Comparison of different stomatal conductance algorithms for ozone flux modelling

P. Büker[1*], L. D. Emberson[1], M. R. Ashmore[1], G. Gerosa[2], C. Jacobs[3], W.J. Massman[4], J. Müller[5], N. Nikolov[6], K. Novak[7], E. Oksanen[8], D. de la Torre[9], J.-P. Tuovinen[10]

** correspondence to: pb25@york.ac.uk*
[1] Stockholm Environment Institute, University of York, UK
[2] Università cattolica del Sacro Cuore, Brescia, Italy
[3] Alterra, Wageningen, The Netherlands
[4] USDA Forest Service, Rocky Mountain Research Station, Fort Collins, CO, USA
[5] Institute of Agronomy and Crop Science, Halle-Wittenberg, Germany
[6] N & T Services, Fort Collins, CO, USA
[7] Forest Ecosystems and Ecological Risk, Swiss Federal Research Institute WSL, Birmensdorf, Switzerland
[8] Department of Biology, University of Joensuu, Joensuu, Finland
[9] Institute for Energetics, Environment and Technological Research (CIEMAT), Madrid, Spain
[10] Finnish Meteorological Institute, Helsinki, Finland

1 Introduction

The ozone deposition model (DO_3SE) that has been developed and applied within the EMEP photo-oxidant model (Emberson et al., 2000, Simpson et al. 2003) currently estimates stomatal ozone flux using a stomatal conductance (g_s) model based on the multiplicative algorithm initially developed by Jarvis (1976). This model links g_s to environmental and phenological parameters with a set of response functions. However, there exist a number of alternative and well established methods to calculate g_s, with the photosynthesis-based algorithm becoming increasingly more popular in situations where carbon-energy flux modelling is required at the regional or global scale. This algorithm uses a semi-mechanistic approach based primarily on the close relationship between g_s and net photosynthetic rate, which provides the link between gas (e.g. H_2O, O_3) influx and the prevailing climatic conditions (Ball et al., 1987); here we use the photosynthesis-based algorithm implemented in the generic leaf-level photosynthesis model LEAFC3 developed by Nikolov et al. (1995).

In order to find the most appropriate algorithm for use in DO_3SE, both g_s modelling approaches have been evaluated focussing on i) the model (input) requirements and ii) the performance of the models in predicting g_s using site-specific data. The models were parameterised for two crop (grapevine and wheat) and two tree (birch and beech) species and have been applied to various datasets covering different European regions (North, Central and South Europe). Ultimately, the performance of the models in predicting total ozone deposition to vegetated surfaces at a regional scale will be tested, similar to comparisons described for grapevine in Emberson et al. (this volume).

2 Parameterisation of the models

The multiplicative g_s algorithm used in DO_3SE is given by equation [1] as described in Emberson et al. (2000).

$$g_{sto} = g_{max} * f_{phen} * f_{PFD} * \max\{f_{min}, (f_{Tair} * f_{VPD} * f_{SWP})\} \quad [1]$$

where g_{sto} is the actual g_s and g_{max} is the maximum g_s occurring during the growing season. The factors

f_{phen}, f_{PFD}, f_{Tair}, f_{VPD} and f_{SWP} represent the modification of g_{max} due to phenological changes, irradiance, air temperature, VPD and soil water potential, respectively. f_{min} is the minimum daytime g_s observed under field conditions. All functions are expressed in relative terms expressed between 0 and 1.

In contrast, the photosynthesis-based algorithm is given by equation [2] as described in Nikolov et al. (1995).

$$g_{sto} = g_{min} + m * A_n * \quad [2]$$

where g_{sto} is the actual g_s, , g_{min} is the minimum daytime g_s observed under field conditions, A_n is the net assimilation rate, m is the species-specific "composite sensitivity" of g_s to A_n, h_b is the relative humidity and C_b is the CO_2 concentration at the leaf surface.

g_s and environmental and phenological parameters can be found in Emberson et al. (2000).

Table 2 shows the main input parameters required by LEAFC3 and its parameterisation for grapevine and birch. The values for V_{m25} (maximum rate of carboxylation at 25 °C) and J_{m25} (maximum rate of potential electron transport at 25 °C) have been derived from a comprehensive literature review. The temperature response functions for the parameters J_{m25}, K_{c25}, K_{o25} and ° (CO_2 compensation point in the absence of mitochondrial respiration) 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).

Since the primary aim of this paper is to compare the predictive abilities of the two g_s algorithms, both

Table 1:
Parameterisation for the multiplicative g_s algorithm based on local data for grapevine and birch (DO_3SE parameterisation in brackets, see references); 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.

Parameter	Grapevine	Birch	Units	Reference
g_{max}	153 (215)	200 (275)	mmol O_3 m^{-2} PLA s^{-1}	UNECE (2004), Emberson et al. (this volume)
f_{min}	0.1 (0.01)	0.1 (0.13)	(fraction)	UNECE (2004), Emberson et al. (this volume
SGS	120	140 (90)	day of year	UNECE (2004), Emberson et al. (this volume)
EGS	300	263 (270)	day of year	UNECE (2004), Emberson et al. (this volume)
f_{phen_a}	0.05 (0.2)	0.05 (0.3)	(fraction)	UNECE (2004), Emberson et al. (this volume)
f_{phen_b}	40 (60)	60 (50)	days	UNECE (2004), Emberson et al. (this volume)
f_{phen_c}	70 (45)	60 (50)	days	UNECE (2004), Emberson et al. (this volume)
light_a	0.002 (0.0076)	0.007 (0.006)	(constant)	UNECE (2004), Emberson et al. (this volume)
T_{min}	9 (9)	9 (-5)	°C	UNECE (2004), Emberson et al. (this volume)
T_{opt}	32 (30)	27 (22)	°C	UNECE (2004), Emberson et al. (this volume)
T_{max}	45 (43)	36 (35)	°C	UNECE (2004), Emberson et al. (this volume)
VPD_{max}	0.6 (1.6)	0.1 (0.93)	kPa	UNECE (2004), Emberson et al. (this volume)
VPD_{min}	6.2 (6.2)	2.3 (3.4)	kPa	UNECE (2004), Emberson et al. (this volume)
SWP_{max}	- (-1.2)	-0.05	MPa	UNECE (2004), Emberson et al. (this volume)
SWP_{min}	- (-0.35)	-1.5	MPa	UNECE (2004), Emberson et al. (this volume)

Table 1 lists the parameterisation required by the multiplicative g_s algorithm and shows DO_3SE and site-specific parameterisation for two of the four species included in this analysis, i.e. grapevine (*Vitis vinifera*) and birch (*Betula pendula*). Definitions of the functions representing the relationships between

models were parameterised for local conditions (see Tables 1 and 2). This is to ensure that model comparisons are affected as little as possible by difficulties associated with establishing parameterisation of model functions (e.g. see Emberson et al. this volume). However, it should be noted that local parameterisa-

Table 2:
Main input parameters required for LEAFC3 and parameterisation for grapevine and birch; 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, m = species-specific "composite sensitivity" of g_s to A_n, Mm soil moisture multiplier [0,1]. Values in brackets represent the range of V_{m25} and J_{m25} derived from a comprehensive literature review.

Parameter	Grapevine	Birch	Units	Reference
V_{m25}	70 (50-100)	60 (28-169)	µmol m^{-2} s^{-1}	Büker et al. (in prep)
J_{m25}	140 (120-260)	120 (80-230	µmol m^{-2} s^{-1}	Büker et al. (in prep)
K_{c25}	404.09	404.09	µmol mol^{-1}	cf. Müller et al. (2005)
K_{o25}	278.40	278.40	mmol mol^{-1}	cf. Müller et al. (2005)
m	8.0	9.0	-	cf. Nikolov et al. (1995)
g_{min}	0.05	0.03	mol m^{-2} s^{-1}	obtained from g_s in dark
Mm	-	-	fraction	not used so far

tion is more easily defined for the multiplicative algorithm (which assumes the model functions are independent of each other) than for the photosynthesis based model (in which parameters such as V_{m25} and J_{m25} are closely related to each other).

When considering the suitability of these models for use in the DO_3SE model intended for application across Europe, it is obviously important to consider how well the generic DO_3SE parameterisation is able to represent individual species at site-specific locations. As such the DO_3SE parameterisation, and where possible, literature based parameterisation of the photosynthesis model has been shown in relation to the local values (Table 1 and 2) and discussed in relation to the results presented in this study.

3 Description of datasets

Four European datasets have been identified to evaluate g_s using the algorithms described above: i) a Mediterranean grapevine dataset from Spain (Jacobs, 1996), ii) a boreal birch dataset from Finland (Oksanen, 2003), iii) a temperate beech dataset from

Table 3:
Origin of datasets and range of main meteorological, physiological and phenological parameters for grapevine, birch, beech and wheat (value in brackets indicates mean).

Parameter	Grapevine	Birch	Beech	Wheat	Units
Location	Tomelloso, E	Kuopio, FIN	Lattecaldo, CH	Alcalá de Henares, E	-
Temperature	13.1 - 40.0 (28.4)	14.8 - 23.6 (20.0)	21.2 - 31.7 (26.8)	13.8 - 43.2 (28.2)	°C
VPD	0.5 - 5.9 (2.7)	0.1 - 1.6 (1.0)	1.0 - 2.8 (1.8)	0.2 - 7.3 (2.3)	kPa
PPFD	2.0 - 2133.0 (784.6)	10.0 - 1870.0 (762.8)	1500.0 (constant)	7.6 - 2349.7 (641.9)	µmol m^{-2} s^{-1}
g_s	1.7 - 251.3 (97.8)	13.5 - 450.6 (181.1)	22.4 - 714.0 (216.9)	14.0 - 681.2 (184.7)	mmol H_2O
A_n	-0.2 - 20.7 (7.9)	-	1.9 - 15.2 (9.1)	-2.7 - 56.7 (12.2)	µmol CO_2 m^{-2} s^{-1}
Measuring period	17/6 - 28/6	18/6 - 1/8	11/5 - 4/10	19/4 - 12/6	-
(no. of measuring days)	(7)	(11)	(9)	(18)	
n	615	1246	272	668	-

Switzerland (Novak, pers. comm.) and iv) a Mediterranean wheat dataset from Spain (De la Torre, 2004). In addition, two further datasets for boreal Scots pine and Mediterranean wheat from Finland (Tuovinen et al., 2000) and Italy (Gerosa et al., 2003) respectively have been acquired. These two datasets contain O_3 deposition data which qualifies them for a comparison of the performance of the different g_s algorithms when used in the DO_3SE model for total ozone deposition modelling.

Table 3 describes the four datasets, listing the range of the main meteorological, physiological and phenological variables. The model runs were performed using both minute-by-minute (i.e. initial time steps of measurements) and hourly mean input data. The conversion to hourly means is intended to ensure 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. The resulting g_s-data were pooled to gain diurnal and seasonal courses of g_s to test the algorithm's ability to account for phenomena such as g_s midday depression and autumnal senescence. Due to limited space, only results for grapevine and birch will be presented in the following.

A common problem with all datasets 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. This assumption is discussed in relation to the results.

4 Performance of algorithms

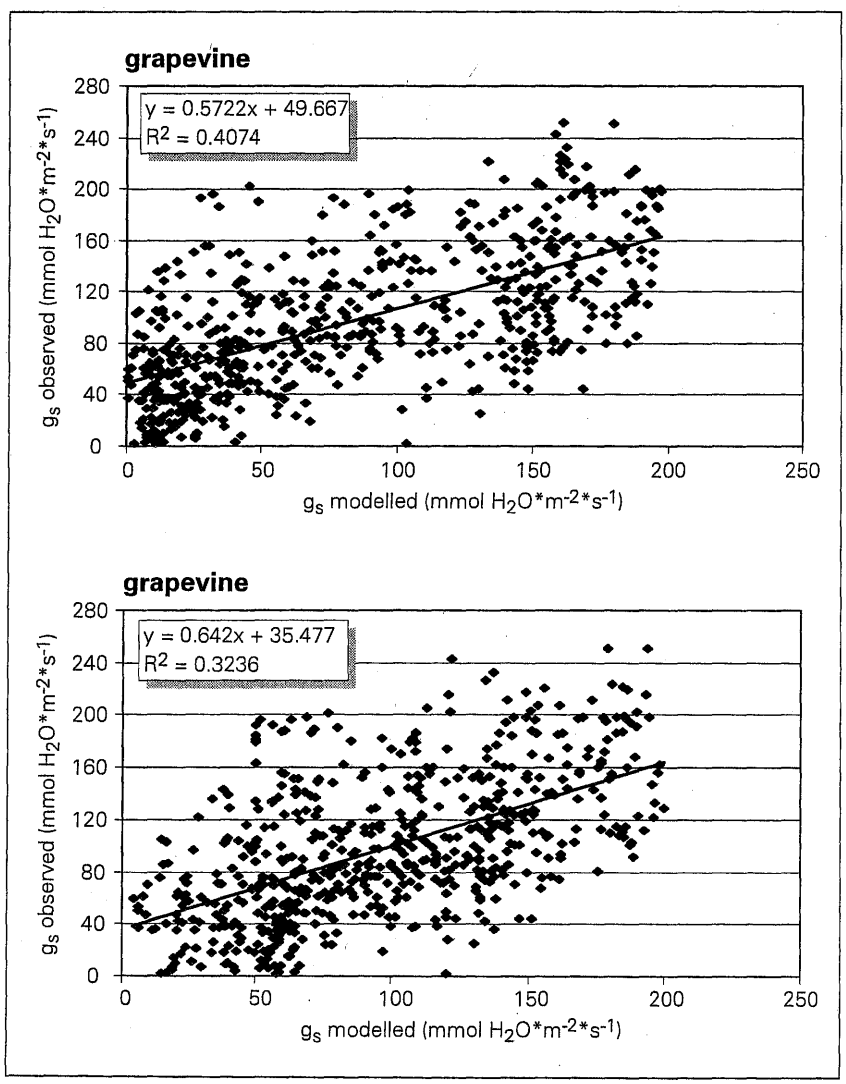

Figure 1:
*Scatter plot of modelled vs. observed g_s (mmol H_2O * m^{-2} * s^{-1}) for grapevine using the multiplicative algorithm (left) and the photosynthesis-based algorithm (right).*

Exemplary for all four datasets, Figure 1 shows the capacity of the multiplicative and photosynthesis-based algorithm in predicting g_s using minute-by-minute input data. Both algorithms tend to overestimate g_s (slopes of the linear regressions are 0.57 and 0.64 for multiplicative and photosynthesis based models, respectively). The models are able to account for only 40% (multiplicative) and 32% (photosynthesis-based model) of the variation in the datasets as denoted by the respective R^2-values. As such, these data would suggest that the multiplicative model performs marginally better than the photosynthesis-based model though neither model could be considered to be performing well.

Diurnal courses for grapevine using hourly means averaged over the course of the measuring campaign (7 days in June 1991) are shown in Figure 2; analysis of these pooled data result in both algorithms providing a much better relationship between observed and modelled g_s. This would indicate that both models can effectively predict diurnal

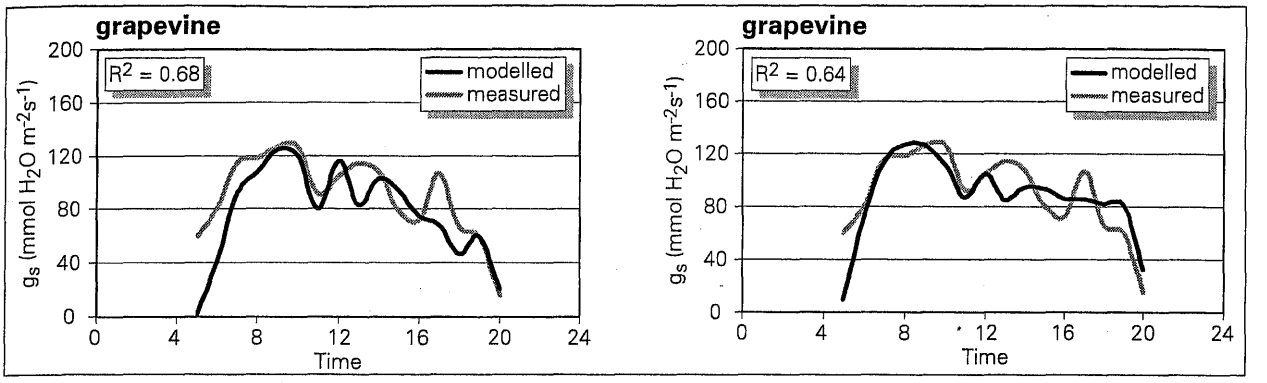

Figure 2:
*Daily course (4:00 until 20:00) of modelled and observed g_s (mmol H_2O * m^{-2} * s^{-1}) averaged over seven days in June 1991 for Mediterranean grapevine using the multiplicative algorithm (left) and the photosynthesis-based algorithm (right).*

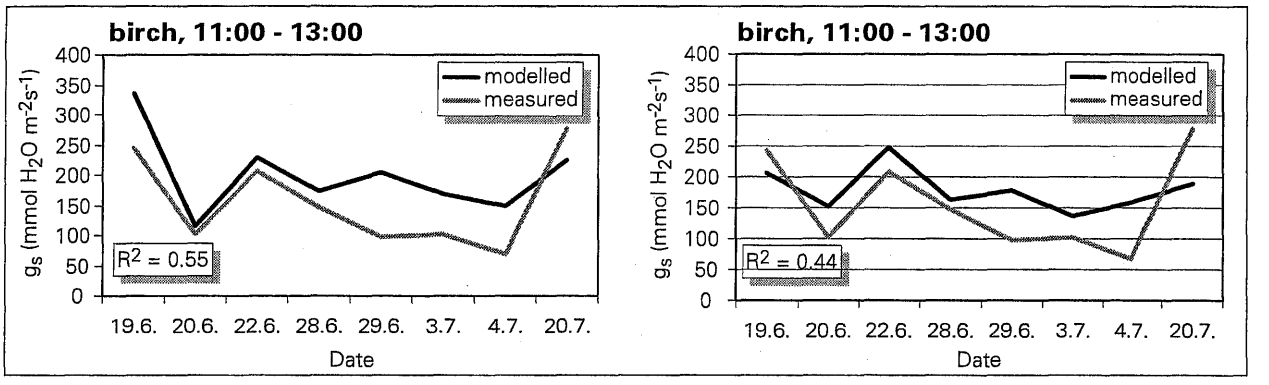

Figure 3:
*Seasonal course (5 weeks during the summer of 2001) of modelled and observed g_s (mmol H_2O * m^{-2} * s^{-1}) averaged over midday hours (11:00 until 13:00) for boreal birch using the multiplicative algorithm (left) and the photosynthesis-based algorithm (right).*

trends. Both models give a good correspondence between observed and modelled g_s for the morning hours (6:00 to 11:00); over the course of the afternoon however, the predictions diverge from the actual mean values and are not able to re-produce the variations in g_s. In fact, the multiplicative algorithm shows shifted peaks after noon whereas the photosynthesis-based algorithm tends to produce a more constant decline in g_s. However, both models are able to predict the observed midday depression of g_s and its decline in the later afternoon.

The birch dataset was selected to show the ability of the algorithms to predict seasonal changes in g_s since this was the dataset recorded over a longer period during the growing season. Figure 3 gives an indication of the seasonal variability of g_s as predicted by both algorithms in comparison with the observed course of g_s. The charts represent the g_s average for the two hours between 11:00 a.m. and 1:00 p.m. for which the models performed well (Figure 2). Although the seasonal period only represents conditions at the height of the growing season (i.e. effects of senescence haven't been observed during the measuring campaign for birch), the graphs show the general ability of the algorithms to predict changes in g_s over longer time periods. In general, both models tend to overestimate g_s.

5 Discussion and outlook

Both algorithms showed a similar performance in predicting g_s for time-steps of various lengths (minute-by-minute, daily and seasonal), with the multiplicative algorithm yielding slightly higher R^2-values for the relationship between observed and modelled g_s. The photosynthesis-based algorithm used in LEAFC3 requires more detailed meteorological (e.g. ambient CO_2-concentration, dew-point temperature) input data and plant-physiological (e.g.

V_{m25}, J_{m25}) parameters. Since the latter are often not available, a site-specific parameterisation accounting for differences in g_s due to plants growing under different climatic conditions is not easy to achieve for this algorithm, i.e. might only be possible via a literature review. Furthermore, the obvious variance (Figure 1) of g_s when using the photosynthesis-based algorithm might be at least partly attributed to the questionable assumption that the g_s is always closely coupled with A_n. Figure 4 shows the variation in the coupling of g_s and A_n over the course of the growing season as observed for beech.

In contrast, the relative weakness of the multiplicative algorithm resulting in similar variances as seen for the photosynthesis-based algorithm lies in its dependence on g_{max}, which is difficult to derive from published literature (see Emberson et al. this volume) and may well vary within species according to prevailing climatic conditions.

For the photosynthesis based algorithm a revised soil moisture deficit function has been published recently (Nikolov & Zeller, 2003), which will be assessed in the near future. However, the soil drought effect for the grapevine and birch dataset was assumed to have been low, because of very deep roots well below the groundwater level for grapevine (Jacobs, pers. comm.) and the low VPD values observed for birch.

The performance of the algorithms in predicting total ozone deposition to vegetated surfaces at a regional scale using the DO_3SE model will be tested using the above described Scots pine and wheat dataset. This will provide further information on how different g_s algorithms compare when used for estimating total O_3 deposition and how the generic DO_3SE parameterisation is able to represent individual species at site-specific locations.

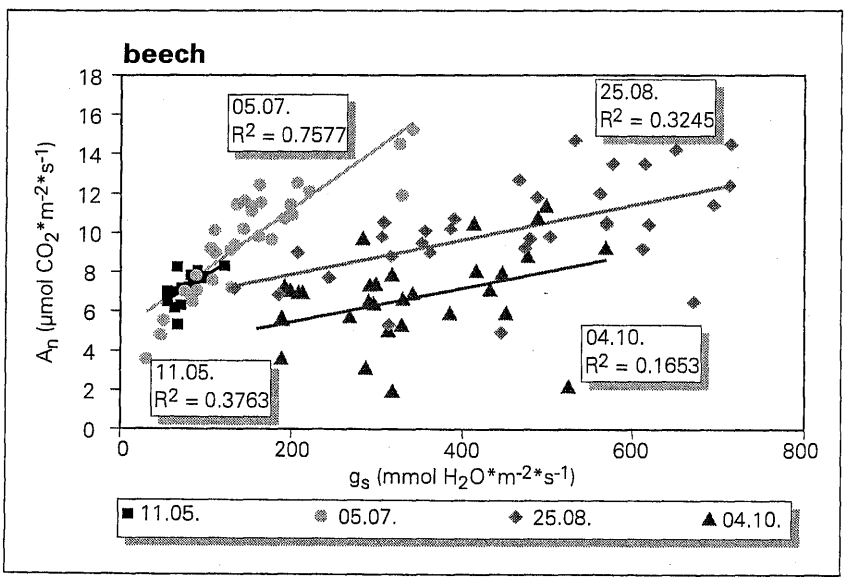

Figure 4:
Coupling of gs and An over the course of the growing season as measured for beech in Switzerland in 2004.

References

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: Progress in Photosynthesis Research, Vol IV, edited by J. Biggens, Dordrecht:Martinus Nijhoff, p. 221-224.

De la Torre D. 2004. Efectos del ozono troposférico sobre la producción relativa de trigo y cebada mediterráneos. Modulación por factores ambientales. PhD thesis. Universidad Autónoma de Madrid, 280p.

Emberson L.D., Simpson D., Tuovinen J.-P., Ashmore M.R., Cambridge H.M. 2000. Towards a model of ozone deposition and stomatal uptake over Europe. Norwegian Meteorological Institute, Oslo, EMEP MSC-W Note X/00, 57p.

Gerosa G., Cieslik S., Ballarin-Denti A. 2003. Micrometeorological determination of time-integrated stomatal ozone fluxes over wheat: a case study in Northern Italy. Atmospheric Environment 37, 777-788.

Jacobs C.M.J., van den Hurk B.I.J.M., de Bruin H.A.R. 1996. Stomatal behaviour and photosynthetic rate of unstressed grapevines in semi-arid conditions. Agricultural and Forest Meteorology 80, 111-134.

Jarvis P.G. 1976. The interpretation of the variations in leaf water potential and stomatal conductance found in canopies in the field. Philosophical Transactions of the Royal Society of London - B 273: 593-610.

Müller J., Wernecke P., Diepenbrock W. 2005. LEAFC3-N: a nitrogen-sensitive extension of the CO_2 and H_2O gas exchange model LEAFC3 parameterised and tested for winter wheat (*Triticum aestivum* L.) Ecological Modelling 183, 183-210.

Nikolov N.T., Massman W.J., Schoettle A.W. 1995. Coupling biochemical and biophysical processes at the leaf level: an equilibrium photosynthesis model for leaves of C3-plants. Ecological Modelling 80: 205-235.

Nikolov N.T., Zeller K.F. 2003. Modeling coupled interactions of carbon, water, and ozone exchange between terrestrial ecosystems and the atmosphere. I: Model description. Environmental Pollution 124, 231-246.

Oksanen E. 2003. Responses of selected birch (*Betula pendula* Roth) clones to ozone change over time. Plant, Cell and Environment 26, 875-886.

Simpson D., Fagerli H., Jonson J.E., Tsyro S. and Wind P. 2003. Transboundary Acidification, Eutrophication and Ground Level Ozone in Europe. Part I Unified EMEP Model Description. Norwegian Meteorological Institute, Oslo, EMEP MSC-W Note 1/2003, http://www.emep.int/publ/common_publications.html, 104p.

Tuovinen J.-P., Simpson D., Mikkelsen T.N., Emberson L.D., Ashmore M.R., Aurela M., Cambridge H.M., Hovmand M.F., Jensen N.O., Pilegaard K., Ro-Poulsen H. 2001. Comparisons of measured and modelled ozone deposition to forests. Water, Air and Soil Pollution: Focus 1, 263-274.

UNECE Revised manual on methodologies and criteria for mapping critical levels/loads and geographical areas where they are exceeded, Chapter 3: Mapping Critical Levels for Vegetation. 2004. Umweltbundesamt, Berlin, Germany. http://www.oekodata.com/icpmapping/html/manual.html, 53p.

authors: P. Büker
L. D. Emberson
M. R. Ashmore
Stockholm Environment Institute
University of York
York YO10 5DD, UK
E-Mail: pb25@york.ac.uk

G. Gerosa
Università Cattolica del Sacro Cuore
Via Musei 41
25121 Brescia, Italy

C. Jacobs
Alterra
Droevendaalsesteeg 3
6708 PB Wageningen, The Netherlands

W.J. Massman
USDA Forest Service
Rocky Mountain Research Station
Fort Collins, CO, USA

J. Müller
Institute of Agronomy and Crop Science
Martin-Luther-University Halle-Wittenberg
Ludwig-Wucherer-Straße 2
D-06099 Halle, Germany

N. Nikolov
N & T Services
6736 Flagler Road
Fort Collins, CO 80525, USA

K. Novak
Forest Ecosystems and Ecological Risk
Swiss Federal Research Institute WSL
Zuercherstraß3 111
8903 Birmensdorf ZH, Switzerland

E. Oksanen
Department of Biology
University of Joensuu
P.O. Box 111, 80101 Joensuu, Finland

D. de la Torre
Institute for Energetics, Environment and Technological Research (CIEMAT)
Avda. Complutense
22 - 28040, Madrid, Spain

J.-P. Tuovinen
Finnish Meteorological Institute
Sahaajankatu 20 E
FIN-00810, Helsinki, Finland