Estimation of Solanum Tuberosum L. carbon assimilation by the Farquhar model : Evaluation of performance and attempts of improvement for water stress episodes

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A Computation of solar elevation

The solar elevation is defined with the following expression :

$$\sin(\beta) = \sin(\lambda)\sin(\delta) + \cos(\lambda)\cos(\delta)\cos(h) \tag{1}$$

Where λ is the latitude, δ the solar declination angle and h is the hour angle. δ is computed with the following expression:

$$\delta = -23.4\frac{\pi}{180}\cos(\frac{2\pi(t_d + 10)}{365}) \tag{2}$$

Where t_d is the number of the day counted from the first of January.

h is obtained by applying the following relation :

$$h = \pi\frac{(t - t_0)}{12} \tag{3}$$

Where t is the hour of the day (regardless of the time zone) and t_0 is the solar noon. It is obtained with :

$$t_0 = 12 + \frac{[4(L_s - L_e) - E_t]}{60} \tag{4}$$

L_s is the longitude of the timezone for a given location, and L_e is the actual longitude. E_t is the result of the following empirical expression :

$$E_t = 0.017 + 0.4281 \cdot \cos(\Gamma_d) - 7.351 \cdot \sin(\Gamma_d) - 3.349 \cdot \cos(2\Gamma_d) - 9.731 \cdot \sin(\Gamma_d) \tag{5}$$

Where Γ_d is the day angle and is given by :

$$\Gamma_d = \frac{2\pi(t_d - 1)}{365} \tag{6}$$

B Solution of the integral for PPFD absorbed by sunlit leaves

I_{lb} can be expressed withe the following expression :

$$I_{lb} = I_{lb}(0) \cdot (1 - \sigma) \cdot k_b \tag{7}$$

Where $I_b(0)$, is the PPFD incident at the top of the canopy per ground area, k_b is the ground surface occupied by $1m^2$ of leaf and (1-σ) is the part of the photosynthetically active radiaton (PAR) effectively absorbed (sum of coefficient of transmission and reflections coefficients) and is equal to 0.85 [-]. The integral for direct beam radiation absorbed is solved as follows:

$$\int_0^{L_t} I_{lb}(L) f_{sun}(L) dL = I_{lb}(0)(1 - \sigma)[1 - e^{-k_b L_t}] \tag{8}$$

For the diffuse PAR absorbed by sunlit leaves, we have the following expression :

$$I_{ld} = I_{ld}(0) \cdot (1 - \rho) \cdot k_b \cdot e^{-k'_d \cdot L} \tag{9}$$

For the diffuse PAR, the coefficient of absorption is considered equal to 1-ρ. It means that the transmission coefficient is equal to 0 for diffuse radiation.

By solving, the integral, we obtain :

$$\int_0^{L_t} I_{ld}(L) f_{sun}(L) dL = I_d(0)(1 - \rho_{cd})(1 - e^{-(k'_d + k_b)L_t}) \frac{k'_d}{k'_d + k_b} \tag{10}$$

$I_d(0)$ is the diffuse part of PAR at the top of the canopy, ρ_{cd} is the reflection coefficient of canopy for diffuse PAR, and k'_d is the extinction coefficient of diffuse PAR modified to take into account the scattering. These two lasts parameters are obtained by integration on multiple leaf classes. For this purpose, 36 class angles are defined by dividing the range between 0 and 180°. ρ_{cd} is then defined as :

$$\rho_{cd} = \sum_{i=1}^{36} 1 - e^{\frac{-2 \cdot \rho_h \cdot \frac{0.5 \cdot C}{\sin(\alpha)_i}}{1 + \frac{0.5 \cdot C}{\sin(\alpha)_i}}} \tag{11}$$

Where $\sin(\alpha)$ comes from the mean angle of each class :

$$\overline{\sin(\alpha)} = \sqrt{1 - \overline{\cos(\alpha)^2}} \tag{12}$$

$$\overline{\cos(\alpha)_i} = \frac{1}{2} \cdot (\cos(\alpha_{i,min}) + \cos(\alpha_{i,max})) \tag{13}$$

With $\alpha_{i,min}$ and $\alpha_{i,max}$ respectively, the lower and the upper limit of the angle class.

The ρ_h parameter is the canopy reflection coefficient of beam PPFD for horizontal leaves and defined as :

$$\rho_h = \frac{1-(1-\sigma)^{\frac{1}{2}}}{1+(1-\sigma)^{\frac{1}{2}}} \tag{14}$$

k'_d is defined with the following expression:

$$k'_d = k_d(1-\sigma)^{\frac{1}{2}} \tag{15}$$

Where k_d is the coefficient of extinction for diffuse PAR unmodified. Its expression is the following :

$$k_d = \int_0^{\pi/2} \frac{0.5 \cdot C}{\sin(\alpha)} d\alpha \tag{16}$$

The last components, the scattered beam PPFD absorbed by sunlit leaves, is defined as follow :

$$I_{lbs} = I_b(0)\left[(1-\rho_{cb}) \cdot k'_b \cdot e^{(-k'_b L)} - (1-\sigma) \cdot k_b e^{-k_b L}\right] \tag{17}$$

The integration result in the following expression :

$$\int_0^{Lc} I_{lbs}(L) f_{sun}(L) dL = I_b(0)\left[(1-\rho_{cb}) \cdot (1-e^{-(k'_b+k_b)\cdot L_c}) \cdot \frac{k'_b}{k'_b+k_b} - (1-\sigma) \cdot \frac{(1-e^{-2k_b L_c})}{2}\right] \tag{18}$$

Where k'_b is the modified extinction coefficient for direct-beam PAR to account for scattering by leaves

$$k'_b = k_b(1-\sigma)^{\frac{1}{2}} \tag{19}$$

and ρ_{cb} is reflection of direct-beam PAR for leaf :

$$\rho_{cb} = 1 - e^{\frac{-2\cdot\rho_h\cdot k_b}{1+k_b}} \tag{20}$$

The total PPFD absorbed by the canopy can be defined with the following expression:

$$I_b(0) \cdot (1-\rho_{cb}) \cdot (1-e^{-k'_b \cdot L_c}) + I_d(0) \cdot (1-\rho_{cd}) \cdot (1-e^{-k'_d L_c}) \tag{21}$$

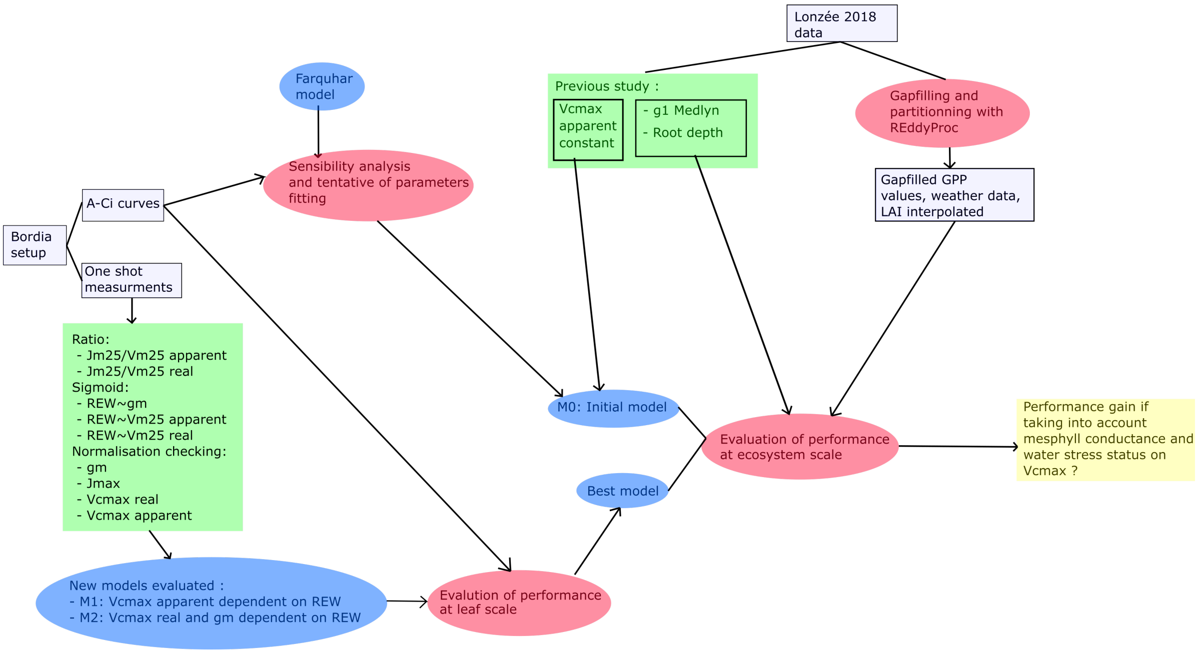
C Value of pressure head and water content for Bordia and Lonzée fields

pF	SWC [%] Bordia	SWC [%] Lonzée
1.00	44.0	42.1
1.60	38.5	38.1
1.85	36.7	39.2
2.00	35.4	36.3
2.48	30.7	30.9
2.85	25.6	26.5
3.00	23.3	24.5
3.70	18.7	18.2
4.18	16.2	16.1

D Soil properties at Bordia and Lonzée in 2013

		Clay (%)	**Silt (%)**	**Sand (%)**	**Density (g/cm³)**	**Organic matter (%)**
Lonzée	0 - 5 cm	11.6	80.2	8.2	1.19	1.912
	5 - 15 cm	11.6	80.2	8.2	1.23	1.854
	15 - 30 cm	10.8	80.7	8.5	1.39	1.857
Bordia	0 - 20 cm	14.0	78.7	7.3	1.48	1.670
	20 - 30 cm	22.2	70.6	7.2	1.48	1.150

E Summary diagram of data use



F Sensitivity analysis and parameters calibration

A sensitivity analysis has been performed on Γ, $\Gamma^*_{25°C}$, ϑ_A, ϑ_J and $V_{max,25°C,app}$. For this purpose, the value of C_i and leaf temperature coming from A_n-C_i curves collected at Bordia have been used to feed the model and produce A_n values.

A variation of $\pm 10\%$ has been used for all parameters except for Γ and $\Gamma^*_{25°C}$. The value of Γ can not go underneath the value of Γ^* (result of Arrhenius equation apply on $\Gamma^*_{25°C}$). Γ minus 10% has thus been replaced by the value of Γ^* and the value of Γ^* plus 10% by the value of Γ.

The sensitivity for a given parameter p is defined as the variation of the output (ΔO) divided by the output (O) for the parameter unchanged and divided by the ratio of the variation of the parameter (ΔP) divided by itself :

$$S_p = \frac{\frac{\sum_{i=0}^{n} \frac{\Delta O_i}{O_i}}{n}}{\frac{\Delta P}{P}} \tag{22}$$

For the analysis, values proposed by (Bernacchi et al. 2001) have been used for Γ and $\Gamma^*_{25°C}$, ϑ_a and ϑ_j come from (De pury and Farquhar 1997) calibration and $V_{cmax,25°C,app}$ comes from previous analysis performed on Lonzée experimental field with *Solanum Tuberosum Agria* and is a value acquired on potato plants in absence of edaphic stress (Beauclaire personnal communication).

After this first analysis, calibration has been tried on the same set of data. The optimisation has been made incrementally from the most sensitive parameter to the least one. The algorithm used is the Broyden-Fletcher-Goldfarb-Shanno algorithm. The Theil's Inequality Coefficient (TIC) between $\mathrm{A_n}$ predicted and observed at Bordia has been used as metric and is defined by:

$$\mathrm{TIC} = \frac{\mathrm{RMSE}}{\sqrt{\sum_{i=1}^{n} \frac{x_i^2}{N} + \sum_{i=1}^{n} \frac{\widehat{x_i}^2}{N}}} \tag{23}$$

with root mean square error (RMSE) equal to :

$$\mathrm{RMSE} = \sqrt{\frac{\sum_{i=1}^{N} (x_i - \widehat{x_i})^2}{N}} \tag{24}$$

This indicator has the advantage of being easily readable, a good prediction as a TIC close to 0 in contrast, a model returning prediction will have a TIC equal to 1.

The result of sensitivity analysis and optimisation is presented in the table below:

	Initial value	**Sensitivity**	**Value after optimisation**
$\mathrm{V_{max,25°C,app}}$	$130 \pm 10\% [\mu\mathrm{molm^{-2}s^{-1}}]$	0.9993	125
Γ	$4.4 \pm 10\% [\mathrm{Pa}]$	0.5698	4.0572 , reset at 4.4 ($< \Gamma^*_{25C}$)
$\Gamma^*_{25°C}$	$4.25 \pm 10\% [\mathrm{Pa}]$	0.1414	1.0667
ϑ_1	$0.7 \pm 10\% [-]$	0.0925	0.5735

G Results of simulation with $\mathrm{V}_{\mathrm{cmax,25°C,constant}}$

Figure 1: Assimilation predicted by model $\mathrm{V}_{\mathrm{cmax,25°C,app}}$ constant and GPP observed on the simulation period

H Results of simulation with $\mathrm{V}_{\mathrm{cmax,25°C,real}}$ and g_{m} depending on REW

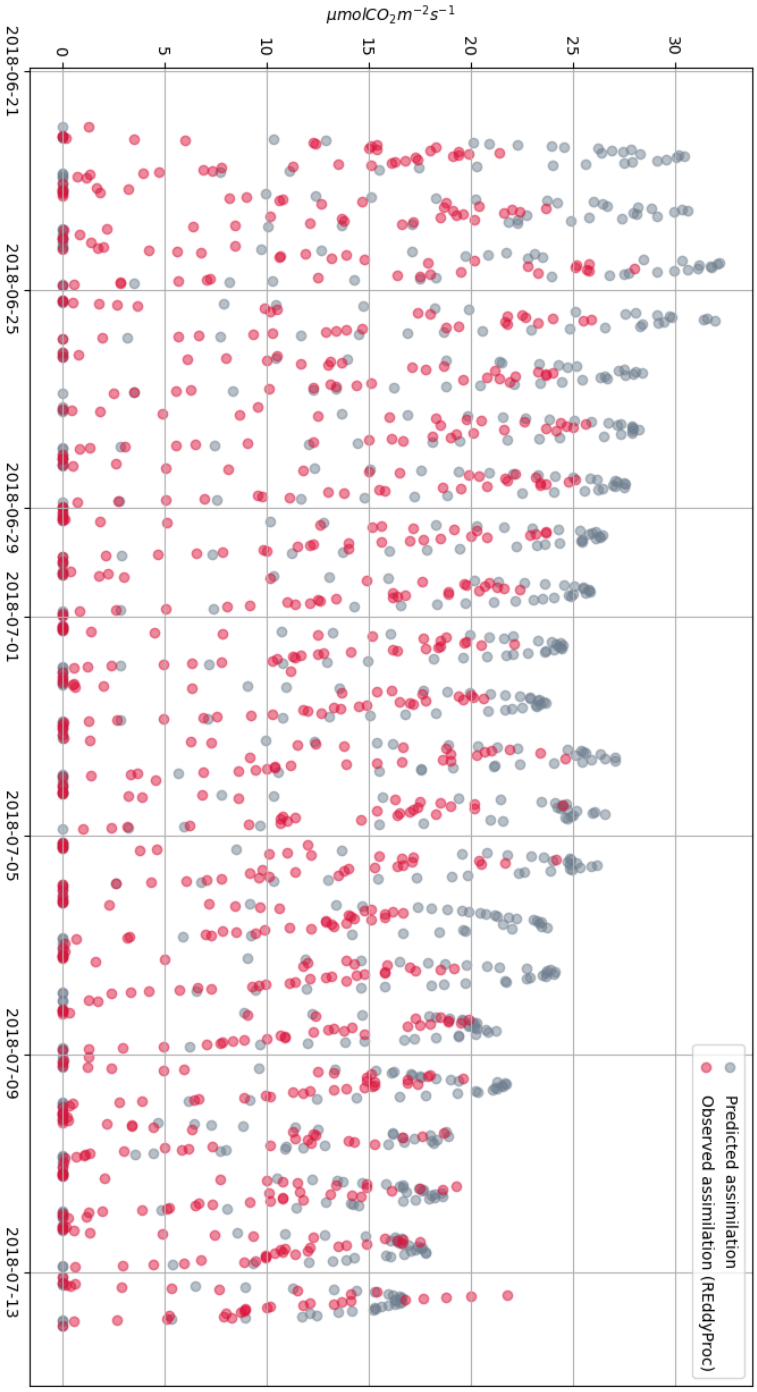


Figure 2: Assimilation predicted by new model and GPP observed on the simulation period