Photosynthesis based stomatal resistance (Rsto)

The objective of the coupled photosynthesis-stomatal conductance model (*Anet*-*gsto*) model is to quantify leaf or canopy scale *gsto* with the help of easily accessible environmental parameters such as air temperature (*Tair*), ambient CO2 concentration (*ca*) and irradiance (*PAR*). The *Anet*-*gsto*  model consists of a combination of two separate models, whose main components are outlined below and include i. the empirical *Anet*-*gsto* model that estimates *gsto* (Leuning, 1990) and ii. the mechanistic and biochemical Farquhar model (Farquhar et al., 1980) that estimates net carbon assimilation or net phostosynthesis (*Anet*).

One of the first coupled *Anet*-*gsto* models was that published by (Leuning, 1990) though some other authors are often cited as the originating sources of the model (e.g. Collatz et al., 1991 and Harley et al., 1992). The models they apparently developed independently are essentially equivalent. The order of description of the *Anet*-*gsto* modelling here follows the order in which they have to be computed.

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# Default Configuration

## Model Flow

<media/photosynthesis_flow_chart.pdf>

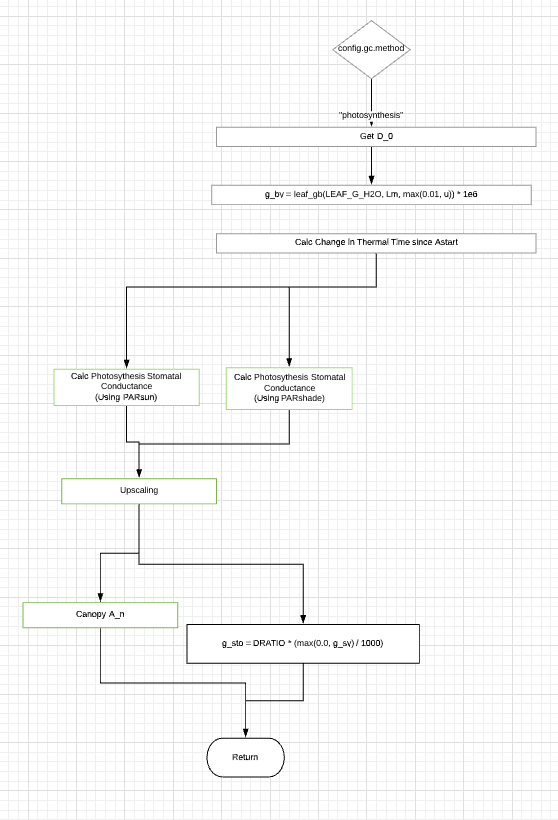
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Figure 1: Calculate Photosynthesis Surface Resistance

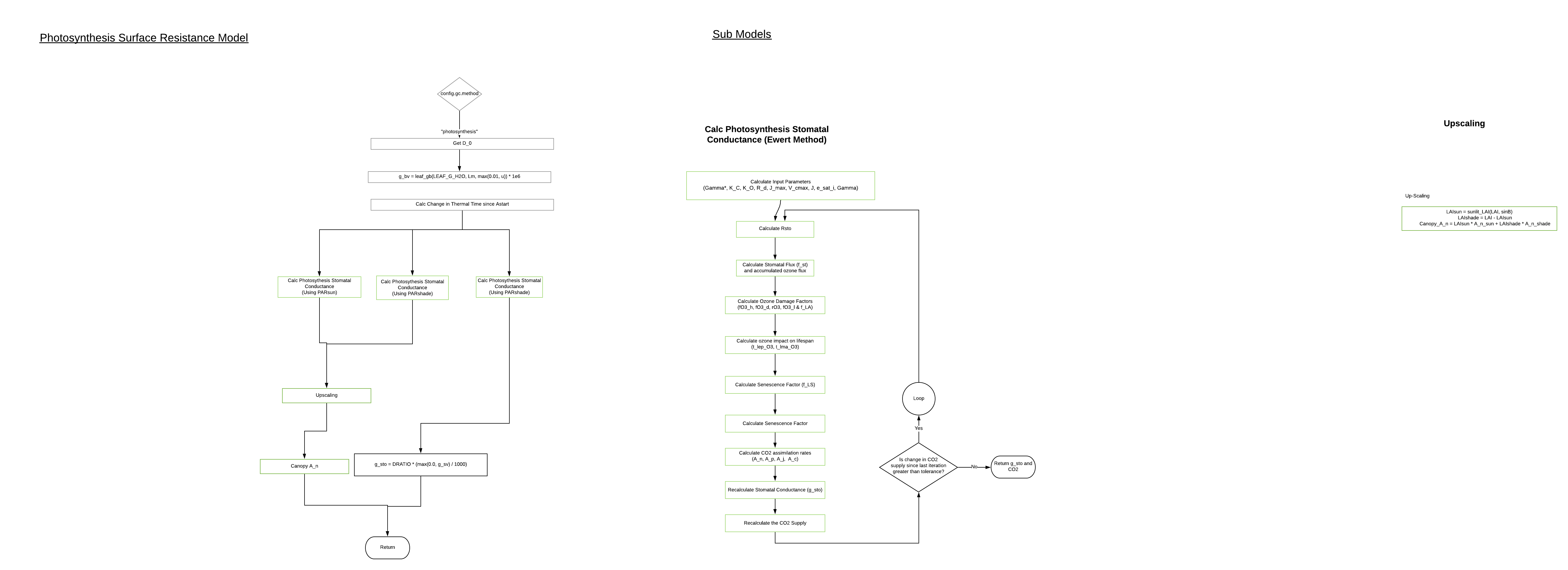


Figure 2: Calculate Stomatal Conductance (Ewert Model)

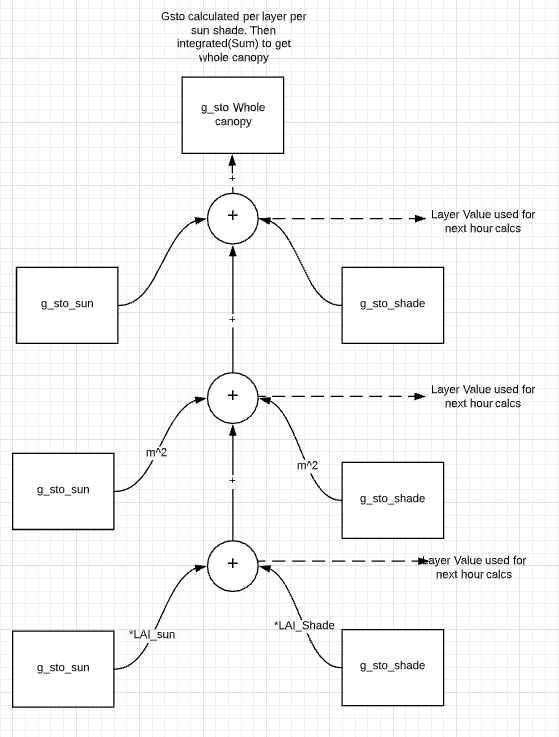


Figure 3: Photosynthesis gsto upscaling

## Coupled photosynthesis-stomatal conductance (*Anet*-*gsto*) model.[2g]

Based on earlier observations of the constant ratio of *gsto* to net CO2 assimilation rate (*Anet*), Ball et al. (1987) discovered an empirical linear relationship, which relates *gsto* to a combination of *Anet* and environmental parameters, such as leaf surface relative humidity (*Dh*) and CO2 concentration (*Ca*) as shown in Figure 2).

Figure 4. The original BWB model. Stomatal conductance plotted against the BWB Index. From Ball et al. (1987).



Leuning (1990 and 1995) modified the original Ball et al. (1987) relationship so that the function used leaf surface CO2 concentration (*Cs*) less the CO2 compensation point (Γ). and. They argued that the use of *Cs* rather than *Ca* (the CO2 concentration outside the leaf boundary layer) eliminates complications arising from the transfer of CO2 through the leaf boundary layer. The introduction of the Γ term allows the correct simulation of stomatal behaviour at low CO2 concentrations which will tend towards zero as *Anet* becomes minimal close to the Γ. The use of humidity deficit (*Ds*) rather than relative humidity *(Dh)* accounts for the fact that stomates respond to humidity deficit rather than surface relative humidity; this response is actually mediated through leaf transpiration (*Etleaf*) but the close link between *Etleaf* and *Ds* means that the use of *Ds* is appropriate for simulations. Leuning (1995) found that a hyperbolic function for *Ds* provided an improved humidity response by accounting for the response of *Ds* to leaf temperature. The resulting formulation they propose is given in eq..

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Leuning 1995 eq (7)

The parameter *g0*is interpreted as the minimal *gsto* (Leuning, 1990) and is equivalent to the intercept of the regression which is sometimes greater, but often close, to zero. The parameter *m* is the so called composite sensitivity of *gsto* to assimilation rate and humidity/CO2 concentration, can be obtained *via* a linear regression of *gsto* against experimental data from steady state gas exchange measurements. The value of *m* is surprisingly consistent amongst many different species, and ranges between 5 and 15 (Kosugi et al., 2003) (if all quantities are in units consistent with Ball et al. (1987) *m* is dimensionless). The parameter is the humidity deficit (or vapour pressure deficit, VPD) as which is reduced by a factor of two (Leuning et al., 1998).

Despite the empirical and non-mechanistic nature of this model it allows for the mathematical quantification of the key environmental feedbacks on stomatal behaviour: (1) Rising irradiance causes stomata to open (incorporated through the positive influence of radiation on *Anet*); (2) Rising CO2 causes stomata to close (incorporated through the negative influence of limited RuBP regeneration); (3) To minimize water loss, stomata close when the transpiration rate rises (incorporated through the response to leaf surface humidity deficit).

However, caution has to be exercised concerning interpretation of the model. It allows for no mechanistic explanation or causal interpretation of the feedbacks between the different parameters (see Aphalo & Jarvis, (1993) for a discussion) and is, strictly speaking, only a statistical correlation.

## Biochemical Farquhar model for net photosynthesis (Anet)[1 & 2f]

The underlying assumption to Farquhars’s 1980 model is that, according to prevailing environmental conditions, either rubisco activity (*Ac*) or the regeneration of ribulose-1,5-bisphosphate (RuBP) which is limited by the rate of electron transport (*Aj*) limits photosynthesis. Subsequent to Farquhar’s 1980 paper, Harley et al. (1992) identified a third limitation resulting from inadequate rate of transport of photosynthetic products (most commonly this is due to triose phosphate utilization) (*Ap*), this limit has now become standard in many models of *Anet* (e.g. Sellers et al., 1996; Cox et al., 1999) and is included here. Taking these influences on photosynthesis into account *Anet* is calculated by determination of the smaller of these theoretical CO2 assimilation rates less the rate of dark respiration (*Rd*) (Farquhar et al., 1980) as in eq. 1 and as described in Figure 1. Note this means that when Ac, Aj or Ap are 0 then Anet is negative.

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**Figure 5** Scheme showing some of the processes that affect photosynthetic rate. For each of the three panels, any process in that panel will cause the photosynthetic rate to vary with [CO2] in the same way. From Sharkey et al. (2007).



Within the literature there are small variations in the precise methods to estimate Ac, Aj and Ap. One important application of our *Anet*-*gsto* model is that it is to be made with empirical data collected at sites across Europe. This provides the opportunity to use empirical data to parametrise the key components of the model; however methods to perform this parameterisation should be consistent with these methods used to estimate *Anet*. Therefore our model will follow the eqs. recently described by Sharkey et al. (2007) since these are expected to represent both the most recent formulations as well as those that are consistent with the derivation of key parameters, described in more detail in section 3. The potential rate of assimilation, limited only by Rubisco activity (*Ac*) is calculated according to Sharkey et al. (2007) as in eq 2.

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Where *VCmax* is the maximum rate of Rubisco activity, *ci* and *Oi* are intercellular concentrations of CO2 and O2 respectively, *Kc* and *Ko* are the Michaelis-Menten coefficients of Rubisco for CO2 activity (in μmol mol-1) and O2 (in mmol mol-1) , respectively, and Γ\* is the CO2 compensation point in the absence of mitochondrial (dark) respiration and they all are calculates as:

*VCmax* = temp\_dep\_inhibit(V\_cmax\_25, deg\_to\_kel(25), H\_a\_vcmax,

H\_d\_vcmax, S\_V\_vcmax, Tleaf\_K, R)

The potential rate of assimilation when RuBP regeneration is limiting is given in eq. 3.

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Where *J* is the electron transport rate, the parameters *a* and *b* denote the electron requirements for the formation of NADPH and ATP respectively. The exact values differ slightly throughout the literature but are all close to *a*=4 and *b*=8 assuming four electrons per carboxylation and oxygenation(Sharkey et al., 2007). *J* is related to incident photosynthetically active photon flux density (*Q*) where the light response of a plants photosystem first follows a linear rise with an increase in radiation *Q* until it reaches an area of saturation where the electron transport rate *J* approaches the maximum value of *Jmax*. Mathematically this is represented by the quadric relationship shown in eq. 4 after Leuning (1990).

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Where α is the quantum yield of electron transport, which determines the slope of the linear rise in the low irradiance regime, and Ø is the curvature of the light response curve normally acquired by experimental fitting. The value of α was fixed at 0.3 mol electrons mol-1 photon, based on an average C3 photosynthetic quantum yield of 0.093and a leaf absorptance of 0.8 (cf. Medlyn et al., 2002). The value of Ø was taken to be 0.90 (Medlyn et al., 2002). These parameter values have only a slight effect on the estimated value of *Jmax*.

Finally, the potential rate of assimilation when the utilization of triose phosphate is limiting assimilation (*Ap*) (i.e. when the chloroplast reactions have a higher capacity than the capacity of the leaf to use the products of the chloroplasts) is estimated rather simply by eq. 5 after (Collatz et al., 1991).

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The key parameters of the model *Jmax* and *VCmax*, as well as the parameters *Kc*, *Ko* and Γ\*, all vary with temperature (Medlyn et al., 2002). *Jmax* and *VCmax* also vary between species, whilst *Kc*, *Ko* and Γ\*are considered intrinsic properties of the Rubisco enzyme and therefore can be assumed constant between species (Harley et al., 1986). Due to the temperature effects on the Rubisco enzyme which catalyses the corresponding process, Γ\* is temperature dependent as well.

The original model of Farquhar et al. (1980) used a purely empirical polynomial from (Brooks & Farquhar, 1985) which approximated the temperature dependence of these different parameters, since then many studies have investigated these temperature dependencies more thoroughly, here we follow the rational of Medlyn et al. (2002) who advised using the temperature relationships provided by Bernacchi et al. (2001) who used an Arrhenius equation to describe the processes and based these functions on measurements made *in vivo* without disturbance of the leaf. The rate of dark respiration *Rd*, Γ\* and the Michaelis-Menten constants for CO2 and O2 (*Kc* and *Ko*) are computed using the standard formulations described in eq 6 and 7.

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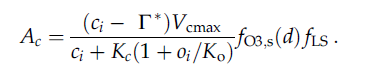
32

where *P* denotes the different quantities, Δ*H* is the activation energy Δ*Hd* is the deactivation energy and Δ*S* is entropy for the processes, values for each process follow those given in Bernacchi et al. (2001). In general this formula describes a normal Arrhenius equation modified to incorporate an inhibition term at high temperatures.

In summary, the Farquhar model mathematically quantifies a detailed mechanistic understanding of the biochemical processes in the chloroplasts which govern photosynthesis. It allows for the estimation and calculation of the CO2 assimilation rate as a function of leaf temperature, irradiance and internal CO2 concentration.

## Effects of ozone on Rubisco limited rate of photosynthesis (Ac) [2f]

Effects of ozone on Rubisco limited rate of photosynthesis (Ac) calculated in the equation (27) is further estimated to see the impact of ozone under the assumption that Ac decreases 1) immediately at high ozone fluxes and 2) with enhanced leaf senescence due to cumulative ozone uptake. It is computed according to the approach used in Ewert’s model (Ewert & Porter 2000);



Where ; V\_cmax – maximum carboxylation velocity

                 c\_i and O\_i – intercellular CO2  and O2 concentration

                 K\_C and K\_O – Rubisco Michaelis-Menten constant for CO2  and O2

                 - CO2 compensation point in the absence of respiration

                 fO3,s  -factor that accounts for daily hour effect of ozone flux on Vcmax at

                              the end of the day

                 f\_LS   -factor that accounts for the effect of leaf senescence on Ac

## Calculating FST

TODO: COMPLETE THIS SECTION

## Short-term ozone response [2a, 2b]

Plants exposed to high doses of ozone for short-term have shown impact on Vcmax, whereas at low ozone doses plants can recover fully via repair system and detoxification without impacting the Vcmax. Therefore hourly short term ozone effect on Rubisco-limited photosynthesis and ozone uptake (fO3,s (h)=1, no effect and fO3,s (h)=0, maximum effect) is calculated hourly as follows:

fO3,s (h) = 1 ;                                                                     for f\_st ≤ γ1 / γ2

fO3,s (h)= 1+ γ1- γ2\* f\_st                                                for γ1/γ2 < f\_st<(1+γ1)/γ 2

fO3,s (h) = 0 ;                                                                     for f\_st ≥ (1+ γ1)/ γ 2

where; f\_st is instantaneous ozone uptake and γ1(0.06) and γ2 (0.0045 nmolm-2s-1)-1) are empirically determined coefficient representing the short-term damage coefficient. f\_st which is computed in DO3SE model while taking into account O3 deposition to the external leaf surface as well as the O3 actually taken up through the stomates. Therefore, if  ozone conductance (Gsto\_l) is 0, then f\_st will also be 0 as ozone won’t be taken up by stomates if there is no conductance, whereas if Gsto\_l>0  then Fst is calculated as follows;

|  |  |
| --- | --- |
|  |  |
|  | Fst =  O3 \* (1/Rsto\_l) \* (leaf\_r / (leaf\_rb + leaf\_r));  leaf\_rb = 1.3 \* 150 \* sqrt(Lm/uh) |
|  | leaf\_r = 1.0 / ((1.0/Rsto\_l) + (1.0/Rext)) |
|  |  |

Where; Gsto\_l    - single leaf ozone conductance (mmol/m3)

               leaf\_rb   - leaf boundary layer resistance (s/m)

               Lm          - leaf dimension (m)

               Uh           - windspeed at canopy (m/s)

               leaf\_r      - leaf resistance (s/m)

               Rsto\_l     - single leaf cuticle resistance (s/m)

               Rext        - external plant cuticle resistance (s/m)

               O3            - Ozone concentration  (nmol/m3)

## Cumulative daylight hour effect of ozone flux on Vcmax(fO3\_d) [2b]

Factor that accounts for the cumulative daylight hour effect of ozone flux on Vcmax(fO3\_d)  is computed as;

fO3\_d = fO3\_S(h)\* rO3,s (If h is not a daylight hour)

fO3\_d = fO3\_S(h)\* previous hour fO3,s(d\_1)  (if h is a daylight hour)

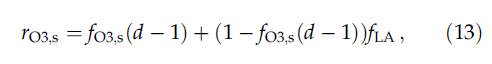
where; fO3,s(d\_1) is effect of ozone on Vcmax of first daylight hour which is calculated based on the assumption that recovery from ozone happens only during night hours (here assumed when PAR>50 W m2­), otherwise the value of fO3,s(d\_1) is same as the cumulative daylight hour effect of ozone flux on Vcmax (fO3\_d) , expressed as;

fO3,s (d\_1) = fO3,s (h) \* rO3,s         for PAR<=50;  and

fO3,s (d\_1) = fO3\_d                           for PAR>50

## Calculation of incomplete recovery from ozone (rO3,s) [2b]

rO3 depends on the leaf age (f\_LA) and the factor which accounts for previous day ozone effect on Vcmax (fO3,s) at the end of the day, calculated as;



Note we use fO­3(d-1)­­ as the daily accumulated damage factor from the previous hour.

We have 2 methods to calculate . The first assumes recovery only at hour 0 (As in Ewert & Porter 2000). The second assumes recovery when there is no daylight.

#### fO3d Method A – Single hour recovery (Ewert & Porter 2000)

where; **Ozone effect on Vcmax at the end of the day (fO3,s)** is computed as follows;



when hour = 2..24;

otherwise 

#### fO3d Method B – Full Night recovery

where; **Ozone effect on Vcmax at the end of the day (fO3,s)** is computed as follows;



when PAR=0;

otherwise ;

and f\_LA  is the factor which accounts for leaf age and is calculated over the life span of leaf (t\_l). Ewert model assumed that young leaf recover fully from ozone damage and didn’t take into account irreversible injury at high ozone concentration, therefore f\_LA is calculated as :

f\_LA= 1;                                                          for    al ≤ tl,em

f\_LA= 1- (al - tl,em )/ tl,ma ;                          for    tl,em< al < tl

f\_LA = 0;                                                         for    al  ≥ tl

where f\_LA – factor which accounts for leaf age

              al –        age of leaf

tl,em –    thermal time interval of emerging leaf

              tl,ma -    thermal time interval of mature leaf

tl -          total life span of leaf

## Long -term ozone response [2c, 2d]

Long-term accumulation of low doses of ozone degrades rubisco enzyme and triggers senescence in mature leaves at early age, which can be explained with the linear relationship between the life-span of a mature leaf and accumulated ozone consumption;

tl,ma = (tl,ep + tl,se)\*fO3,l

and tl,se also changes with tl,ma which is given by

tl,se = 0.33 tl,ma

Where; tl,ma -    thermal time interval of mature leaf

               tl,se    - thermal time interval of senescence leaf

               tl,ep   - thermal time interval of expanded leaf

               fO3,l -  factor which accounts for long term ozone impact on Vcmax

We also calculate the tl\_ep value.

tl,ep = tl,ma +  tl,se

We recalculate t\_lma, t\_lse and t\_lep with the impact of ozone (fO3\_l). These new values are then used for calculating the new senescence factor below.

Factor which accounts for long term ozone impact (fO3,l )is calculated using the i) empirical factor γ3=0.5(µmolm-2)-1 (which describes reduction in life-time of a mature leaf per unit accumulated ozone) and ii) integrated ozone uptake value which changes with respect to age of the leaf which gives integrated f\_st from the beginning to the total life span of the leaf and represented as follows:

## Effect of leaf senescence on Ac (f\_LS calculation) [2e]

Factor which accounts for effect of leaf senescence on A\_c (fLS) is calculated as

fLS = 1;                                                                         for al  ≤ tl,em + tl,epO3

for for tl,em+tl,epO3<al<tlO3

fLS= 0;                                                                          for al≥ tlO3

 This is based on Ewert equation below:

where; al        - age of  leaf (°Cday)

              tlO3     -life span of leaf after ozone damage

              tl,ma -    thermal time interval of mature leaf

              tl,seO3     - thermal time interval of senescence leaf after ozone damage

              tl,epO3    - thermal time interval of expanded leaf after ozone damage

              tl,em   - thermal time interval of emerging leaf

Note that we replaced the t\_lse and t\_lep values in the Ewert & Porter eq 18 with their ozone damaged values. This resulted in the correct relationship between f\_LS and ozone.

### Micrometeorological CO2 supply model [2h]

It becomes clear that to calculate *gsto*, the value of *Anet* is needed and for the calculation of *Anet*  it is necessary to know *gsto*. Baldocchi (1994) found an analytical solution for parts of the problem, and Su et al. (1996) and Nikolov et al. (1995) developed solutions for other sets of coupled equations. Still the vast majority of published models had to use numerical loops to iteratively guess values for different parameters that satisfy the different equations as the available analytic solutions are limited to certain sets of given environmental quantities and model formulations. An additional cross dependency is added to the model when *Tleaf* values have to be computed from *Tair*, as transpiration is a main driving force for leaf surface temperature control. Therefore *gsto* is needed to calculate *Tleaf* , which can only be calculated when *Anet* is known and for this, again, *Tleaf* is needed (see Nikolov et al. (1995) for a solution).

To facilitate the calculation of the internal (*Ci*) and surface (*Cs*) CO2 from ambient CO2 concentrations (*Ca*) a boundary layer model equivalent to that used for calculating the exchange of O3 across the same physical pathway is used. *Cs* is calculated as a function of *Ca*, *Anet* and *gb*; *Ci* also requires an estimate of gsto. These equations also follow those described in von Caemmerer & Farquhar (1981) and are as described in eq. and .

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The *gb* and *gsto* conductance values are for water vapour and therefore eqs. and use the factors 1.37 and 1.6 (which are the ratios of the diffusivity of CO2 and water vapour in semi turbulent air and still air respectively; the former value equates to 1.62/3 and results from the Pohlhausen analysis of mass transfer from a plate in laminar parallel flows (Kays, 1966)). See also 2.3.2 for methods on how to estimate gb, the values used here are rounded up.

Finally, the leaf surface humidity deficit *Ds* also has to be calculated. This relies on estimates of leaf temperature and standard equations to convert relative humidity into leaf to air vapour pressure deficits (humidity deficit). **EXPLAIN HOW WE CLACULATE LEAF ToC…..**

are similar to those used for ambient air humidity (see Nikolov et al. (1995)).

(19)

where ei is the water-vapor pressure in the intercellular air space of the leaf, es(Tleaf) is the saturation vapor pressure at leaf temperature and ea is the vapor pressure in the ambient air (all in Pa). This implies that the air inside the leaf boundary layer is at leaf temperature. In the case of a wet leaf, Eq. 20 still holds (assuming that the CO2 exchange through stomatal pores is not significantly affected by water droplets residing on the leaf surface), but then Eq. 19 does not apply because the air next to a wet surface is normally vapor-saturated and, therefore, *hs* = 1.

**\/\/\/\/\/\/Not Checked \/\/\/\/\/\/**

# Advanced Configurations

## Canopy Level stomatal ozone flux for forest trees (Canopy AFst)[[p8]](" \l "_msocom_8)

AFst based risk assessments for forest trees might be improved by estimating whole-canopy rather than leaf-level stomatal flux. This is due to the fact that whole tree sensitivity to ozone may not be adequately represented through the calculation of uptake by only the sunlit leaves of the upper canopy; rather the uptake of sun and shade leaves of the entire canopy may have to be considered. As such, here we define ***provisional methods*** to estimate canopy stomatal flux (canopy AFst). Since these methods are only provisional they are only recommended to be used to provide ***comparisons*** with leaf level AFst estimates to give an indication of whether the geographical distribution of ozone risk to forest trees may be altered when using canopy *vs.* leaf level fluxes. For comparative purposes, leaf level stomatal ozone fluxes should be estimated without the use of the threshold (Y) since there is evidence of that detoxification capacity may change with age dependant changes in leaf/needle morphology (e.g. Wieser et al. 2002).

However, measurement data suggest that a more appropriate division of leaf and needle populations within a canopy would be made according to leaf/needle morphology (i.e. sun and shade leaves/needles). This is supported by data which shows shade needles to have significantly lower gmax (ca. 70%) compared to sun needles. Based on data from Schulze et al. (1977) a simple 60:40 (sun:shade) split is suggested, applicable all year round, for provisional modelling of canopy AFst. It is noted that these proportions are likely dependent on tree type, stand density and other factors, and efforts should be targeted in the future to refining these canopy fractions as new data become available.

The incorporation of leaf/needle morphology in estimates of canopy stomatal flux would improve methods used to scale up from the leaf to the canopy for both coniferous and deciduous forests. A simple method described below assumes that sun and shade leaves/needles are evenly distributed over the tree canopy.

gmax\_shade = 0.6 \* gmax\_sun

                                                                                                                        [2]

Canopy gsto = 0.6 \* gmax\_sun + 0.4 \* gmax\_shade

which can be simplified, assuming a 60:40 (sun:shade) split to :-

gmax\_canopy = 0.84 \* gmax\_sun                                                               [3]

The estimation of forest tree canopy stomatal ozone flux would be made using [3] in combination with existing up-scaling methods in the DO3SE dry deposition model.  These methods use standard algorithms to define light extinction with canopy depth to estimate the fraction of- and irradiance to- sunlit and shaded leaves within the canopy (e.g. Emberson et al. 2000). Resulting flight values for both sunlit and shaded fractions are then scaled to the canopy level using an estimate of LAI; hence definition of this parameter is crucial in canopy level stomatal ozone flux estimates. Values for LAI for each “Real” species are given by climate region in the parameterisation table provided in the following sections. Further details of the up-scaling methods used can be found in Simpson et al. (2003).

In the future methods that define the LAI fractions of sun and shade leaves/needles with canopy depth can be combined with estimates of sunlit and shaded fractions of the canopy to refine these up-scaling methods. However, the increased complexity of these methods would warrant larger datasets with which to parameterise the fractional distribution of leaf/needle morphologies within the canopy and hence will not be considered here.

**/\/\/\/\/\/\/\/\/\ NOT CHECKED /\/\/\/\/\/\/\/\/\/**

**\/\/\/\/\/\/\/\/\ NOT CHECKED /\/\/\/\/\/\/\/\/\/**

## Parameterisation

The parameters ΔHa and ΔHd (energy for activation or deactivation of the process) describe the shape of the response function. Their values are species dependent and have to be fitted to experimental laboratory datasets. Medlyn et al. (2002) give a review of experimental values, (Leuning, 2002) assesses uncertainties incorporated by using mean values and (Wohlfahrt et al., 1999) quantifies the mistakes caused by a wrong parameterisation. The value of the two quantities at T=25°C, PT,ref can be more easily determined *via* gas exchange measurements. Wullschleger, (1993) reviews several experimental datasets and reports a wide set of values for different species.

[this is the bit that needs most work…..perhaps start off with the Sharkey paper and the parameterisation details…and refer largely to this?...plus als add table of values from review literature….to be expanded as research is ongoing.]]

As the first step, empirical relationships are used to calculate the maximum electron

transport rate *Jmax* as a function of ambient irradiance *PAR* and *Tleaf*. and further maximum rubisco activity is calculated from *Tleaf* in a similar manner as a function of leaf temperature (add *Tleaf* calculation details). The actual shape of the response functions differs significantly between species (see Figure 1) and has to be determined empirically for each species.



**Figure 6.** Temperature response of Jmax and Vcmax for different species. From (Medlyn et al., 2002b).

In total the combined model incorporates a total of 18 parameters (see table 1). Out of these, only the parameters determining the shape of the temperature response of the Michaelis Menten constants (equation 2) , and the universal gas constant R can be assumed to be constant throughout all species and environmental conditions and can therefore be taken from the literature. The characteristic size of the leaf can be estimated independently via measurements or from published values. Q and a, the two parameters governing the light response curve of the photosystem are nearly always assumed to be reasonably consistent amongst different species.

It is significantly harder to estimate the remaining six parameters. Especially the values of *m*, *Jmax*and *Vcmax* have turned out to differ significantly and to be quite sensitive to the model results. Approaches to parametrize these parameters and the complications arising from spatial and temporal differences of the parameters are discussed in the proceeding chapter.

#### Slope parameter m

The parameter m, the slope of the BWB relationship (equation 1), can be estimated relatively straightforward via linear regression of measured stomatal conductance against assimilation rate, humidity and CO2 concentration at leaf surface as described above (chapter 2.1). Still, reported values have all been within a small range (5-15) so authors assume its value to be roughly consistent within species and use literature values. Leuning (1995) and Kosugi et al. (2003) review a small set of estimated values for different species.

Despite the strong sensitivity of the stomatal conductance model to this parameter

(gsto is directly linearly dependent on m) there has been surprisingly little research on changes within one species (spatial or temporal). Falge et al. (1996) found a change in stand age, though their analysis is based solely on two different stands of differing age. Kosugi et al. (2003) found changes between developments stages of perennial trees during the growing season by a factor of two to three. Additionally Kosugi et al. (2006) report significantly differing values of m during the phenological stage of leaf expansion, but no further change during the growing season (see also Kosugi et al. (2003)).

Still, throughout the literature, it is assumed that *m* is considerably constant amongst well watered plants. Due to the observation that plants under water stress control their stomatal openings via processes which are not included in the BWB approach (like signal transmission from the roots to the leaves), several authors try to incorporate the effects of soil water stress on the behavior of the stomatal conductance model. Tenhunen et al. (1990, 1994) found that m is significantly smaller at the end of a prolonged drought period and hypothesized that plants alter their stomatal response to environmental conditions to reduce water loss during drought. Similar observations are reported by Kosugi et al. (2006). Sala Serra & Tenhunen (1996) fitted values of m for several diurnal gas exchange courses during different regimes of soil water content and found a roughly linear relationship between xylem water potential and optimized values for m. Several others (Wang (1998),Van Wijk et al. (2000) and Tuzet et al. (2003)) include scaling factors into the BWB model (equation 1) which vary between 0 and 1 according to soil water content or soil water potential Y, which is technically equivalent to a direct modification of m. All response functions of these factors to Y are purely empirical but are similar in their general shape (a value of zero for very low Y and a gradual rise into a saturation in well watered regimes). Challenging these findings, Xu & Baldocchi (2003) found no significant alteration of m during periods of drought.

#### Temperature response of Jmax and Vcmax

One major advantage of the Farquhar model is its detailed representation of the temperature response of photosynthesis. This response is mainly governed by the exact shape of the T response curve of Jmax and Vcmax (equation 3). Additionally, the actual shape and scale of this function also crucially influences which process the model “choses“ to be rate limiting and therefore uses for the calculation of Anet . In the following chapter different methods to estimate these two parameters and the factors influencing their actual size are discussed.

The most direct way to determine the temperature response of Jmax and Vcmax is to measure several response curves of Anet to a change in ambient CO2 ci at different temperatures (Medlyn et al., 2002a) under a regime of high irradiance. Under the assumption that Rubisco activity is limiting at low CO2 concentration, equations 3, 5 and 8 are used to gain best fit estimates for Vcmax at given temperatures to low ci values. With these values set fixed, Jmax values are fitted with the same method to the whole ci response curves. Finally estimates for Ha, Hd and PT=25 for both parameters are calculated by fitting equation 3 to the data. This procedure yields parameter values which are relatively independent from the data which is most often later used for modeling, but the calculations are rather complicated and lengthy measurements directly at the leaf scale are necessary, which are often not available. One option, used by Kosugi et al. (2003), is to use field measurements to determine Vcmax and use a often published constant ratio of Vcmax/Jmax (see, for example, Wullschleger (1993), Medlyn et al. (2002a) or Leuning (1997)) to estimate Jmax.

The majority of authors who follow this approach only acquire Vcmax;25 and Jmax;25 in this manner and use published values for Ha and Hd (the two parameters influencing the shape of the rise and decline of the function). Concerning similar plants (like different trees for example (Medlyn et al., 2002a)), it seems to be justifiable to assume similar responses, but Leuning (2002) demonstrated that the response of these parameters can differ significantly between different types of plants, especially in the range of temperatures above 30°C.

Some authors (for example Nikolov et al. (1995) or Falge et al. (1996)) simply fit the parameters to parts of measured time series of assimilation rates or stomatal conductance. This approach should be seen very critically due to the huge amount of parameters with a direct interdependency on best-fit-model results and the resulting high equifinality of estimated parameter values.

#### Influencing factors

The first generation of *Anet*-*gsto* models, published in the beginning of the 1990s, all described *gsto* for independent (temporal) point measurements at the scale of the single leaf. Leuning (1990, 1995), for example, fitted their models to single day time-series of different leaves independently. As soon as the focus moved more towards canopy scale models or models on longer timescales like the whole growing season, it became clear that the optimized parameter values Jmax and Vcmax differ significantly not only between different species but also between different leaves of one single plant, or between positions within the canopy. Furthermore they change during plant development and are highly dependent on environmental conditions during growth of the plant. A wide array of studies have been conducted since to mathematically incorporate these effects into the model.

**Growth temperature** As the Rubisco enzyme governs assimilation in all C3 plants its enzyme kinetics are assumed not to vary between different plants Bernacchi et al. (2001), and the same equations and parameter values are usually taken to calculate Vcmax. On the the contrary, the temperature response of Jmax has been found to vary significantly according to temperatures during growth as a result of the high potential of adaptation to its local environment of each individual plant. June et al. (2004) found a significant rise of the temperature optimum of the electron transport rate with higher growth temperature. In agreement with these findings, Bernacchi et al. (2003) found a slower rise of Jcmax with temperature in plants grown in warmer environments (tobacco was found not to reach an optimum in the measured range of temperatures below 40°C). In these experiments values of Jmax for a given temperature differed by a factor of 1.5-3 between species grown at 15 and at 25°C.

**Leaf position** Even in one single plant, variations in photosynthetic activity have been found in different leaves of this plant. Schultz (2003) measured gas exchange differences between sun and shade leaves of a grapevine stand and found up to two times higher values for Vcmax and Jmax of sun leaves, compared to leaves within the stand. Leaf nitrogen content varied in a similar manner and could explain parts of the variation. Similar findings are reported by Wilson et al. (2000) who explain this effect by a rise in leaf thickness in upper parts of a tree canopy.

**Seasonality** Based on the observation that the two key photosynthetic parameters Jmax and Vcmax change significantly during the growing season especially under field conditions, a large group of authors tried to find correlations between the two parameters and factors like leaf age, leaf nitrogen content, leaf position, ambient temperature or phenological development stage. During interpretation of these results it should be kept in mind that these parameters are not independent of each other and statistical correlation should not be mistaken as causal explanation. Leaf nitrogen con tent for example is strongly correlated with leaf age and position of the leaf (sun/shade leaf) and ambient temperature follows seasonal changes in most parts of the world. Medlyn et al. (2002b) found a roughly linear relationship between leaf nitrogen content and values for Vcmax and Jmax for a yearly time series of evergreen pine trees. At the same time nitrogen content was significantly lower during summer months due to nitrogen relocation during times of growth of new needles. Due to the seasonality of the temperature, the authors could as well construct a reciprocal linear relationship between values of the two parameters and ambient temperature. They argue that this could have been, on the one hand, caused by acclimatisation of the plant to ambient climate conditions which caused lower photosynthetic activity with higher temperatures.

On the other hand changes could have also been induced by phenological changes in

nitrogen content and photosynthetic activity. Similar results have been reported by Schultz (2003) for gravepine, by Xu & Baldocchi (2003) for blue oak and by Kosugi et al. (2003, 2006) or Wilson et al. (2001) for several evergreen trees. In general the seasonal pattern showed a sharp rise of photosynthetic activity and the size of Jmax and Vcmax during leaf development and a gradual decline during the summer months. In accordance to the findings of Medlyn et al. (2002b), Xu & Baldocchi (2003) found the same pattern in leaf nitrogen content and reasoned that about 70% of the observed variation in Vcmax could be attributed to changing nitrogen content. In all studies both parameters changed by a factor between 2 and up to 4 during the growing season. In addition Xu & Baldocchi (2003) reported a gradual decline in the ratio of Jmax/Vcmax, which is often assumed to be constant, from 2.5 at the beginning down to 1 at the end of the season.

Motivated by all these findings Mueller et al. (2005) developed a modification of the model in which they varied Vcmax seasonally according to leaf nitrogen content in different leaves and during different stages of plant development. They based their calculations on a remarkable linear correlation (R2 = 0.97) they found between Vcmax;25 and nitrogen content.

**Comparison of methods with JULES (UK Joint Land Surface Ecosystem Model).**

The JULES model uses very similar formulations to estimate photosynthesis for C3 plants; they also include methods for C4 photosynthesis estimation. These follow Collatz et al., (1991) for C3 plants and (Collatz et al., 1992) for C4 species. The specifics of these methods used in JULES are described in Sellers et al. (1996), Cox et al. (1999) and Clark et al. (2011).

**/\/\/\/\/\/\/\/\ NOT CHECKED /\/\/\/\/\/\/\/\/\**

# Appendix

## Gas units

The Ewert model works with CO2 gas for calculations while the DO3SE model primarily works with O3. This means that we must convert gsto\_O3 inputs to CO2 to run the Ewert photosynthesis model then convert the resulting gsto back to O3 to use elsewhere in the model.

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