







# **TECHNICAL NOTE 85.75**

Higher Plant Chamber Prototype for the MELiSSA Pilot Plant: Updated Prototype Mathematic Model

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## 1. Introduction

This document outlines the status of the mathematical model based on the Thornley model for canopy photosynthesis.

## 2. Control Law and Expected Performance of the HPC

Recent advances have been made in the use of the Thornley canopy photosynthesis model which is an extension the rectangular hyperbola model (Thornley and Johnson, 2000). In collaboration with ESA-ESTEC, the Thornley model has been coded in EcosimPro software and the predicted responses have been compared to empirical carbon exchange data collected in the SEC-2 chambers in 2004 (Ordóñez *et al.*, 2004; Favreau *et al.*, 2005). Results indicate that the Thornley model is superior to the Modified Energy Cascade Model reported upon in the cited papers. Higher plant modeling efforts for space-related applications have been limited within NASA to the Modified Energy Cascade (MEC) model by Cavazzoni (Cavazzoni, 1999). However, the predictive control strategy that has been foreseen for MELiSSA imposes additional constraints to the model. A first principles model is therefore necessary to extend the capabilities of the control law to operational points beyond the limits of historical on-the-ground research. This allows a more effective control and the development of an adequate optimization strategy.

Thornley and Johnson's work proved to be a very valuable source of information. All the aspects of the growth of plants are reviewed, giving mathematical models for photosynthesis, leaf growth, respiration, light interception, temperature effect, transport processes, root growth, and transpiration. Although not all the models proposed are based on physiology, a first principles model is proposed for photosynthesis, which is the main process driving plant growth.

## 2.1. Models of Gas Exchange of the HPC

The transport of  $CO_2$  into the leaf interior is governed by the pathway conductance. Equations 8.1.1 and 8.1.2 are established considering that, at equilibrium, the diffusion rate of  $CO_2/O_2$  into/from the leaf must be equal to the photosynthesis rate (in congruent units)



$$P_n = \frac{C_a - C_i}{r_{dc}}$$

Equation 2.1.1

 $P_n = \frac{O_i - O_a}{r_{do}}$ 

Equation 2.1.2

Equations 8-1 and 8-2 variables have the following meaning:

 $\begin{array}{l} P_n: \mbox{ Net photosynthesis rate} \\ C_a: \mbox{ CO}_2 \mbox{ concentration in the ambient air} \\ C_i: \mbox{ CO}_2 \mbox{ concentration in the leaf} \\ r_{dc}: \mbox{ CO}_2 \mbox{ diffusion coefficient from air to leaf} \\ O_a: \mbox{ O}_2 \mbox{ concentration in the ambient} \\ O_i: \mbox{ O}_2 \mbox{ concentration in the leaf} \\ r_{do}: \mbox{ O}_2 \mbox{ diffusion coefficient from leaf to air} \end{array}$ 

In a simplified model of the Calvin Cycle, it is supposed that an enzyme X is activated by light. Its activated form, X\*, fixes  $CO_2$  into the carbohydrate recovering its original form. A constant dark respiration rate is assumed. Considering these three reactions as equilibrium reactions with equilibrium constants  $k_1$ ,  $k_2$  and  $k_3$  respectively;

$$P_n = \frac{\alpha \cdot I \cdot \left(\frac{C_i}{r_x} - \frac{O_i}{r_p}\right)}{\alpha \cdot I + \frac{C_i}{r_x} + \frac{O_i}{r_p}} - R \qquad \text{Equation 2.1.3}$$

 $\alpha$ ,  $r_x$ , and  $r_p$  are constants derived from the equilibrium constants, the depth of the leaf (h), and the total concentration of enzyme  $X_0$  ( $X_0=X+X^*$ ). This is:

$$\alpha = h \cdot k_1 \cdot X_0; \quad r_x = h \cdot k_2 \cdot X_0; \quad r_p = h \cdot k_3 \cdot X_0$$

R is the respiration rate and is treated below.

Given the respiration rate and the boundary conditions (light intensity,  $O_2$  and  $CO_2$  concentration in the atmosphere) equations 8.1.1, 8.1.2 and 8.1.3 allow solving the system for  $P_n$ ,  $C_i$  and  $O_i$ .

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The leaf photosynthesis model has to be extended to canopy level. Assuming a high planting density, the canopy can be considered as a murky medium. The light attenuation through a murky medium follows a Beer-Lambert law (exponential decay), given by equation 8.1.4.

$$I(l) = I_0 \cdot \frac{k}{1-m} \cdot e^{-k \cdot l}$$
 Equation 2.1.4

where:

I(l): Light intensity at leaf area index 1
I<sub>0</sub>: Light intensity at leaf area index 0 (top of the canopy)
I: Cumulative leaf area index
k: extinction coefficient
m: transmission coefficient

The leaf area index (l) represents the density of leaves in the canopy (measured as  $m^2$  of leaf over  $m^2$  of ground). It is supposed to be null at canopy height, and the sum of all the leaf areas at ground level. The light is thus attenuated while absorbed by the leaves. The extinction coefficient *k* is related to three parameters: the leaf transmission coefficient *m*, and two geometrical parameters  $\xi$  and  $\zeta$  related to the leaf distribution and inclination within the canopy respectively (equation 8.1.5)

$$k = (1-m) \cdot \xi \cdot \zeta$$
 Equation 2.1.5

The knowledge of the light distribution within the canopy allows the integration of the leaf photosynthesis to obtain the total photosynthesis in the canopy;

$$P = \int_{0}^{l} \left[ \frac{\alpha \cdot I_{0} \cdot e^{-k \cdot l} \cdot \left( \frac{C_{bs}}{r_{x}} - \frac{O_{bs}}{r_{p}} \right)}{\alpha \cdot I_{0} \cdot e^{-k \cdot l} + \frac{C_{bs}}{r_{x}} + \frac{O_{bs}}{r_{p}}} - R \right] \cdot dl$$
 Equation 2.1.6

Although a constant dark respiration could be assumed, the reproduction of the experimental results required the introduction of a respiration model. The approach consists of separating the respiration into two components. The first component is known as "growth respiration" and it is proportional to the photosynthesis rate, while the second component is the so called "maintenance respiration", and is proportional to the total biomass,





 $R = k_n \cdot P_n + c \cdot W$ 

Equation 2.1.7

where:

R: Respiration P<sub>n</sub>: Net photosynthesis rate W: Canopy dry mass

The three sub-models presented above allow the implementation of a canopy model whose results will be compared against experimental data. Three additional parameters are needed to evaluate the leaf area growth from the net photosynthesis: the specific leaf area ( $m^2 leaf / g leaf$ ), the carbon content of the plant (g C / g plant), and the percentage in weight of leaves in the plants.

 $\frac{dl}{dt} = \frac{P \cdot L_{plant} \cdot SLA}{C_{leaf}}$  Equation 2.1.8

where:

l: Leaf area index
P: Photosynthesis rate
L<sub>plant</sub>: Leaf content of the plant (% in dry weight)
SLA: Specific Leaf Area (m<sup>2</sup> leaf / g leaf)
C<sub>leaf</sub>: Carbon content of leaf (% in dry weight)

Empirical data were used to validate the Thornley model with initial inputs of canopy density, initial leaf area, light intensity as a function of time, and the atmospheric conditions (pressure, temperature, atmosphere composition). The results of the comparison are shown in the figures below.



Figure 2.1-1. Comparison between lettuce experimental results (blue) and simulation results (pink) - Accumulated Carbon Gain (mol C)



## Figure 2.1-2: Comparison between lettuce experimental results (blue) and simulation results (pink) - Daily Carbon Gain (mol C / d)





The table below show the results of the tuning, giving the values for the parameters resulting from the fitting exercise.

Parameter	Value	Units
С	1000	ppm
0	21	%
lo	7.5 10 <sup>-4</sup>	m <sup>2</sup> leaf / m <sup>2</sup>
α	4.5 10 <sup>-8</sup>	kg CO <sub>2</sub> / J
k <sub>ρ</sub>	0.005	No units
С	5.0 10 <sup>-8</sup>	S <sup>-1</sup>
k	0.9	No units
m	0.1	No units
rdc	25	s / m
SLA	225	m²/g
L <sub>plant</sub>	95	%
Cleaf	40	%
rdo	50	m <sup>2</sup> kgO <sub>2</sub> /kgCO <sub>2</sub> /g
rp	$1.67 \ 10^4$	s/m
rx	5	s/m

 Table 2.1-1. Lettuce model parameters

The model was also compared to experimental trials with beet. Results are shown in Figure 2.1-3 and Figure 2.1-4. shows the values of the parameters which resulted from fitting the beet model to experimental data. Table 2.1-2 presents estimations of model parameters for fits on beet experimental data.



Figure 2.1-3: Comparison of beet experimental results (blue) with simulation results (pink) - Accumulated Carbon Gain (mol C)



Figure 2.1-4: Comparison of beet experimental results (blue) with simulation results (pink) - Daily Carbon Gain (mol C / d)





Parameter	Value	Units
С	1000	ppm
0	21	%
l <sub>o</sub>	5.0 10 <sup>-3</sup>	m <sup>2</sup> leaf / m <sup>2</sup>
α	3.2 10 <sup>-8</sup>	kg CO <sub>2</sub> / J
k <sub>ρ</sub>	0.12	No units
С	5.5 10 <sup>-9</sup>	S <sup>-1</sup>
К	0.9	No units
m	0.1	No units
rdc	24	s / m
SLA	110	m <sup>2</sup> /g
L <sub>plant</sub>	50	%
Cleaf	40	%
rdo	50	m <sup>2</sup> kgO <sub>2</sub> /kgCO <sub>2</sub> /g
rp	$1.82 \ 10^4$	s/m
rx	3.45	s / m

#### Table 2.1-2. Beet model parameters

Despite the fact that the model implemented is at an early stage of development, preliminary results indicate a good performance as shown by the ability to reproduce independently derived experimental results. Several capabilities remain to be added to the model including i) temperature dependence, ii) carbohydrate partitioning models, iii) water uptake, and iv) the ability to simulate staged and integrated canopies.

### 2.2. Models of Nutrient Uptake by the HPC

Under closure of a hydroponics system it has been found that ion imbalances may result from the indiscriminate control capability afforded by conventional electrical conductivity and pH feedback sensing. Since both commercial greenhouse and advanced life support systems target closure of the hydroponics loop, compensatory nutrient addition to the crop root zone needs to be balanced by uptake. While the design team are also investigating the role of specific ion sensing technologies such as in-line HPLC and ion-specific electrodes, there is the parallel development of predictive models of nutrient uptake that can be integrated into a model and sensor driven control system. An advantage of working in sealed environments is that canopy gas exchange may be readily monitored with conventional gas analysis equipment. This gives rise to opportunity for correlating canopy photosynthetic activity with nutrient uptake. Ideally, mass dynamics in closed environment system designed for life support could be expressed as a function of a single variable, Net Carbon Exchange Rate.

The theory of steady state nutrition, as proposed by Ingestad and Agren (1988) provides a mechanism by which dynamics in nutrient uptake may be predicted from the carbon exchange of plant canopies. The theory, originally developed for aspen (populus tremuloides), proposes that the relative growth rate (RGR) of plant stands and the relative





nutrient uptake rate (RUR) of a given nutrient are equivalent. Ingestad and Agren (1988) explain that the theory of steady state nutrition holds if two conditions are met i) the relative proportions of different plant parts (tuber, roots, flowers etc.), whose mineral concentrations may differ, remains constant during the period of study and ii) the nutrient composition of each different plant part must itself remain constant or the relative proportions of the plant parts adjust to offset any mineral changes. It is very difficult to confirm adherence to steady state nutrition using mineral analysis of plant parts and tissues. First, high numbers of plants must be cultured to generate sufficient biomass for destructive growth analysis and secondly, plant parts must be harvested at regular intervals in order to assess any drift in tissue concentrations as a result of departures in steady state theory.

It can be shown that non-destructive estimations of crop RGR can be determined from NCER as follows:

$$RGR(t) = \frac{NCER(t)}{\int_{t=0}^{t} NCER(t) \cdot dt}$$
 Equation 2.2.1

where NCER(t) is an instantaneous estimate of plant Net Carbon Exchange Rate at any age t. Ingestad and Agren's (1988) concept of steady state nutrition states that Relative Nutrient Uptake Rate (RUR) is equivalent to RGR. Under the assumption of steady state nutrition, the ion uptake rate,  $U\tilde{\eta}(t)$  may be estimated by non-destructive means as follows:

$$U\eta(t) = \frac{NCER(t)}{\int_{t=0}^{t} NCER(t) \cdot dt} \cdot \int_{t=0}^{t} U\eta(t) \cdot dt$$
 Equation 2.2.2

where  $U\tilde{\eta}(t)$  is the instantaneous uptake rate of any ion,  $\tilde{\eta}$ , at time t.

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Figure 2.2-1. Patterns of the ln transform of nutrient uptake for beet canopies grown in a sealed environment chamber.



Figure 2.2-2. Relative nutrient and carbon uptake for beet canopies grown in a closed environment

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## Figure 2.2-3. Reltaionships between relative nutrient uptake rate and relative carbon uptake rate derived from NCER analysis.

Preliminary analysis of the data presented above indicates that congruence between the stand RGR and RUR as postulated in may hold. While there exists for each experiment conducted in 2004 nutrient uptake and gas exchange data much of them remain to be analyzed. Work on the application of steady state nutrition to model driven control of hydroponics solution will continue using NCER as the main predictor and by linking the canopy photosynthesis models described above to ion uptake dynamics.