological conditions since it is acknowledged that changes in g_s will often lag behind changes in environmental variables and are consistent with the time step used in regional scale deposition modelling. Additional analysis was also performed with pooled g_s data to provide diurnal and seasonal time courses of g_s allowing analysis of the algorithm's ability to predict the general temporal trends in stomatal conductance. Note that the beech data set contains a constant PPFD-value of 1500 μmol m^{-2} s^{-1}.

A common problem with all data sets was the lack of information describing soil water status, a variable necessary as input to both g_s models. As such, it has been necessary to assume that water availability was not limiting to g_s over all observation periods. Although this might reduce the predictive performance of the g_s models, the results should still be comparative between models since the assumption of non-limiting soil water is consistent between algorithms.

3. Modelling

3.1. Model formulation

The multiplicative g_s algorithm currently used in the DO_3SE model is given in Eq. (1) and described in more detail in Emberson et al. (2000).

$$g_{sto} = g_{max} f_{phen} f_{light} \max\{f_{min}(f_{temp} f_{VPD} f_{SWP})\} \tag{1}$$

where g_{sto} (mmol O_3 m^{-2} s^{-1}) is the actual g_s and g_{max} (mmol O_3 m^{-2} s^{-1}) is the maximum g_s occurring during the growing season. The factors f_{phen}, f_{light}, f_{temp}, f_{VPD} and f_{SWP} represent the modification of g_{max} due to leaf phenology, irradiance, air temperature, vapour pressure deficit (VPD) and soil water potential (SWP), respectively. f_{min} represents the minimum daytime g_s observed under field conditions before the onset of permanent wilting point (PWP). All the f functions are expressed in relative terms between 0 and 1.

The photosynthesis-based algorithm is given in Eq. (2) as described in Nikolov et al. (1995).

$$g_{sto} = g_{min} + mA_n\frac{h_b}{C_b} \tag{2}$$

where g_{sto} (mmol O_3 m^{-2} s^{-1}) is the actual g_s, g_{min} (mmol O_3 m^{-2} s^{-1}) is the minimum daytime g_s observed under field conditions, A_n (μmol CO_2 m^{-2} s^{-1}) is the net assimilation rate and m is a dimensionless slope representing the species-specific composite sensitivity of g_s to A_n, the CO_2 concentration at the leaf surface (C_b; μmol mol^{-1}) and the relative humidity at the leaf surface (h_b; decimal fraction). A_n can either be supplied from measured data or, as in LEAFC3, modelled as a function of irradiance and temperature according to Farquhar et al. (1980). These two environmental parameters define the plant's biochemical activity by directly influencing the species-specific maximum rate of carboxylation (V_{cmax}) and electron transport (J_{max}).

3.2. Model parameterisation

When considering the suitability of the two algorithms described above for use in DO_3SE and hence application at the regional scale, it is important to consider how well a generic parameterisation is able to represent individual species at specific locations. As such the default parameterisation of the multiplicative model (i.e. the current DO_3SE parameterisation), and where possible, literature based parameterisation of the BWB-model is shown in relation to local values in Tables 3 and 4. The use of local parameterisation in the model runs performed ensured that model comparisons were affected as little as possible by difficulties associated with establishing parameterisation of model functions for site-specific locations. However, it should be noted that local parameterisation is

Table 2
Range of main meteorological, physiological and phenological parameters for grapevine, wheat, beech and birch (value in brackets indicates mean)

Parameter	Grapevine	Wheat	Beech	Birch	Units
Temperature	13.1–40.0 (28.4)	18.0–43.2 (30.5)	21.2–31.7 (26.8)	14.8–23.6 (20.0)	°C
VPD	0.5–5.9 (2.7)	0.2–7.3 (2.7)	1.0–2.8 (1.8)	0.1–1.6 (1.0)	kPa
PPFD	2.0–2133.0 (784.6)	65.0–2349.7 (1360.0)	1500.0 (constant)	10.0–1870.0 (762.8)	μmol m^{-2} s^{-1}
g_s	1.7–251.3 (97.8)	21.8–504.0 (169.4)	22.4–714.0 (216.9)	13.5–450.6 (181.1)	mmol H_2O m^{-2} s^{-1}
A_n	−0.2–20.7 (7.9)	−0.4–46.5 (11.9)	1.9–15.2 (9.1)	–	μmol CO_2 m^{-2} s^{-1}
Measuring period (no. of measuring days)	17/6–28/6 (7)	19/4–12/6 (16)	11/5–4/10 (9)	18/6–1/8 (11)	–
n	615	193	272	1246	–

Table 3
Parameterisation of the multiplicative g_s algorithm based on local data for grapevine, durum wheat, beech and birch (values in brackets represent default DO$_3$SE parameterisation as described in Simpson et al. (2003) and Emberson et al. (2005a,b)

Parameter	Grapevine	Wheat	Beech	Birch	Units
g_{max}	153 (215)	310 (450)	340 (140)	200 (275)	mmol O$_3$ m^{-2} PLA s^{-1}
f_{min}	0.1 (0.01)	0.03 (0.01)	0.1 (0.13)	0.1 (0.13)	Fraction
SGS	120 (120)	109 (119)	120 (90)	140 (90)	Day of year
EGS	300 (300)	164 (174)	310 (270)	263 (270)	Day of year
f_{phen_a}	0.05 (0.2)	0.5 (0.8)	0.1 (0.3)	0.1 (0.3)	Fraction
f_{phen_b}	40 (60)	35 (15)	100 (50)	30 (50)	Days
f_{phen_c}	70 (45)	12 (40)	40 (50)	30 (50)	Days
light_a	0.002 (0.0076)	0.01 (0.0105)	0.026 (0.006)	0.001 (0.006)	Constant
T_{min}	9 (9)	7 (12)	17 (−5)	−5 (−5)	°C
T_{opt}	32 (30)	34 (26)	25 (22)	20 (22)	°C
T_{max}	45 (43)	50 (40)	39 (35)	39 (35)	°C
VPD$_{max}$	0.6 (1.6)	2.3 (1.2)	1.1 (0.93)	0.9 (0.93)	kPa
VPD$_{min}$	6.2 (6.2)	6.9 (3.2)	3.0 (3.4)	3.0 (3.4)	kPa

SGS = start of growing season, EGS = end of growing season, f_{phen_a} = minimum of f_{phen}, f_{phen_b} = number of days for f_{phen} to reach its maximum, f_{phen_c} = number of days for f_{phen} during decline to again reach the minimum. PLA = Projected Leaf Area.

more easily defined for the multiplicative algorithm (which assumes model functions to be independent of each other) than for the photosynthesis-based algorithm (in which parameters such as V_{cmax} and J_{max} are closely related to each other (cf. Leuning, 2002)).

Table 3 lists the input parameters required by the multiplicative g_s algorithm and their site-specific parameterisation for grapevine, durum wheat, beech and birch. The site-specific parameterisation was achieved by fitting boundary lines to the g_s relationships that gave optimal model performance in comparison with observations. The default DO$_3$SE parameterisation representing mean European growing conditions is shown in brackets. Definitions of the functions representing the relationships between g_s and environmental and phenological parameters can be found in Emberson et al. (2000). It should be noted that the wheat site-specific parameterisation is for *T. durum*, whereas the DO$_3$SE model is only parameterised for *Triticum aestivum.*

Table 4 shows the main input parameters required by LEAFC3 and its parameterisation for the same species as mentioned above. Note that apart from m all shown parameters are related to the photosynthesis module of LEAFC3. To represent local conditions, the parameters m, V_{m25} (V_{cmax} at 25 °C) and J_{m25} (J_{max} at 25 °C) were adjusted: m has been calculated according to a methodology described in Müller et al. (2005) which uses measured data. However, for birch no measured A_n data were available, and therefore a value provided by Nikolov (1997) for deciduous trees was used. V_{m25} and J_{m25} were varied within a data range (see brackets) derived from a comprehensive literature review, always ensuring a ratio J_{m25}/V_{m25} of 2.0 ± 0.6 as suggested by Leuning (2002). The temperature response functions (not shown) for the parameters J_{m25}, R_d (mitochondrial respiration), Γ (CO$_2$ compensation point in the absence of mitochondrial respiration), K_{c25} and K_{o25} (Michaelis–Menten constant of Rubisco for carboxylation and oxygenation at 25 °C, respectively) were taken from a recently published revision of LEAFC3 by Müller et al. (2005), whereas the temperature response function for V_{m25} remained the same as in Nikolov et al. (1995). For C$_3$ plants the parameters K_{c25} and K_{o25} (Table 4) only vary within a small range and therefore were considered to be constant here with values according to Bernacchi et al. (2001).

4. Results

Based on both algorithms, Table 5 shows the percentage of the variation in observed values that is explained by the two models, averaged over hourly, daily and seasonal time steps. This comparison reveals a substantial amount of unexplained variation, in particular for the data set of hourly means, for which the unexplained variation ranges from 77% (wheat using the multiplicative algorithm) to 33% (beech using

Table 4
Parameterisation of LEAFC3 for grapevine, wheat, beech and birch based on published data and calculations using local data (italics)

Parameter	Grapevine	Wheat	Beech	Birch	Units	Reference
m	*6.14*	*8.12*	*16.83**	13.5	–	*After* Müller et al. (2005), Nikolov et al. (1995)
V_{m25}	*100* (50–100)	*180* (25–261)	*30* (28–66)	*35* (28–169)	μmol m^{-2} s^{-1}	*See text*
J_{m25}	*225* (120–260)	*400* (87–522)	*60* (52–128)	*70* (80–230)	μmol m^{-2} s^{-1}	*See text*
K_{c25}	404.09	404.09	404.09	404.09	μmol mol^{-1}	Bernacchi et al. (2001)
K_{o25}	278.40	278.40	278.40	278.40	mmol mol^{-1}	Bernacchi et al. (2001)
g_{min}	*0.05*	*0.02*	*0.03*	*0.03*	mol m^{-2} s^{-1}	*Obtained from g_s in dark*

m = Species-specific composite sensitivity of g_s to A_n, V_{m25} = maximum rate of carboxylation at 25 °C, J_{m25} = maximum rate of potential electron transport at 25 °C, K_{c25} and K_{o25} = Michaelis–Menten constant of Rubisco for carboxylation and oxygenation at 25 °C, respectively. Values in brackets represent the range of V_{m25} and J_{m25} derived from a comprehensive literature review.

Table 5
Performance (R^2-values of observed vs. modelled g_s) of both algorithms applied to four different data sets representing grapevine, wheat, birch and beech

	Hourly means		Diurnal course		Seasonal course	
	Multiplicative	BWB	Multiplicative	BWB	Multiplicative	BWB
Grapevine (*Vitis vinifera*)	0.39 (9.49; *10.13*)	0.40 (4.83; *5.16*)	0.77	0.78	–	–
Wheat (*Triticum durum*)	0.23 (−59.79; *31.19*)	0.29 (11.44; *5.97*)	0.72	0.82	–	–
Birch (*Betula pendula*)	0.30 (40.04; *23.08*)	0.33 (2.37; *1.37*)	0.48	0.32	0.55	0.45
Beech (*Fagus sylvatica*)	0.67 (−26.76; *12.01*)	0.04 (18.62; *8.36*)	0.95	0.62	0.77	0.03

The values in brackets represent the mean residual g_s (observed minus modelled) in mmol O_3 m^{-2} s^{-1} and the percentage of this value of the mean observed g_s (italics). Diurnal time courses are based on hourly mean values for g_s for all measuring days (cf. Table 2), seasonal time courses are based on hourly means of all measuring days representing the hours from 11:00 until 13:00 and 10:00 until 14:00 for birch and beech, respectively.

multiplicative algorithm) (Table 5). Apart from the beech data set, which was of limited use for testing the BWB-algorithm due to its constant PPFD-value, the differences in performance between multiplicative and BWB-algorithm were small.

The mean residuals (observed minus modelled) of hourly g_s values were higher for the multiplicative than the BWB-algorithm, with the application of the former leading on average to an over-prediction of g_s for wheat (31.19% of mean observed g_s) and beech (12.01%) and an under-prediction for birch (23.08%) and grapevine (10.13%) (Table 5). The BWB-algorithm on average underpredicted g_s for all species. However, the residuals were always less than 10% of the mean observed g_s.

The ability of the models to predict mean diurnal time courses of g_s was consistently greater than their ability to predict individual hourly mean values (Table 5), except for the BWB-algorithm with birch. The diurnal g_s-profiles based on hourly means showed good correspondence between observed and modelled data for grapevine and wheat (Table 5, Figs. 1 and 2). In terms of grapevine, both algorithms performed well for the morning hours before showing an increase in divergence between observed and modelled data in the afternoon (Fig. 1). Only the observed g_s-peak at 4 p.m., which is the mean of two measuring days, wasn't predicted by either algorithm. The multiplicative algorithm generally led to an over-prediction of g_s for wheat (Fig. 2) and an under-prediction for birch (Fig. 3), whereas the BWB-algorithm over-predicted g_s for the midday hours but under-predicted it in the morning (only for wheat) and afternoon for both wheat and birch. In general, the modelled diurnal g_s-courses for birch showed only small amplitudes when compared with observed data (Fig. 3). Fig. 4 again demonstrates the difficulties of applying the BWB-algorithm to the beech data set, whereas the multiplicative algorithm performs much better with a slight over-prediction of g_s between 10 a.m. and 12 a.m. However, no statements can be made regarding the performance of both algorithms for afternoon hours because of a lack of data for that time-period.

In order to test the algorithms' ability to account for the variation in g_s over the course of the growing season due to changes in plant-physiological activity, seasonal profiles of modelled and observed midday-g_s for birch and beech are shown in Figs. 5 and 6, respectively. For birch, the fit between modelled and observed g_s was improved using daily means when compared with individual hourly means (Table 5). Though generally showing a good fit, the modelled g_s increasingly differed from the observed g_s later in the growing season. In contrary, for beech the multiplicative algorithm performed better from August on as compared with the beginning of the growing season, whereas the BWB-algorithm could not reproduce the observed seasonal variation at all.

A similar comparison for the crop species was not possible due to the nature of the input data.

5. Discussion

The performance of both modelling approaches, when assessed on an hourly mean basis, is generally rather similar, with the exception of beech for which the multiplicative model performs far better than the BWB-algorithm (with R^2 values of 0.67 and 0.04, respectively). However, in comparison with the

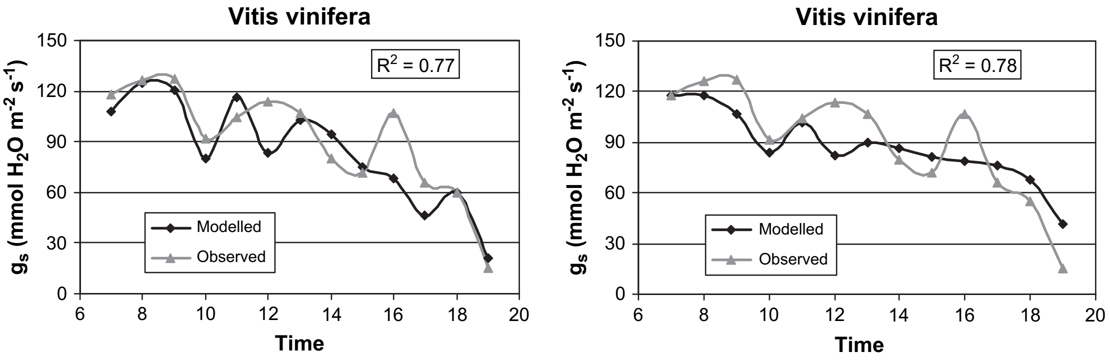

Fig. 1. Daily time course (07:00–19:00 hrs) of modelled and observed g_s (mmol H_2O m^{-2} s^{-1}) averaged over 7 days in June 1991 for Mediterranean grapevine using the multiplicative algorithm (left) and the BWB-algorithm (right).

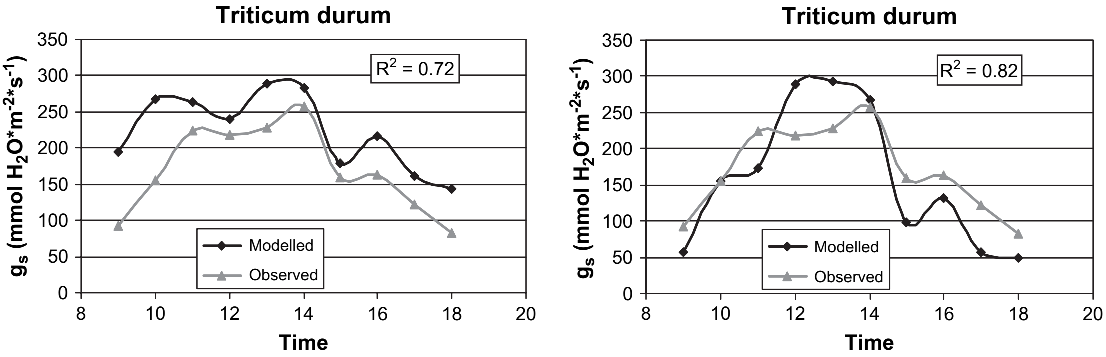

Fig. 2. Daily time course (09:00–18:00 hrs) of modelled and observed g_s (mmol H_2O m^{-2} s^{-1}) averaged over 16 days between April and June 2000, 2001 and 2002 for Mediterranean durum wheat flag leaves using the multiplicative algorithm (left) and the BWB-algorithm (right).

BWB-algorithm, there is greater systematic bias in the g_s predictions using the multiplicative algorithm (Table 5). It is evident that both models are not performing as well as have been found in other similar studies (e.g. Van Wijk et al., 2000; Misson et al., 2004; Uddling et al., 2005). Jacobs et al. (1996) applied a photosynthetic-based algorithm to the grapevine data set presented here and obtained R^2 values of up to 0.66 between predicted and observed values of g_s. The better performance of all these studies may well be due to their site-specific scope, developing formulations (not just parameterisations) that may be more representative of local conditions at particular sites. This was not possible or desirable in this study since the intention here is to compare predictive capabilities of the models designed for generic application over broad geographical scales.

However, when the models are compared over diurnal and seasonal time courses the results appear to improve, indicating that both modelling approaches are capable of capturing major temporal trends in conductance. The commonly observed midday depression for g_s – as seen here for wheat, birch and to a lesser extent grapevine, but not for beech – and the decline of g_s in the afternoon hours was predicted by both algorithms.

Arguably, in terms of modelling stomatal ozone uptake these general trends are more important than individual hourly means, as ensuring that the appropriate co-variation in g_s with the variation in ozone concentrations is crucial since the advantage of the flux-based approach is often cited as the ability to predict when stomatal responses will constrain ozone uptake at elevated ozone concentration. In using seasonal cumulative flux indices, it is the ability to predict diurnal and seasonal variations with precision that is more important than the ability to predict every hourly mean value accurately.

The fact that both models seem capable of predicting afternoon closure of the stomata, which is likely to be driven by increasing atmospheric water deficits (e.g. as observed for grapevine and wheat), might indicate that appropriate g_s responses are being modelled for prevailing environmental conditions. In addition, the ability of the models to simulate the rather constant g_s values of birch (which are probably due to the measurement period being only between the hours of 10.00 and 15.00 hrs) also indicates that the models can simulate near optimal conditions reasonably well (the observed g_s values are close to the maximum for this species).

The improved model results for wheat using the BWB-algorithm may be explained by the optimisation of the LEAFC3 model parameterisation for this species published by Müller et al. (2005), which was implemented where appropriate in the modelling applied in this analysis. For beech, the multiplicative model performs better diurnally; the poor performance of the BWB-algorithm is most likely related to the fact that the saplings were observed under constant saturated light conditions, which will result in a lack of variation in g_s since light is a key driver of A_n.

Over the seasonal time course the multiplicative model consistently outperformed the BWB-algorithm for both beech and birch. This is to be expected since the multiplicative model incorporates a phenology function in contrast to the

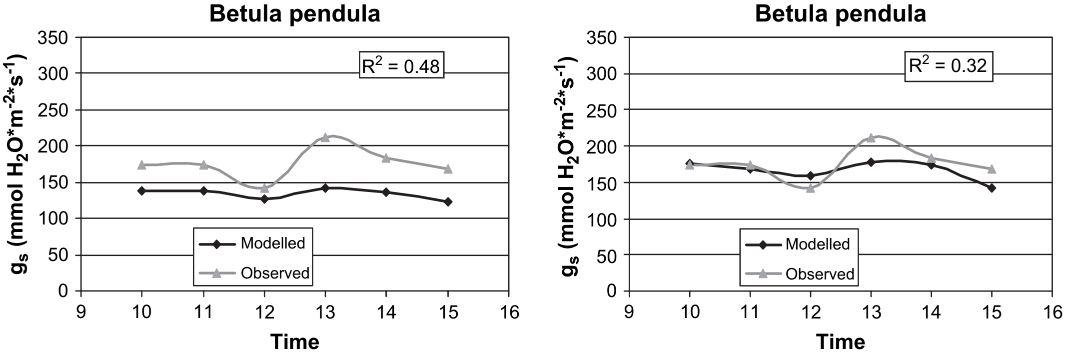

Fig. 3. Daily time course (10:00–15:00 hrs) of modelled and observed g_s (mmol H_2O m^{-2} s^{-1}) averaged over 11 days between June and August 2001 for boreal birch using the multiplicative algorithm (left) and the BWB-algorithm (right).

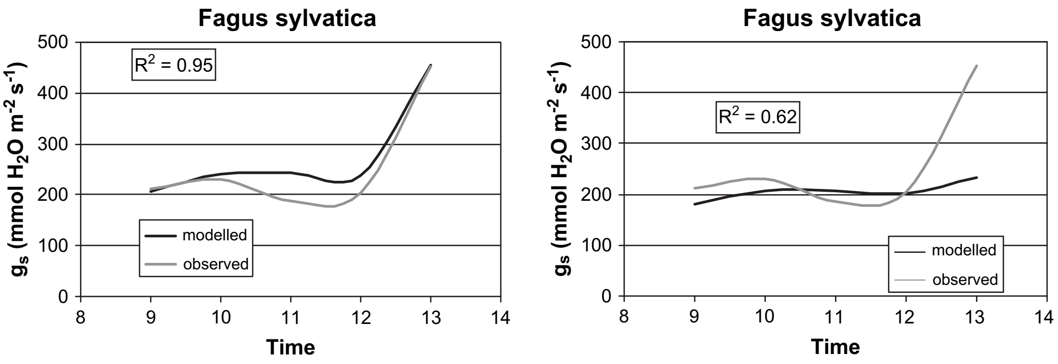

Fig. 4. Half-daily time course (09:00–13:00 hrs) of modelled and observed g_s (mmol H_2O m^{-2} s^{-1}) averaged over 9 days between May and October 2004 for beech using the multiplicative algorithm (left) and the BWB-algorithm (right).

BWB-algorithm. The inability to account for seasonally determined modulation in g_s is often cited as a problem related to the BWB-type models. One way to overcome this problem is the introduction of a parameter representing the variation in photosynthetic capacity over the course of the growing season, such as the leaf nitrogen content. For example, Müller et al. (2005) have developed a nitrogen-sensitive extension of the LEAFC3 model which improved the predictive performance when being applied to wheat.

One of the key issues in the overall comparison work performed here is that of parameterisation of the models. Firstly, it should be recognised that re-parameterisation for local conditions is far easier to achieve for the multiplicative model since this algorithm assumes that all required variables are independent of each other. However, this is also a weakness of the multiplicative algorithm, since in nature the variables are often dependant and act synergistically. Previous studies (e.g. Emberson et al., 2000; Tuovinen et al., 2001) have highlighted the strong dependency of the multiplicative model on g_{max}. In the modelling performed here the uncertainty in this parameter is reduced since g_{max} is here derived from the data sets. However, the importance of this parameter is clearly demonstrated by this analysis since the local g_{max} values for grapevine, wheat and beech are rather different from the DO3SE model default g_{max} values, although in the case of beech this may well be explained by growth of the saplings in open top chambers. The difference between observed and predicted daily courses of g_s using the multiplicative algorithm for wheat and birch is likely to be related to the fact that the g_{max} values used in this study were derived from primary data sets, hence might not represent optimal species-specific gas exchange conditions.

In terms of the other multiplicative model parameters, those that deviate most from the default values are the f_{temp} and f_{VPD} functions. In terms of wheat, this is not surprising since the default data are for *T. aestivum*, whereas this study used *T. durum*. The latter is better adapted to local Mediterranean conditions which require the capacity to maintain gas exchange at higher temperatures and atmospheric water deficits than more temperate counterparts. This is also the case for the grapevine cultivar used here, which is well adapted to Mediterranean climates, whereas the default parameterisations account for grapevine grown in Central Europe.

For the BWB-algorithm, the key species-specific parameters (i.e. V_{m25}, J_{m25} and their associated temperature response functions) were defined based on published values. Table 4 shows that the range in these values, even within species, is large and the local parameterisation tends towards the extremes of the range. In addition, the parameterisation of the parameter m of the BWB-algorithm is essential because it defines the "composite sensitivity" of g_s to A_n. Several studies (Wohlfahrt et al., 1998; Kosugi et al., 2003; Müller et al.,

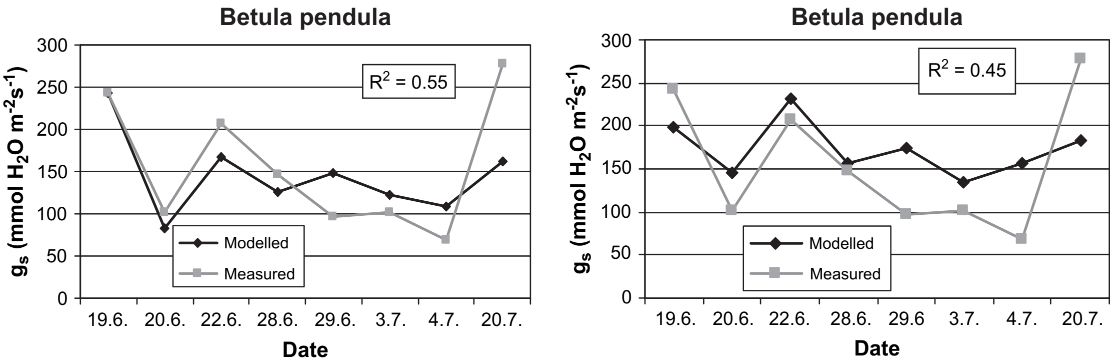

Fig. 5. Seasonal time course (5 weeks during the summer of 2001) of modelled and observed g_s (mmol H_2O m^{-2} s^{-1}) averaged over midday hours (11:00–13:00 hrs) for boreal birch using the multiplicative algorithm (left) and the BWB-algorithm (right).

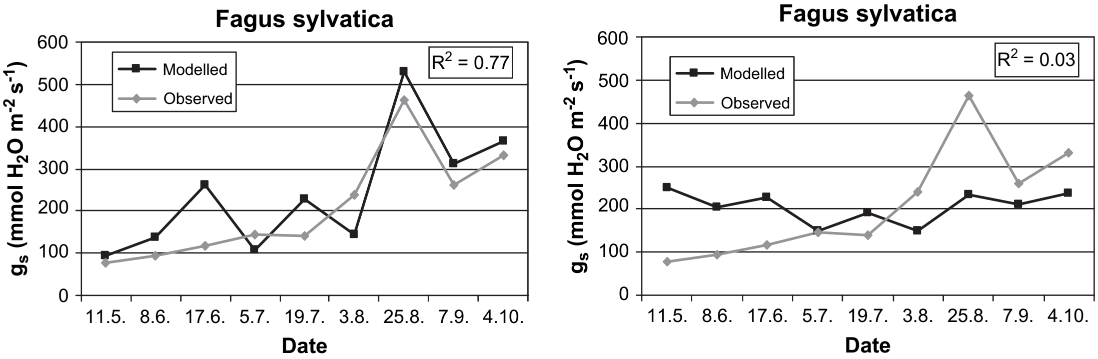

Fig. 6. Seasonal time course (5 months during the summer of 2004) of modelled and observed g_s (mmol H_2O m^{-2} s^{-1}) averaged over midday hours (10:00–14:00 hrs) for beech using the multiplicative algorithm (left) and the BWB-algorithm (right).

2005) have shown that this parameter might change with leaf age, which was not accounted for in this study. However, the parameterisation of m for the four species used here is in good agreement with published values for various crop and tree species (cf. Wullschleger, 1993).

Leuning (1995) stressed the theoretical weakness of the BWB-type models because of their reliance on relative humidity rather than VPD. It has been shown that evaporative loss is a main driver for stomatal aperture, which can be expressed by VPD changes but not by changes in relative humidity. However, there is evidence that when applying BWB-type models to field data showing varying VPD values due to temperature changes, as is the method used here, the predictive performance of both approaches (relative humidity vs. VPD) is very similar.

One of the key limitations to this comparison has been the inability to incorporate the effects of soil moisture deficit (SMD) on g_s. Although not used in this analysis due to the lack of data describing the water status of the soil system, both algorithms do have the capability to predict drought effects on g_s. The multiplicative algorithm used in DO$_3$SE incorporates a relationship relating soil water potential (derived from g_s observations with pre-dawn leaf water potential) to g_s, whereas LEAFC3 accounts indirectly for the effect of SMD on stomata via the alteration of m as a function of leaf water potential (Nikolov et al., 1995).

Finally, the main purpose of this paper was to assess both models, performance in the context of their applicability for use within a regional scale ozone deposition model (e.g. DO$_3$SE). The higher input requirements of the BWB-algorithm are an obvious limitation (both in terms of input and parameterisation data) to application at the regional scale. The main reason for this is that net photosynthesis (A_n) is required as an input parameter. Since information on A_n is not always readily available, and certainly not available on a regional scale, BWB-type models are often connected with photosynthesis models (e.g. LEAFC3) which require detailed and species-specific plant-physiological input parameters (e.g. V_{m25}, J_{m25}, K_{c25}, K_{o25}) which are often difficult to obtain. In fact, in the absence of experimental plant-physiological (primary) data, users usually have to rely on secondary data from the literature. As such, even though the semi-mechanistic nature of the BWB-algorithm provides a more process-based approach to modelling g_s, this may not be perceived as reason enough given the increased data requirements and model run times that would be necessary for a regional scale application of the model for ozone deposition studies. In addition, since the results presented in this paper do not show significant improvements in the prediction of g_s using the BWB-algorithm compared with the multiplicative algorithm (in some cases the predications are less favourable, especially over a seasonal time course) it would not seem appropriate to suggest using such models in present-day regional scale deposition modelling schemes.

However, while the multiplicative algorithm might be favourable for regional scale g_s predictions, the photosynthesis-based algorithm might give beneficial additional information on the relationship between ozone flux and impacts on a local scale, provided that key parameters are available. In particular, photosynthesis-based models provide a means of linking ozone uptake directly to effects on photosynthesis making it possible to perform process growth modelling to understand ozone sensitivities to carbon dynamics, e.g. carbon allocation assessments (e.g. as possible with the TREGRO model of Weinstein et al., 1991).

In the longer term, photosynthesis-based models may also have the advantage in estimating g_s under future climate change conditions, since the influence of elevated CO$_2$ is directly incorporated in the g_s algorithm.

6. Conclusions

In summary, the comparison of observed and modelled g_s for durum wheat, grapevine and birch showed a similar performance for both the multiplicative algorithm and the BWB-algorithm, with the former slightly outperforming the latter in calculating seasonal courses of g_s. The beech data set proved to be unsuitable for the BWB-algorithm due to its constant irradiance values. In general, both algorithms were able to predict the observed trends over the course of the day and the season, i.e. a steady increase in g_s in the morning, followed by a midday depression, a subsequent recovery and a steady decline from mid-afternoon on, as well as a steady increase in g_s at the beginning of the growing season as shown for beech. The main drivers for these trends are thought to be the temperature and VPD. Furthermore, SMD, which couldn't be taken into account in this study, is expected to have a strong effect on the seasonal time course of g_s.

However, the performance of the algorithms was not as good as reported in previous studies. This result might be attributed to site-specific model alterations (i.e. not only parameterisation) in previous studies and to the nature of the data used in this study.

A site-specific parameterisation of the algorithms accounting for local growing conditions, which is desirable to validate ozone deposition modelling on a regional scale, reveals the higher input requirements of the BWB-algorithm as compared to the multiplicative algorithm because of the need of the former to first model net photosynthesis (A_n). The most important input parameters that require precise parameterisation are g_{max} for the multiplicative and V_{cmax}, J_{max} and m for the BWB-algorithm.

In conclusion, this study shows that for present-day applications there is no obvious advantage in replacing the multiplicative with a BWB-algorithm for regional scale ozone deposition modelling schemes. However, advances in data acquisition techniques (e.g. remote sensing and global carbon modelling systems) combined with a more urgent need to include the influence of CO_2 under climate change conditions might favour the photosynthesis-based algorithm in the future.

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