ENVI-met implementation of the Jacobs $A - g_s$ Model to calculate the stomata conductance (Working paper)

Michael Bruse

16th February 2004

1 Implementation of the Jacobs $A - g_s$ Model to calculate the stomata conductance

1.1 Introduction

Modelling the stomata resistance r_s (or conductance g_s) of plants is one of the most important factors when simulating fluxes from vegetation layers into the atmosphere. As plants are complex, active biological systems, the correct estimation of the stomatal behavior under different environmental conditions is far from being trivial. A correct model for stomatal behaviour must be able to include the effect of short-term variations (light, temperature) as well as long-term changes (e.g. increase of atmospheric CO_2) when calculating the plants transpiration.

Many of the influencing factors produce synergistic effects- For example it is known that an increase of atmospheric CO_2 increases the plants sensitivity to light and temperature and possibly other factors, too (Meidner and Mansfield, 1968). The correct representation of such effects is not only of relevance when looking at the global increase of CO_2, but also for estimating the plants behavior in polluted environments such as urban streets with dense car traffic.

Emperical models like those presented by Deardorff (1978) or Jarvis (1976) calculate the stomata conductance by scaling it down from its maximum possible value using a set of response functions $f(x)$ where x is the influencing factor.

The disadvantage of these models is, that they normally cannot include synergistic effects between different stimuli because the factors $f(x)$ are treated independently from each other. In addition, they are obtained from statistical analysis of emperical data, which cannot be measured over the full range of possible conditions (Jacobs, 1994 ; Jarvis, 1976). Most of the models treat the complete plant canopy as a single "big leaf" exposed to a uniform microclimate and calculate the average response of this canopy layer. This is not realistic, especially not for heterogenous climate conditions like those found in urban areas. Therefore is is not viable to downscale these canopy models to a single-leaf scale. For that reason, the classical Deardorff stomata resistance model used in ENVI-met have been replaced with a so called $A - g_s$ model, which allows a more accurate simulation of the plant physiological activity at leaf-scale base and under the influence of varying environmental conditions.

$A - g_s$ models overcome most of the restrictions mentioned in the section above, as they use the observed relationship between the photosynthetic rate A_n and the stomatal conductance g_s of a plant. These two parameters are not directly linked from a plant physiological of view, but represent the plant's strategy to balance water use and CO_2 assimilation in order to maximise carbon gain and minimize water loss (Jacobs 1994). In addition to the photosynthesis rate, the ratio of leaf internal CO_2 concentration (C_i) to external concentration (C_s) can be used to include the humidity response of the stomata in the model.

$A - g_s$ models are valid over a wide range of environmental situations, including stress conditions. Possible synergetic effects are included implicitly by calculating the photosynthesis rate of the plant.

The basic hypothesis of the $A - g_s$ model can be roughly be written as

$$g_s = 1.6 \frac{A_n}{C_s - C_i}$$

where A_n is the net photosynthesis rate, C_s and C_i are the CO_2 concentrations at

the leaf surface and inside the leaf. The factor 1.6 results from the differing diffusivity of CO_2 and H_2O in the air.

The unit of the stomatal conductance g_s is $[mms^{-1}]$ and therefore the transformation into the stomatal resistance r_s value is

$$r_s = \frac{1}{g_s} \cdot 1000$$

1.2 Excurse: Photosynthesis

The basic equation of the photosynthesis is

$$6\mathrm{CO_2} + 12\mathrm{H_2O} \overset{h \cdot \nu}{\rightarrow} \mathrm{C_6H_{12}O_6} + 6\mathrm{O_2} + 6\mathrm{H_2O}$$

with a total enthalpy of $\Delta G^{0'} = +2872$ kJ.

Hydrogen is separated from the water and transferred to the CO_2 molecule releasing O_2. It is obvious, that this reactions has three limiting parameters: CO_2, $h \cdot \nu$ (Light) and water, where the latter one is the less critical under normal conditions.

To extract energy from the absorbed (sun)light, the plant uses chlorophyll α and β (plus some other receptor devices) which changes its internal energy state by absorbing quantum energy. The energy gained is transferred into the biochemical reaction system known as "*Light Reaction*", forming NADPH and ATP. Although the dominating processes are quite complex and still not fully understood, it is sufficient accurate to say that around 48% of the incoming sun radiation will be accepted for photosynthesis [1]. We call this fraction the *Photosynthetically Active Radiation* (PAR).

In the so-called "Dark Reaction", NADPH and ATP are used to generate $(CH_2O)_n$ sugars out of CO_2 molecules. This cyclic reaction is called the "*Calvin Cycle*".

The counter process, the "*Dark respiration*" releases the energy stored in the sugar molecules As this process mainly takes place in the dark it is distinguished from the "*Photorespiration*" which also releases CO_2 and certain conditions, but during daylight.

1.3 Calculating Net Assimilation A_n

In nature, the assimilation rate A_n can be restricted by two factors: missing light and missing CO_2. If light is the limiting factor, A_n can be written as

$$A_n = \varepsilon I_a - R_d \tag{1}$$

where I_a is the physically active radiation PAR reaching the leaf surface. In the model equations used in this model, PAR is related to the input on a horizontal surface in height z:

$$PAR(z) = 0.48 \cdot (\sin\phi R_{sw,dir}(z) + R_{sw,dif}(z))$$

with $R_{sw,dir}$:shortwave direct radiation on a surface perpendicular to the incoming sun, $R_{sw,dif}$: diffuse shortwave radiation (including horizon obstruction and reflection from walls) and ϕ elevation of the sun (see Radiation chapter for details).

R_d is the energy loss due to dark respiration and ε the initial quantum use efficiency and can be calculated with:

$$\varepsilon = \varepsilon_0 \frac{C_i - \Gamma}{C_i + 2\Gamma} \tag{2}$$

[1] Which does not mean that this energy is actually used in the biochemical reactions. Net energy transferred through the biosystem is around 0,05% of the sun radiation.

Here, ε_0 is the maximum quantum use efficiency based on the theoretical efficiency of the Calvin cycle (≈ 0.025 mg J^{-1} PAR), corrected with a loss factor. For C_3 plants ε_0 is 0.017 mgJ^{-1}, for C4 plants it is 0.014 mgJ^{-1}(see also Table 1). Γ is the "*Compensation Point*" [ppm]. In case that only CO_2 is the limiting factor, the photosynthetic rate at light saturation (A_m) is linearly related to the CO_2 concentration:

$$A_m = 0.001 g_m \cdot (C_i - \Gamma)\, \phi_{co2} \tag{3}$$

Putting together both equations, the final expression for A_n, including both the effect of limited light and CO_2 is:

$$A_n = (A_m + R_d)\left(1 - \exp\left(\frac{-\varepsilon I_a}{A_m + R_d}\right)\right) - R_d \tag{4}$$

The respiration rate R_d is simply defined as $R_d = A_m/9$ (van Heemst, 1986).

Finally. A_m must be limited to a maximum value to avoid unrealistic values at hight light intensities and hight CO_2 concentrations. A smooth transition between (3) and the maximum value $A_{m,\max}$ is therefore used:

$$A_m = A_{m,\max}\left(1 - \exp\left(\frac{-0.001 g_m \cdot (C_i - \Gamma)\, \phi_{co2}}{A_{m,\max}}\right)\right) \tag{5}$$

A_m, A_n and $A_{m,\max}$ are in [$mgm^{-2}s^{-1}$].ϕ_{co2} is a conversion factor transforming the CO_2 concentration from [ppm] (or [$\mu molmol^{-1}$]) into [mgm^{-3}]:

$$\phi_{co2} = \frac{M_{co2} \cdot \rho_{a,v}}{M_a} \simeq 1.96 \tag{6}$$

where M_{co2} and M_a are the molecular masses of CO_2 and air (44.0 and 28.9 $gmol^{-1}$). The density of air is calculated taking into account the vapour content:

$$\rho_{a,v} = \frac{P}{R_a \cdot x}$$

with $x = T_a\left(1 + R' \cdot \frac{q}{1000}\right)$ and $R' = \frac{R_v}{R_a} - 1$. R_v and R_a are the gas constants for air and vapour pressure (461.51 and 287.05 $Jkg^{-1}K^{-1}$) and P is the air pressure in [Pa].

1.3.1 Temperature response of the leafs

The temperature dependency of photosynthesis is taken into account by using temperature dependent scaling functions for Γ, g_m and $A_{m,\max}$, the so called Q_{10} functions[2]. These functions describe the proportional increase of a parameter X value for a 10 degrees increase in temperature (Berry and Raison, 1982).

For Γ the Q_{10} function is

$$\Gamma(T_l) = \Gamma(@25)\, Q_{10}^{(T_l - 25)/10} \tag{7}$$

[2]Index for temperature dependence of a chemical process. Defined as the increase of reaction velocity by temperature increase of 10 K. Temperature independent process have a Q_{10} value of 1. Most chemical processes have Q_{10} values of 2 and higher (reaction velocity is doubled or more)

Table 1: Parameters of the Q_{10} functions for C_3 and C_4 plants (Jacobs 1994)

	Parameter	$X(@25)$	Q_{10}	$T_1(°C)$	$T_2(°C)$
C_3	$\varepsilon_0[mgJ^{-1}PAR]$	0.017	-	-	-
	$\Gamma[ppm]$	45	1.5	-	-
	$g_m[mms^{-1}]$	7.0	2.0	5	28
	$A_{m,\max}[mgm^{-2}s^{-1}]$	2.2	2.0	8	38
	f_0	0.85	-	-	-
C_4	$\varepsilon_0[mgJ^{-1}PAR]$	0.014	-	-	-
	$\Gamma[ppm]$	2.8	1.5	-	-
	$g_m[mms^{-1}]$	17.5	2.0	13	36
	$A_{m,\max}[mgm^{-2}s^{-1}]$	1.7	2.0	13	38
	f_0	0.50	-	-	-

where $\Gamma(@25)$ is the reference value of Γ at $T_l = 25°$C. For the parameter g_m and $A_{m,\max}$ the function is

$$X(T) = \frac{X(@25)Q_{10}^{(T_l-25)/10}}{(1+\exp(0.3\,(T_1-T_l)))\,(1+\exp(0.3\,(T_l-T_2)))} \tag{8}$$

The reference values for the functions according to Jacobs (1994) are given in table 1 for C_3 and C_4 plants.

1.3.2 Calculating the internal CO_2 concentration C_i

To solve the equation set, the leaf "internal" CO_2 concentration must known. It can be be calculated from the ratio of internal and external CO_2 concentration:

$$\frac{C_i}{C_s} = f + (1-f)\,\frac{\Gamma}{C_s} \tag{9}$$

where factor f takes into account the stomatal response to humidity and is defined as

$$f = f_0\left(1-\frac{D_s}{D_{\max}}\right) + f_{\min}\left(\frac{D_s}{D_{\max}}\right) \tag{10}$$

D_s is the saturation deficit of the air at the plant surface with $D_s = q^*(T_l) - q_a$. For $D_{\max}$ a maximum value of 45 gkg^{-1} is used to represent then humidity response for crops and deciduous forests (Choudhurry and Monteith, 1986). For other plants, values might vary.

f_0 is the value of f at D_s=0 gkg^{-1} which is 0.85 for C_3 plants and 0.50 for C_4 plants.

The minimum $f_{\min}$ is calculated with

$$f_{\min} = \frac{g_c}{g_c+g_m} \tag{11}$$

where g_c is the cuticular conductance, controlling the diffusion of water vapour from the leafs without using the stomatal mechanism.The values for g_c may differ from plant to plant. For crops, g_c lies between 0.1 and 0.4 mms^{-1}, for trees and xerophytes it is smaller. (Jacobs 1994). Usually g_c is set constant to a value of 0.25. The resulting internal CO_2 concentration can finally be calculated using (9):

$$C_i = f\cdot C_s + (1-f)\cdot\Gamma$$

1.4 Estimating the stomatal response

The correlation between the assimilation rate A_n and the stomata conductance for H_2O (g_s) for can be written as

$$g_s = 1.6 * 1000 g_{sc}$$

The conductance g_{sc} $[ms^{-1}]$ of the leaf to CO_2 transfer can be calculated as

$$g_{sc}^{'} = \left(A_n - A_{m,\min} \cdot \frac{D_s}{D_{\max}} \cdot \frac{A_g}{A_{m,g}} + R_d \left(1 - \frac{A_g}{A_{m,g}} \right) \right) \frac{1}{(C_s - C_i)\,\phi_{co2}} \quad (12)$$

with

$$\begin{aligned} A_g &= A_n + R_d \\ A_{m,g} &= A_m + R_d \\ A_{m,\min} &= 0.001 g_m \cdot (C_{\min} - \Gamma)\,\phi_{co2} \end{aligned}$$

where $C_{\min}$ is the value of C_i at $D_s = D_{\max}$ calculated using (9,10,11):

$$C_{\min} = \frac{g_c C_s + g_m \Gamma}{g_c + g_m} \quad (13)$$

The value of A_n is obtained from (4), with the additional condition

$$A_n = \max\left(A_{m,\min}, A_n\right) \quad (14)$$

to avoid negative conductance values.

The total leaf stomatal conductance for vapour, including the cuticular conductivity, can then be calculated as

$$g_s = 1.6 \cdot 1000 g_{sc}^{'} + g_c \quad (15)$$

1.4.1 Interactions between CO_2 and H_2O

In, addition, the interactions between CO_2 and H_2O diffusion are taken into account (Calvet, 2000; Calvet et al., 1998): ,

$$g_{sc} = g_{sc}^{'} + m \cdot \frac{C_s + C_i}{2\,(C_s - C_i)\,\phi_{H_2O}} 10^{-6}$$

with

$$\phi_{H_2O} = \frac{M_{H_2O} \cdot \rho_{a,v}}{M_a}$$

where M_{H_2O} is the molecular masses of vapour (18 gmol^{-1}). m is the transpiration of the plant givening $[mgm^{-2}s^{-1}]$:

$$m = \rho_a g_s D_s$$

with $D_s = q_* - q_a$ in $[gkg^{-1}s^{-1}]$

The final solution is found by inserting new values of g_{sc} into (15) and iterating.

This module is unused at the moment.

1.5 Interactions with atmospheric CO_2

The uptake and release of CO_2 due to assimilation and respiration effects the atmospheric CO_2 concentration inside and downstream the vegetation stand. In order to allow an accurate simulation of the diurnal CO_2, a prognostic equation for CO_2 was added to the atmospheric model. The basic equation is equivalent to the standard advection- and diffusion equations of the atmospheric system:

$$\frac{\partial[CO_2]}{\partial t} + u\frac{\partial[CO_2]}{\partial x} + v\frac{\partial[CO_2]}{\partial y} + w\frac{\partial[CO_2]}{\partial z} = \frac{\partial}{\partial x}\left(K_{\chi,CO2}\frac{\partial[CO_2]}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_{\chi,CO2}\frac{\partial[CO_2]}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_{\chi,CO2}\frac{\partial[CO_2]}{\partial z}\right) + Q_{\chi,CO2}(x,y,z) \quad (16)$$

The unit of $[CO_2]$ in the atmospheric prognostic equation is [mgkg^{-1}] whereas in the plant system CO_2 is needed in [ppm].

The conversion between the different units used is

$$ppm \leftarrow \cdot 1/\phi_{co2} \leftarrow \frac{mg}{m^3} \rightarrow \cdot 1/\rho \rightarrow \frac{mg}{kg} \rightarrow \cdot \rho/\phi_{co2} \rightarrow ppm$$

with ϕ_{co2} given by (6). The Source/Sink term $Q_{\chi,CO2}$ linked to the plants net assimilation by

$$Q_{\chi,CO2}(x,y,z) = -A_n \cdot LAD(x,y,z) \cdot \frac{1}{\rho} \quad (17)$$

Where A_n is the CO_2 flux per leaf area unit and $Q_{\chi,CO2}$ is the local source/sink rate in [mgkg^{-1}s^{-1}]. The exchange coefficient for CO_2 is calculated from the coefficient for water vapour K_v taking into account the differing molecular diffusivities in air:

$$K_{\chi,CO2} = 0.625 K_v \quad (18)$$

The conversion from mgkg^{-1} to ppm depends on the local temperature and vapour contend of the air. As the internal calculations of the $A - g_s$ model also work with mgkg^{-1}, it is important to use the same T and q for both conversions.

The initial CO_2 field is taken from the given background concentration in [ppm] using the temperature and humidity in approximately 2 m from the reference profile (1D model). The boundary conditions are the initial background concentration at all model borders, except the lateral outflow borders, where a zero-gradient condition is used.

1.6 Extension to include soil water stress

The Jacobs model as it was described up to now, does not take into account the water conditions of the soil. If the soil layers inside the root zone are not able to supply enough water, transpiration will be reduced even if the stomata could be open wide under the given atmospheric conditions.

The ISBA-$A - g_s$ model (Calvet et al., 1998) uses one additional factor to include soil water stress. This was done by changing the parameterizations of the mesophyll conductance g_m:

$$g_m = \xi \cdot g_m^{'} \quad (19)$$

where $g_m^{'}$ is the mesophyll conductance from the original Jacobs model obtained by applying (8)..

The available soil water is calculated as an normalized value ξ:

$$\xi = \frac{\eta - \eta_{wilt}}{\eta_{fc} - \eta_{wil}}$$

Here, η is the volumetric soil water contend in the root zone and η_{wilt},η_{fc} its value at wilting point and field capacity respectively.

As different layers might contain different soils with varying hydraulic properties, an average value $\bar{\xi}$ is calculated over the root zone in ENVI-met. The minimum value of ξ is set to 0.1 (=10%) to avoid unrealistic behaviour of the model system.

As a special case, plants might stand on roofs. In this special case, water availability is a function of the external irrigation.

1.6.1 Plants on roofs

If a plant stands on a roof, the Rooftop-Watering coefficient ϱ_{water} going from 1 (total irrigation) to 0 (total stress) replaces $\bar{\xi}$ in (19). This formulation is conform with the use of ϱ_{water} in the Deardorff-approach (see there).

1.7 Acknowledgements

The author thanks Jean Christophe Calvet from METEO France for his help in implementing the $A - g_s$ model.

Literaturverzeichnis

Berry, J. A. and Raison, J. K. (1982). Responses of macrophytes to temperature. In Lange, O. L. e. a., editor, *Encyclopedia of Plant Physiology. New Series*, pages 277–338, Berlin. Springer Verlag.

Calvet, J.-C. (2000). Investigating soil and atmospheric plant water stress using physiological and micrometeorological data. *Agric. For. Meteorol.*, 103:229–247.

Calvet, J.-C. et al. (1998). An interactive vegetation SVAT model tested against data from six contrasting sites. *Agric. For. Meteorol.*, 92:73–95.

Choudhurry, B. L. and Monteith, J. L. (1986). Implications of stomatal response to saturation deficit for the heat balance of vegetation. *Agric. For. Meteorol.*, 36:215–225.

Deardorff, J. W. (1978). Efficient prediction of ground surface temperature and moisture with inclusion of a layer of vegetation. *J. Geophys. Research*, 83:1889–1903.

Jacobs, C. M. J. (1994). *Direct impact of atmospheric CO_2 enrichment on regional transpiration*. PhD thesis, Wageningen Agricultural University.

Jarvis, P. (1976). The interpretation of leaf water potential and stomatal conductance found in canopies in the field. *Phil. Trans. R. Soc. Lond.*, 273:593–610.

Meidner, H. and Mansfield, T. A. (1968). *Physiology of Stomata*. McGraw-Hill, London.

van Heemst (1986). Potential crop production. In van Keulen, H. and Wolf, J., editors, *Modelling of agricultural production: Weather, soil and crops*, Wageningen. Pudoc.