2004-01-2351

MELiSSA Higher Plants Compartment modeling using EcosimPro

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ABSTRACT

This paper introduces two modeling approaches in consideration for the MELiSSA Higher Plants Compartment. This includes an empirical light response curve modeling approach and the Modified Energy Cascade (MEC) model. The MEC model was translated into EcosimPro and evaluated for its performance under a range of environment conditions. The model demonstrated an adequate response to changes on the environmental conditions (temperature, CO_2 concentration and light flux) predicting the gas exchange (O_2 production, CO_2 consumptions, and water vapor transpiration)

INTRODUCTION

The use of regenerative Life Support Systems becomes inevitable when long-term manned space flights are considered. Bio-regenerative systems such as MELiSSA [1] are particularly attractive due to their capacity to provide the crew needs for life support following a closed loop approach. However, no possibility of closure can be foreseen without the connection of several processes and therefore, an overall strategy of control is needed. The implementation of a predictive control [2] strategy for the MELiSSA loop requires detailed knowledge of the dynamic models for the different compartments.

Regarding the Higher Plants Compartment, the top-level plant growth models currently available are, among others, Empirical Light Response [3] and the Modified Energy Cascade [4, 8]. Both models follow specific approaches and therefore their performance and compliance with MELiSSA requirements must be assessed. This paper presents a preliminary assessment for both alternatives.

The empirical light response model is based on the response of full canopies to variation in light intensity. Light is considered one of the important variables from a control perspective since it is an environment variable that may be easily changed to throttle plant photosynthesis. The knowledge and description of how crop canopies respond to light intensity at various stages of growth is the key to a successful predictive control strategy. Figure 1 shows a typical light response function for a single leaf, given by equation (1). This exponential model has been applied to single leaf data with great success [11] but data relating to its extension to full canopies is limited.

$$P_n = Pg_{\max} \cdot \left(1 - e^{-\frac{f \cdot F_l}{Pg_{\max}}}\right) + R_d \qquad (1)$$

where P_n is the net photosynthetic rate (μmol CO_2 m^{-2} s^{-1}) of the photosynthesizing leaf surface, Pg_{max} is the maximum gross photosynthetic rate (μmol CO_2 m^{-2} s^{-1}) at light saturation, f is the quantum yield (initial slope of the light response curve, (μmol CO_2 / μmol PAR), Rd is the dark respiration rate (μmol CO_2 m^{-2} s^{-1}) and $F_?$ is the PPF (μmol m^{-2} s^{-1} PAR).

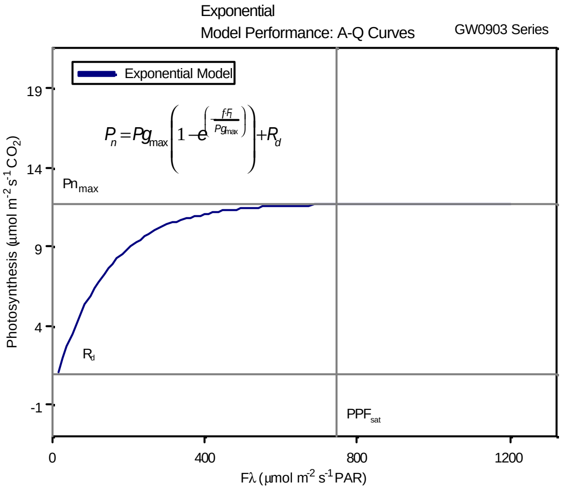

Figure 1. An empirically based, exponential light response model

A challenge in modeling the photosynthetic rate of full canopies is the quantification of the effective photosynthetic surface. In scaling up the exponential model from the leaf to the full canopy, or indeed in dealing with the growth of canopies, the following points may be considered.

- As the canopy biomass increases the total maintenance respiratory load increases and so too does Rd (becomes more negative)
- If canopy growth is to occur P_n must be positive
- In a growing canopy Pg_{max} must increase over time if Rd becomes more negative
- Due to mutual shading of leaves it becomes increasingly difficult to achieve light saturation in the canopy. This results in an increasing light saturation (PPF_{sat}) point.

With the growth of the canopy comes a change in at least two of its parameters – Rd and Pg_{max}. The exponential may account for this by allowing Pg_{max} and Rd to vary with time or another non-destructively measured variable such as integrated carbon gain. The empirical modeling approach is to generate surface responses for the canopy by generating light curves at various staged of development. In this way the behavior of the canopy to changes in light intensity may be assessed. A similar argument may be made for CO_2 response. The task is considerably easier if two additional points are considered. First, the operational range of light intensities may mean that light responses are within the 'linear' portion of the exponential function. This simplifies the structure of the empirical model to a planar surface when time or accumulated carbon gain is considered as an independent variable in the model along with light intensity. Secondly, if staged planting is used, the dynamic in Pg_{max} and Rd is restricted to a range that is much narrower than that for a batch planted canopy. This means that the light and CO_2 response profiles are relatively stable. Finally, the empirical modeling approach will allow for the determination of Apparent Quantum Yield (AQY) defined as the gross canopy photosynthetic rate per unit of incident photons within the PAR range. This avoids the need for estimating light absorption by the canopy using a second model.

The more mechanistic Modified Energy Cascade (MEC) model is also being investigated for its potential. The MEC calculates daily carbon gain (or the daily integral of the net canopy photosynthetic rate) as follows [4]:

$$DCG = 0.0036 \cdot H \cdot CUE_{24} \cdot APAR \cdot CQY \cdot PPF \quad (2)$$

where DCG is defined as the Daily Carbon Gain of the canopy (moles C m^{-2} day^{-1}), 0.0036 is a unit conversion factor, H is the photoperiod in hours, CUE_{24} is the Carbon Use Efficiency of the canopy over a 24 hour period (DCG/ daily gross photosynthesis) and as such includes night-time respiratory losses. The units of CUE_{24} are mole C $mole^{-1}$ C), APAR is the fraction of incident light absorbed by the canopy, CQY is the Canopy Quantum Yield (mole C $mole^{-1}$ PPF) and PPF is the Photosynthetic Photon Flux (µmol m^{-2} s^{-1} PAR). CUE_{24} is defined as the ratio of net photosynthesis to gross photosynthesis, which is assumed constant in the MEC model. CQY is defined as the gross photosynthesis per absorbed photon within the PAR range.

Values for CUE_{24} are assumed independent of CO_2 concentration, PPF and temperature. They are crop specific and are held constant throughout the crop growth period. Values of CQY_{max} were determined from crop photosynthesis data and involved the generation of multivariate polynomials to describe the dependency of CQY on light intensity, temperature and CO_2 concentration. The physiological basis for a description of CQY in terms of a multivariate polynomial of high degree is not understood. Given the dependencies of these parameters, the model allows for user defined light- and dark-cycle temperatures, irradiance, photoperiod, CO_2 concentration, planting density, and relative humidity.

The MEC model faces a similar challenge as the exponential model in describing the effective leaf surface for a developing canopy. The MEC model approach uses the Beer extinction law for light attenuation in dense canopies and an estimate of the increment in leaf area to estimate the time to canopy closure t_A (LAI = 1). The value of t_A is determined from input environmental conditions in the crop specific growth models. The fraction of absorbed PPF, APAR, is assumed to increase following Beer's law until canopy closure and retains the value A_{max} until harvest. Similarly, CQY is assumed to be at a maximum through the onset of senescence (t_Q) and then decreases linearly through to harvest, t_M.

A preliminary comparison of empirical and MEC approaches to crop modeling yielded the following results:

- The MEC model demands the development of crop specific growth sub-models that relate some of its key parameters to environment conditions using multivariate regression.
- The MEC model has a significant number of parameters to be estimated or defined

- The MEC model relies heavily on the light absorption co-efficient estimate since DCG is calculated in terms of absolute quantum yield rather than apparent quantum yield
- The MEC has a daily temporal resolution which may make control efforts difficult
- The empirical model conserves the typical light response functions used at the leaf level and makes allowance for dynamics in quantum yield, dark respiration and canopy light saturation points. In this way the kinetics of the canopy is described in the same way as that of a leaf but with different parameter values
- The empirical model does not require an estimate of the light absorption co-efficient (which is in turn based on the LAI of the stand) since the model is parameterized using the apparent quantum yield and non-destructive estimates of carbon gain. Non destructive estimates of LAI can not be achieved in cases when LAI > 1
- Insufficient data exist for the evaluation of this model at the present time

Given the immediate availability of the MEC models for the crops considered in this paper, an initial attempt at modeling the HPC using the MEC model was made with EcosimPro [5].

On the basis of the early-developed MELiSSA Library for EcosimPro [5], the authors have created a global Higher Plant Compartment component including different crop specific growth models. In addition, the component has been provided with the adequate ports allowing the connection with other components of the loop and consequently the integration of the model in the global simulator.

In the first part of the paper, the model is introduced and validated, while the second part tests its performance by the analysis of simulation results, covering steady state response and reactions to step changes.

MEC MODELS IN ECOSIMPRO

The first step taken for this work has been the implementation of the existing Cavazzoni models (Mathematica) into EcosimPro. Only six of the nine crops were selected (wheat, rice, soybean, lettuce, white potato and tomato) because they form part of the eight crops in the initial design of the MELiSSA Higher Plant Compartment (HPC).

In order to validate the translation, EcosimPro results have been compared against the Mathematica results presented by Cavazzoni. Figures 1-6 represent the relative differences between the results obtained by the two software tools, during a harvest cycle. The variables selected for the comparison were the biomass and the yield, and the relative difference was calculated following equation:

$$d_X = \frac{\left(X_{Mathematica} - X_{E\,cosim\,Pro}\right)}{X_{Mathematica}} \qquad (3)$$

The fact that the difference is always below the default relative tolerance of EcosimPro (10^{-6}) demonstrates that both models are eventually identical, independently of the mathematical solver and the software used.

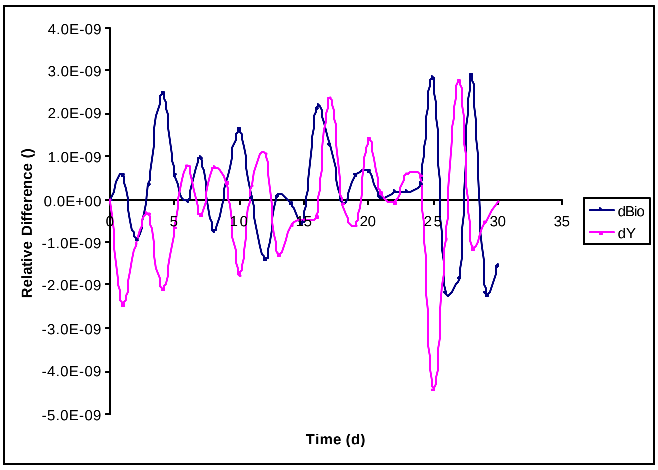

Figure 1: Lettuce Model Relative Differences

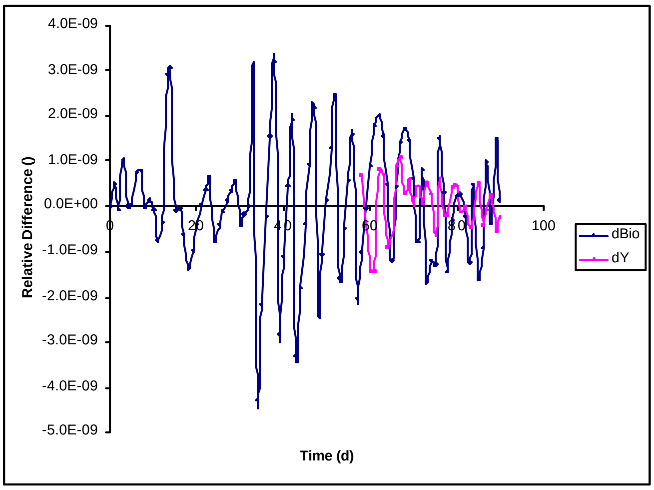

Figure 2: Rice Model Relative Differences

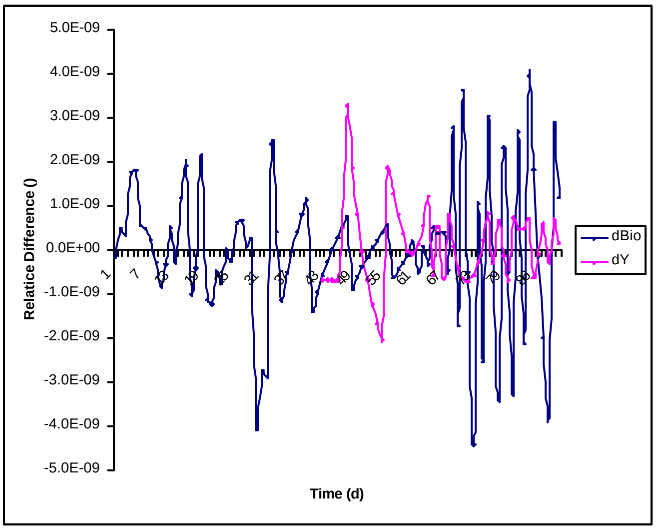

Figure 3: Tomato Model Relative Differences

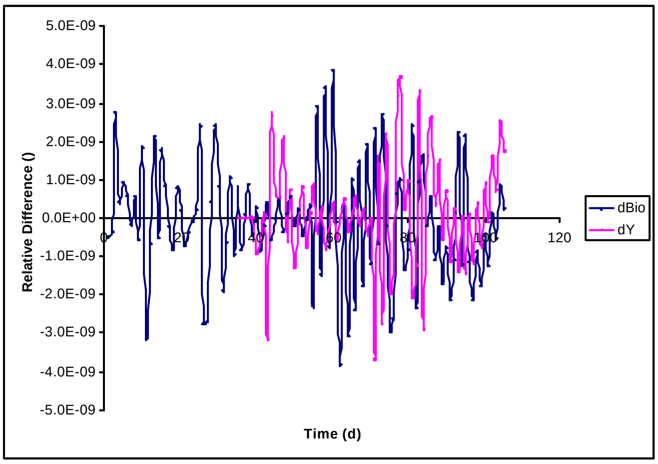

Figure 4: Potato Model Relative Differences

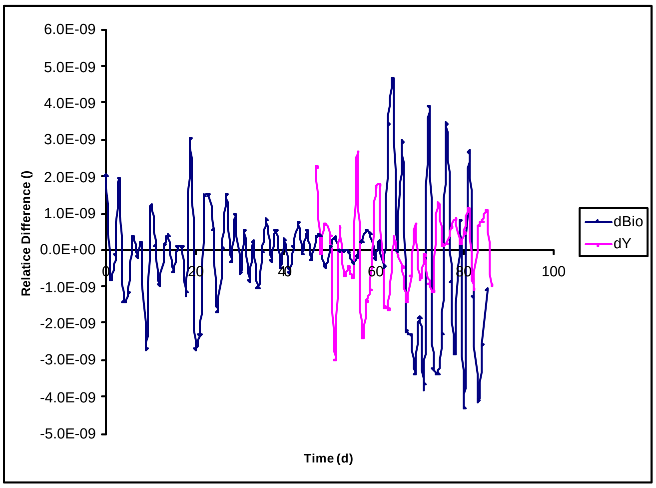

Figure 5: Soybean Model Relative Differences

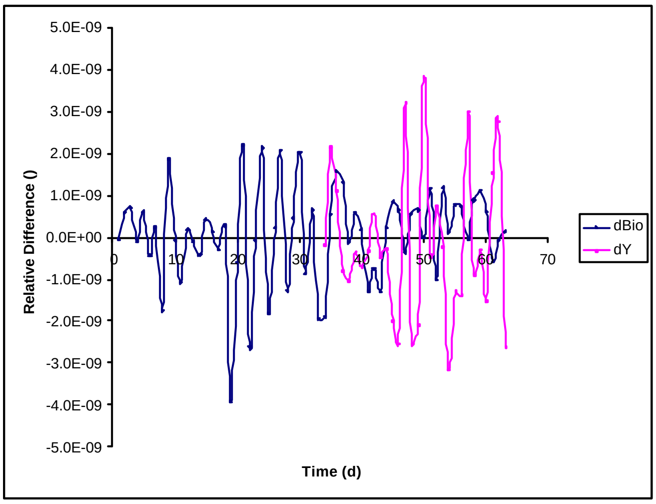

Figure 6: Wheat model Relative Differences

HPC MODEL

The Higher Plants Compartment model was implemented by following the steps listed below:

1. Enhance the individual crop models by introducing harvesting cycles as well as a staggered (staged) planting strategy.

2. Integrate the individual models into a global model including all the different crops.

3. Model the gas phase behavior by introducing momentum conservation law and mass balance equation for each compound (H_2O, N_2, O_2, CO_2) Energy mass balance has not been taken into account.

4. Add three PID control set-ups, in order to control CO_2 concentration, Relative Humidity, and total pressure.

5. Provide the code with the appropriate warnings and failure messages, in order to avoid the limits of application of the models (CO_2 concentration, light flux and temperature ranges)

The main parameters to define when running simulations on the global model are:

- Number of harvesting cycles per crop. A number of 5 stages per crop class is used by default

- Light flux (in PPF). Due to the fact that different minimum and maximum values of PPF apply to the different crop models, a duty variable was defined (0 = x = 1). x = 0 means all the light fluxes set to the minimum value, while x = 1 means all the light levels set at their maximum values. The minimum and maximum values are taken from Jones et al [8] and are listed in table 1. A default value of 0.75 has been established

- CO_2 set point (in ppm) The default value is 1200 ppm.
- Relative Humidity set point (by default, 70 %)
- Pressure set point (by default $P_{setpoint}$ = 101300 Pa)
- Photoperiod (h / d). Although the optimal value is not equal for all the crops, 12 h / d have been considered for all the crops.
- Temperature (in C). Due to difficulties for the pressure control, the same temperature has been considered during light at dark periods. 21 degrees has been used as default value.
- Harvesting dates (in hours). Six different values, one for each crop. Default values are taken from Jones et al [8] and can be read in table 2.
- Area fraction (one value for each crop). Default values are given by Poughon [6] and listed in table 1.
- Airflow through the chamber (l / h). By default it is set to 10 times the volume of the chamber per hour
- Growth area (by default, 5 m^2)
- Chamber height (by default, 1 m)

Crop	PPF_{min}	PPF_{max}	Harvest Date (h)	Area fraction[1]
Lettuce	200	500	720	0.050
Potato	200	1000	2880	0.221
Rice	200	2000	2112	0.280
Soybean	200	1000	2064	0.056
Tomato	200	1000	1920	0.012
Wheat	200	2000	1488	0.381

Table 1: Default values of parameters for different crops: maximum and minimum PPF (μmol / m^2 / s), harvest date, and area fraction

SIMULATION RESULTS

HPC SIZING

The HPC sizing may be attempted with three different objectives. The first objective is the provision of food for the crew in the context of MELiSSA. Another objective may be the recycling of the gas phase, and the third objective is the recovery of water by transpiration.

Solid Loop Closure

For this purpose, the sizing of the Higher Plants compartment was performed with the help of Microsoft Excel Solver ® routine. The exercise is similar to the one presented by Poughon in [6]. However, two main differences may be found: only six crops were taken into account in this case, because of the lack of models for onion and spinach, and the temperature was included as a variable for the optimization.

The dependence of yield production against temperature was calculated by running the HPC model at different temperatures and fitting the data by regression curves for temperatures between 20 and 26 degrees. This dependence is shown on figure 7.

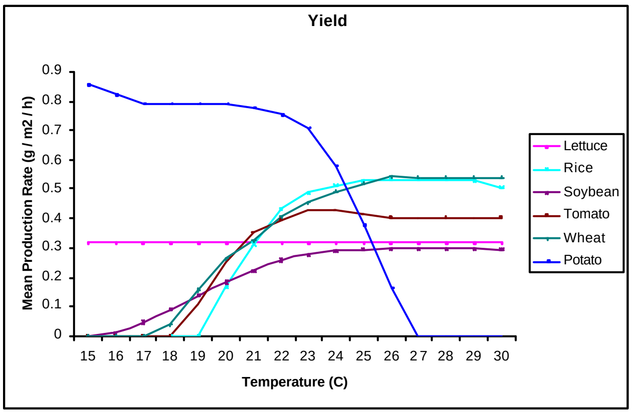

Figure 7: Yield production vs. T for different MELiSSA crops

The HPC was designed according to the following objectives:

- Minimize the crop area
- Allow biomass consumption in the diet, but limit the nucleic acids consumptions to less than 4 g / d.
- Fit into an energy consumption of 3000 kcal / d (15% proteins, 30% fats, 55% carbohydrates) []. Fats may be supplied from an external source.
- Different crops' fraction limited as proposed by Poughon [6]

In addition, the subsequent assumptions were made:

- Plants composition as reported in [6].
- Biomass production of 1440 g dw / m^2 / d []
- Biomass composition of Spirulina Platensis as reported by Poughon [6]

The results obtained are listed in tables 2 and 3. The optimal temperature for the HPC happened to be 23 C.

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[1] Reference [6] considers a diet based on eight different crops. As neither onion nor spinach models were available, the percentages were calculated eliminating onion and considering lettuce model valid as well for spinach

Percentage Diet	
Source	**Fraction (%)**
HPC	73.36
Biomass	15.00
External (fat)	11.64

Table 2: Percentage of the diet from different sources

Crop	Area (m^2)	Area percentage
Tomato	0.48	1.19
Rice	6.12	15.09
Lettuce	0.65	1.59
Potato	8.67	21.40
Soybean	2.39	5.89
Wheat	22.23	54.84
Spirulina	69.35 l	--

Table 3: Area of different Crops, Spirulina bioreactor volume.

A total area of 40.5 m2 / CM is on the range of values obtained before. The only explanation is that the productivity values calculated from the model are higher than those reported elsewhere.

Atmosphere Regeneration

A diet of 3000 kcal / d / CM has been considered. The daily oxygen consumption and CO_2 production of one crewmember can be calculated from the fraction of proteins, fats and carbohydrates as reported by [7].

The values resulting from this calculation are 0.902 kg O_2 / (d CM) and 1.018 kg CO_2 / (d CM) respectively.

Two different goals may be analyzed. One objective is to achieve the production of enough oxygen, using the rest of the CO2 for other purposes. The second one is the reduction of all the CO2 generated, using the extra O2 with a different objective. The biomass production processes taking part in other compartments have not been taken into account.

The optimal temperature for this case is 21 C, at which total biomass production reaches its maximum. The CO2 consumption and O2 production in this case are 66.6 g CO_2 / m^2 / d and 54.7 g / m^2 / d. Area needed is then:

Oxygen closure: 16.5 m^2

CO_2 closure: 15.3 m^2

Water Regeneration

Water usage by the crew may have different origins. It is common practice to consider a water need of around 4 l per crewmember per day for physiological reasons (water re-hydration for food and drinking water) [10]. The needs of water for hygiene purposes range from 0.5 l / (CM d) for short manned missions (only WC flush water) to 25 l / (CM d) for long duration missions as planetary bases (considering clothes and dish washing) [9]. The latter will be considered here, due to the fact that MELiSSA is intended for these sorts of missions. In this case, the optimal temperature is 23 degrees. At this temperature, the water production of the HPC is 3.0 l / (m2 d), which immediately implies an area of 9.84 m^2.

STEADY STATE

The HPC model performance has been analyzed by running a simulation for two years long period. The values for the different parameters for this simulation have been the ones obtained for the solid loop closure.

Figures 9 to 11 show the behavior of different variables during the simulation period. As it can be seen, after a transient period of about 3000 hours, a steady state is reached. The transient time frame corresponds to about the longest harvest time (potato). Here, steady state means that the HPC production rates of O_2 and water vapor, as well as the consumption rate of CO_2, oscillate around a mean value. The oscillations come from the harvesting / re-planting operations.

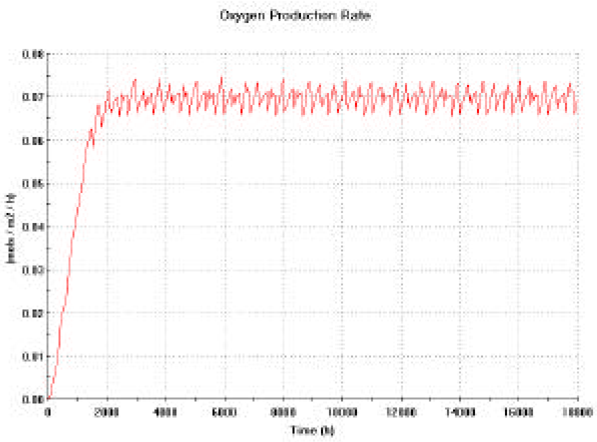

Figure 8: O_2 production rate

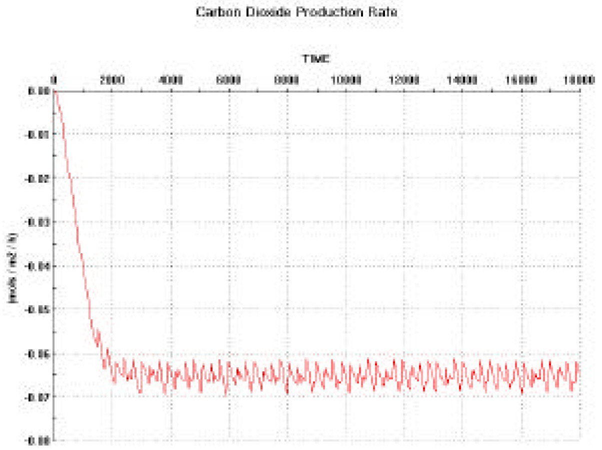

Figure 9: CO_2 production rate

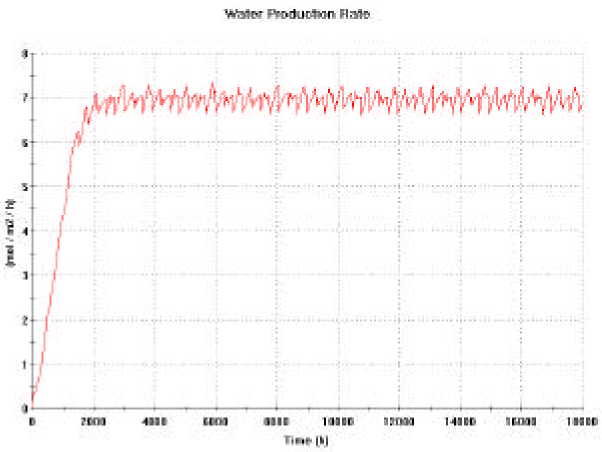

Figure 10: water vapor production rate

An additional exercise that can be performed is the Fourier analysis of the oscillations that appear in the CO2 consumption. One would expect to find peaks at the frequencies corresponding to the harvesting cycles (this is, harvesting dates divided by number of stages). Figure 11 shows the results of this analysis, and the different peaks corresponding to the different crops are marked.

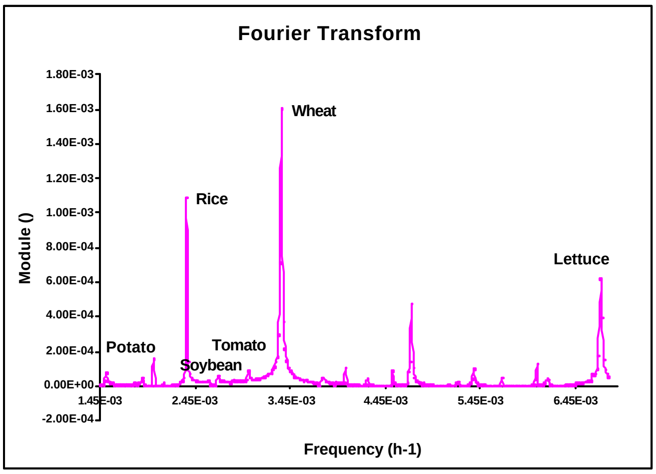

Figure 11: Fourier Transformed of the CO_2 production signal

For the analysis, the transient part of the simulation has been eliminated. Table 2 shows the periods calculated and expected, as well as the relative error, which is always below 0.5 %. The origin of the other peaks has not been investigated yet, but it is probably due to interferences.

Crop	Calculated Period (h)	Actual Period (h)	Relative Difference (%)
Lettuce	719	720	0.08
Wheat	1485	1488	0.19
Tomato	1923	1920	0.16
Potato	2069	2064	0.24
Rice	2113	2112	0.03
Soybean	3297	3312	0.46

Table 4: Signal periods (calculated, real)

RESPONSE TO STEP CHANGES

Step in CO_2 concentration set point

In this simulation, the HPC is started with a CO_2 concentration set point of 1200 ppm. Once the steady state is reached, the set point is sequentially changed to 500, 800, and back to 1200 ppm each 3000 h. Figure 9 shows the evolution of the carbon dioxide production rate during the simulation. The first 3000 hours are needed to achieve the steady state, in which constant mean value of the production rate is achieved. The oscillations are due to the harvesting of mature plants and re-planting of the new plants. At Time = 3000 hours, the first step is introduced. The growth rate of the plants consequently decreases. Following step changes on the CO_2 concentration set point increase the CO_2 consumption, at the end having the initial state.

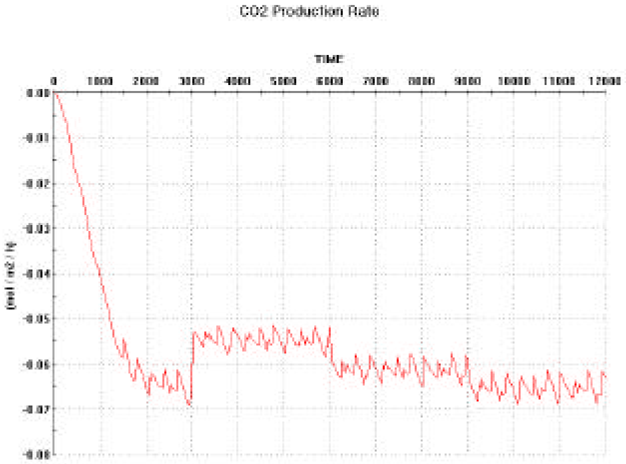

Figure 12: carbon dioxide production rate

Step in Light Flux

The following simulation case is similar to the one presented before, but this time the variable subject to step changes is the light flux. The simulation starts with the duty variable at 0.5 (this means, a mean value between the minimum and maximum flux) and when the steady state is reached, step changes to 0.75, 1.0 and finally to the initial value were simulated separated by intervals of 3000 h.

Figure 15 shows the behavior of the water transpiration rate during the simulation period. On a very similar way, the HPC achieves its steady state, having, as expected, different transpiration rates according to the different PPFs.

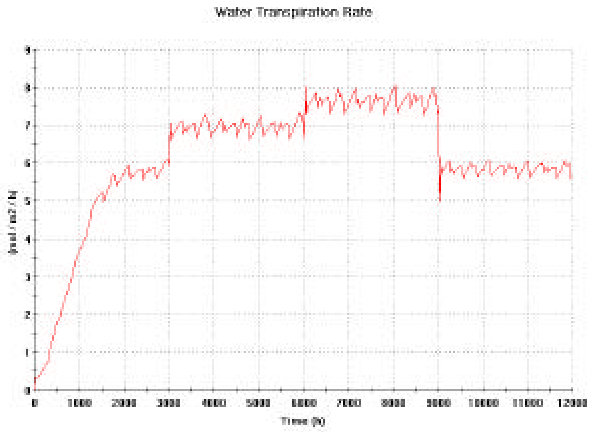

Figure 13: water transpiration rate

CONCLUSION

An easy to use model has been built under EcosimPro, whose main advantages are the ability to change most of the parameters (light flux, plants density, number of stages, and planted area of different crops) and the compatibility with existing models of the other MELiSSA compartments, allowing the simulation of the whole MELiSSA loop.

The model demonstrated an adequate response to changes on the environmental conditions (temperature, CO_2 concentration and light flux) predicting the gas exchange (O_2 production, CO_2 consumptions, and water vapor transpiration)

Further work will be focused on the development of empirical models and the comparison of both empirical and mechanistic approaches with experimental results in order to decide the final modeling strategy.

ACKNOWLEDGMENTS

The authors would like to thank the MELiSSA partners for the information given.

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ACRONYMS

CM:	Crewmember
HPC:	Higher Plants Compartment
MELiSSA:	Micro-ecological Life Support Alternative
LAI:	Leaf Area Index
PAR:	Photosynthetically Active Radiation
PPF:	Photosynthetic Photon Flux
PPF_{sat}:	Saturation Photosynthetic Photon Flux