Parameterisation and Terms

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# 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 3.** 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).

# Non-Stomatal resistance terms Rsoil, Rinc and Rext

## External leaf-resistance (rext)

A value for rext has been chosen to keep consistency with the EMEP deposition modules “big-leaf” external resistance, Rext = 2500/SAI, where SAI is the surface area index (green + senescent LAI). Assuming that SAI can be simply scaled:

rext = 2500 (s m-1)

There are two different methods for estimating stomatal resistance (or its inverse, stomatal conductance): i. the multiplicative model and ii: the coupled photosynthesis-stomatal conductance model. These are described in the following sections.

The external plant resistance (Rext) represents the resistance of O3 deposition to all the external parts of the plant, including cuticles, twig, bark, mosses, etc. Massman (2004) reviewed the literature detailing investigations of Rext. This revealed that Rext was dependent upon variables such as relative humidity, the presence of leaf hairs and dust on the leaf surface, the thickness of the leaf cuticle, the type and amount of epiphytes and micro-organisms present on the leaf surface, and the length of time over which the surface is exposed to O3.

In view of the uncertainties surrounding deposition rates to canopies, either dry or wet, we assign a single value to describe the external plant resistance to O3 deposition, irrespective of the land-cover category and water status of the cuticles :-

Rext = 2500 s/m.

For a canopy with LAI = 5, this corresponds to a conductance of 0.2 cm/s.

## In-Canopy resistance (*Rinc*)

The in-canopy resistance (*Rinc*) determines the resistance to ozone transfer within the canopy and hence the amount of ozone available for deposition to the surface underlying the vegetation (e.g. bare soil or leaf litter). Since this deposition pathway is controlled by the transfer through the canopy, it depends on the density and height of the surface elements. To estimate *Rinc*, a highly simplified parameterisation is used after that suggested by Erisman et al. (1994) based on the analysis of maize field data by van Pul & Jacobs (1994). The in-canopy resistance is estimated by eq. 30.

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Where *b* = 14 m-1 and is an empirical constant derived from data obtained in association with a maize canopy and *h* is the vegetation height taken as constant for each land-cover class. The *LAI* in the original formula has been replaced here by the *SAI* to account in a simple way for leaves, twigs, bark, etc…. It must be emphasised that this parameterisation is based on one data set for a maize field with a rather limited range of *SAI* h/u\*.

## Soil resistance (Rsoil)

For bare soil a large range of resistance values has been observed and these have been documented by Massman et al. (2004) as shown in Fig x. This variation appears to be strongly influenced by soil wetness with drier soils tending to have lower resistances, evidence also suggests that soil type is important (Galbally & Roy, 1980). Soil wetness is thought to limit O3 deposition by reducing the effective reactive surface due to the low solubility of O3 in water.

**Fig. x. Summary of observationally based inferences for the intrinsic soil resistance (Rsoil) from Massman et al. (2004). The dotted line represents the DO3SE model value of 200 s/m.**



However, given the variability in the published values for Rsoil the data seem too inconclusive for a detailed treatment of this deposition pathway and therefore single values for base values for Rsoil\_Base for different land-cover types have been identified by Simpson et al. (2003) as described in Table x.

|  |  |
| --- | --- |
| **Land-cover type** | **Rsoil\_Base (s/m)** |
| Forests (CF, DF, NL, BL) | 200 |
| Crops | 200 |
| Moorland | 400 |
| Grassland | 1000 |
| Mediterranean Scrub | 200 |

These Rsoil\_Base values are modified to account for low temperature and snow cover conditions according to :-

Rsoil = Rsoil\_Base + Rlow + 2000 δsnow

Where δsnow is represented by δsnow = 1 when snow is present and zero otherwise. Rlow is calculated as :-

Rlow = 1000 e-(ToC+4)

For the DO3SE interface is assumed that Rsoil = Rsoil\_Base since it is unlikely that the information on snow cover will be available as input to the modelling.

An Rsoil\_Base value of 200 s/m corresponds to a conductance of 0.5 cm/s, i.e. a potentially rather efficient deposition velocity. However, as discussed above, deposition is limited by the in-canopy resistance in series with Rsoil.

**Table (x) Default deposition land-cover and species class parameters for fVPD (VPDmin and VPDmax) and fSWP (SWPmin and SWPmax) calculations.**

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Land-cover type & Species** | **Climate region** | **VPDmax** | **VPDmin** | **VPDcrit** | **SWPmax** | **SWPmin** | **Reference** |
|  |  |  |  |  |  |  |  |
| **Coniferous Forests (CF)** |  | 0.6 | 3.3 | - | -0.76 | -1.2 | Simpson et al. (2003) |
| Norway spruce  (*Picea abies*) | Northern Europe | 0.8 | 2.8 | - | 15\* | 1\* | UNECE (2004); Hansson et al. (in prep); Zimmerman et al; Sellin. (1997). (1988); |
| Scots Pine  (*Pinus sylvestris*) | Atlantic Central Europe | 0.6 | 2.8 | - | -0.7 | -1.5 | UNECE (2004); Beadle et al. (1985); Sturm et al. (1998); Ng. (1979); Whitehead et al. (1984) |
| Norway Spruce  (*Picea abies*) | Continental Central Europe | 0.5 | 3.0 | - | -0.05 | -0.5 | UNECE (2004); Zweifel et al. (2000,2001,2002); Braun et al. (in prep) |
| **Deciduous Forests**  **(DF)** |  | 0.93 | 3.4 | - | -0.55 | -1.3 | Simpson et al. (2003) |
| ***Generic Deciduous*** | ***All Europe*** | ***1.0*** | ***3.25*** | ***-*** | ***fSWP=1*** | ***fSWP=1*** | ***UNECE (2004)*** |
| Silver birch  (*Betula pendula*) | Northern Europe | 0.5 | 2.7 | - | 15 | 1 | UNECE (2004); Uddling et al. (2005a) |
| Beech  (*Fagus sylvatica*) | Atlantic Central Europe | 1.0 | 3.25 | - | -0.8 | -1.5 | UNECE (2004) |
| Oak  (*Quercus petraea & robur*) | Atlantic Central Europe | 1.0 | 3.25 | - | -0.5 | -1.2 | UNECE (2004) |
| Beech  (*Fagus sylvatica*) | Continental Central European | 1.0 | 3.1 | - | -0.05 | -1.25 | UNECE (2004) |
| Beech  (*Fagus sylvatica*) | Mediterranean Europe | 1.0 | 4.0 | - | -2.0 | -3.8 | UNECE (2004) |
| **Needleleaf Forests**  **(NF)** |  | 0.4 | 1.6 | - | -0.4 | -1.0 | Simpson et al. (2003) |
| Aleppo Pine  *(Pinus halepensis)* | Mediterranean Europe | 1.0 | 3.2 | - | -0.5 | -1.0 | UNECE (2004); Gimeno. (pers.comm); Picon et al 2006. |
| **Broadleaf Forests**  **(BF)** |  | 1.8 | 2.8 | - | -1.1 | -2.8 | Simpson et al. (2003) |
| ***Generic Evergreen Mediterranean*** | ***All Europe*** | ***2.2*** | ***4.0*** | ***-*** | ***fSWP=1*** | ***fSWP=1*** | ***UNECE (2004)*** |
| Holm Oak  (*Quercus ilex*) | Mediterranean Europe | 2.2 | 4.0 | - | -1.0 | -4.5 | UNECE (2004); Sala & Tenhunen. (1994);Tognetti et al. (1998); Vitale et al. (2005); Manes et al. (1997); Elvira et al. (2005); Bussotti & Ferretti. (2007); Alonso et al. (2007) |
| **Temperate crops**  **(TC)** |  | 0.9 | 2.8 | - | -0.3 | -1.1 | Simpson et al. (2003) |
| ***Generic crop*** | ***All Europe*** | ***1.2*** | ***3.2*** | ***8*** | ***fSWP=1*** | ***fSWP=1*** | ***UNECE (2004)*** |
| Wheat  (*Triticum aestivum*) | All Europe | 1.2 | 3.2 | 8 | -0.3 | -1.1 | UNECE (2004); Gruters (1995);Weber (1996); Bunce (2000); Teubner (1995);  Gollan et al. (1986); Emberson (1997); |
| **Mediterranean crops**  **(MC)** |  | 1.0 | 2.5 | - | -0.11 | -0.8 | Simpson et al. (2003) |
| Maize  *(Zea mays)* | All Europe | 0.0 | 5.0 | - | -0.12 | -0.8 | ICP Vegetation contract report (2006); Olioso et al. (1995); Tardieu et al. (1992a); Davies et al. (1994) |
| Sunflower  *(Helianthus annuus)* | All Europe | 1.2 | 4.0 | - | -0.25 | -1.65 | ICP Vegetation contract report (2006); Ward & Bunce (1986); Turner et al. (1984); Tuebner, F. (1985); Quick et al. (1992); Hirasawa et al. (1992); Fambrini et al. (1994); Sadras et al. (1993); Zhang (1989); Gollan et al. (1986); Trifilo et al. (2003) |
| Tomato  *(Solanum lycopersicum)* | All Europe | 1.0 | 2.7 | - | -0.3 | -1.0 | ICP Vegetation contract report (2006); Boulard et al. (1991); Bakker (1991); Romero-Aranda et al. (2001); Katerji et al. (1998); Haupt-Herting & Fock (2000); Makela et al. (1998) |
| Grape vine  *(Vitis vinifera)* | All Europe | 1.6 | 6.2 | - | -0.35 | -1.2 | ICP Vegetation contract report (2006); Correia et al. (1995); During (1987); Massman et al. (1994); Jacobs et al. (1996); Medrano et al. (2003); Schultz (2003); Winkle & Ramble (1993); Quick (1992) |
| **Root crops**  **(RC)** |  | 0.31 | 2.7 | - | -0.44 | -1.0 | Simpson et al. (2003) |
| Potato  (*Solanuum tuberosum*) | All Europe | 2.1 | 3.5 | 10 | -0.5 | -1.1 | UNECE (2004); Tuebner (1985); Vos & Oyarzun (1987) |
| **Semi-Natural / Moorland**  **(SNL)** |  | 88.8 | 99.9 | - | - | - | Simpson et al. (2003) |
| **Grassland**  **(GR)** |  | 1.3 | 3.0 | - | -0.49 | -1.5 | Simpson et al. (2003) |
| Perennial rye grass  (*Lolium perenne*) | All Europe | 2.0 | 4.0 | - | -0.49 | -1.5 | ICP Vegetation contract report (2009) |
| Clover  (Trifolium repens) | All Europe | 2.8 | 4.5 | - | -0.49 | -1.5 | ICP Vegetation contract report (2009) |
| **Mediterranean scrub** |  | 1.3 | 3.0 | - | -1.1 | -3.1 | Simpson et al. (2003) |