PRELIMINARY STATIC AND DYNAMIC ANALYSIS OF MELISSA COMPONENTS USING ECOSIMPRO

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ABSTRACT

This paper documents the development of an EcosimPro Library to model a bio-regenerative Life Support System.

The objective of this Library is the validation of EcosimPro for this kind of simulations by a comparison between an existing MELiSSA model in Matlab / Simulink and the EcosimPro model.

In addition, three simulations are shown:

- Controlling a photo bioreactor
- Introducing pH analysis
- Closing the gas loop (steady state)

EcosimPro: Multi-disciplinary simulation tool developed by Empresarios Agrupados (Madrid, Spain) under ESA contract.

MELiSSA: Micro Ecological Life Support Alternative. It is a microorganism and higher plants based ecosystem intended as a tool to gain understanding of the behaviour of artificial ecosystems, and for the development of the technology for a future biological life support system for long term manned space missions [1,2].

LSS: Life Support Systems. In this context it encompasses the systems, which are necessary to ensure atmosphere revitalisation, waste management, water management and food management in a sustainable fashion for a crew in a closed and controlled habitat.

1   BACKGROUND

The Melissa project started in 1989. The following is a short description of the complete Melissa Loop.
The loop is conceived as five interconnected compartments, following the schema of figure 1. In a first stage the waste (faeces, urea and non-edible parts of plants), is treated by anaerobic bacteria (Compartment I) in order to reduce it to organic molecules of lower molecular weight. These molecules (mainly fatty acids) will be degraded to CO_2 by Rhodobacter (Compartment II). The ammonia appearing as a result of the degradation in Compartment I needs to be oxidised to nitrate, in order to be used by Higher Plants and photoautotrophic bacteria. This oxidation takes place in the Nitrifying Compartment (Compartment III). The photosynthesis occurs in Compartment IV, which is fed by the CO_2 coming from different compartments. Compartment V represents the crew, which consume O_2, H_2O and food, producing CO_2, wastewater, as well as urea and faeces, which feed the first compartment, closing the loop.
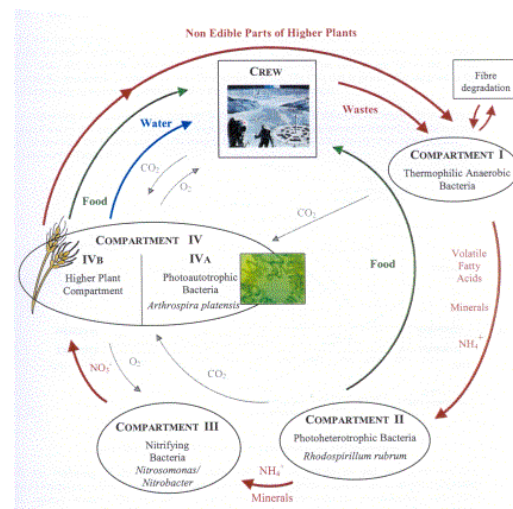

Figure 1. MELiSSA Loop

For more information, see [2].

2   MODELLING BIOREACTORS

The MELiSSA library makes use of a unique hydraulic port.

The port is able to take into account two different kind of compounds: monophasic compounds, being dissolved in the liquid phase of the stream; and biphasic compounds, which exist in both liquid and gas phases.

The phenomena considered when dealing with the biphasic compounds are: gas - liquid equilibriums, acid - base equilibriums and the reactions block, while monophasic compounds dynamics depends only on the reactions block[1].

The most important limitations of the model are:

- Constant pH. This assumption is justified because reactors are usually controlled to maintain a constant pH, to allow for optimal growing conditions of the bacteria, as well as to positively influence the gas/liquid equilibrium.
- Constant Temperature. No thermal considerations are taken into account in these models because reactors are maintained at constant temperature in order to optimise conditions for bacteria growth.
- No variations on the main compound of the liquid and gas phases (water and inert gas). The concentration is usually so big, that the variation can be neglected. When performing a mass balance analysis, water dissociation has been taken into account.

2.1   GAS-LIQUID EQUILIBRIUM

The equilibriums are modelled for compounds that are present in both liquid and gas phases [3].

The flow from liquid to gas phase (ϕ_i) can be calculated from equation (1).

$$\Phi_i = KlA_i \cdot \left(\frac{a_i \cdot n_0 \cdot V_M(T)}{KpartN_i(T)} - b_i^{pure} \right) \quad (1)$$

Where:
- *KlA* is the transfer coefficients, depending mainly on the working conditions of the reactor.
- *KpartN* is the partition coefficient, obtained by an Antoine law for the vapour pressure (2), which coefficients are determined from experiments and are valid for a determined range of temperatures.

$$Ln(KpartN) = A - \frac{B}{C+T} \quad (2)$$

- n_0 is the number of moles in a litre of water.
- V_M is the molar volume of a perfect gas.
- *a* is the concentration on gas phase and b^{pure} is the concentration of pure molecular forms on the liquid phase, which is calculated from the acid – base equilibrium.

2.2   ACID – BASE EQUILIBRIUM

This equilibrium is considered instantaneous, and it is described by means of a dissociation constant k_i, depending on the conditions of pH and temperature, and the character of the compound [3].

The global concentration on liquid phase (b_i) has to be split into the concentration of ionic forms and the concentration of pure forms of the compounds. This is:

$$b_i^{pure} = \frac{b_i}{1 + k_i(pH,T)} \quad (3)$$

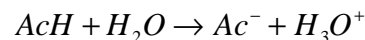$$b_i^{ionic} = \frac{k_i \cdot b_i}{1 + k_i(pH,T)} \quad (4)$$

For basic compounds (such as ammonia), the equilibrium reaction takes the form:

$$BaseOH + H^+ \rightarrow Base^+ + H_2O$$
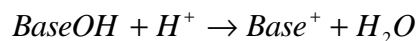
So the equilibrium constant becomes:

$$k_i = \frac{k(T)}{k_w(T)} 10^{-pH} \quad (5)$$

For acid compounds (such as fatty acids),
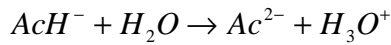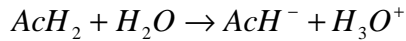
$$AcH + H_2O \rightarrow Ac^- + H_3O^+$$

So the equilibrium constant:

$$k_i = \frac{k(T)}{10^{-pH}} \quad (6)$$

There are some compounds, like carbon dioxide, that can accept either one or two

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[1] The acid – base quilibrium for monophasic compounds with a strong acid-base character should be taken into account for the pH variations but, as it will be mentioned below, the reactors are considered to be pH controlled, mainly because the bacteria are only active in very restricted conditions of pH.

protons. For this compounds (bi-acids), the equilibrium is double:

$$AcH_2 + H_2O \rightarrow AcH^- + H_3O^+$$

$$AcH^- + H_2O \rightarrow Ac^{2-} + H_3O^+$$

The equilibrium constant taking the form:

$$k_i = \frac{k_1(T)}{10^{-pH}} \cdot \left(1 + \frac{k_2(T)}{10^{-pH}}\right) \qquad (7)$$

All the temperature dependant expressions follow an Antoine law:

$$Lnk = \frac{A}{T} + B \cdot LnT + C \cdot T + D \qquad (8)$$

2.3   REACTIONS BLOCK

The reactions block consists on the calculation of the creation rates of different compounds from the biomass creation rate. The relationship is based upon the stoechiometric and rate coefficients of the biomass synthesis reaction and the biomass composition [3]. In addition, the biomass growth rate depends on the light flux in PBRs, and concentration of limiting substrates.

2.4   GLOBAL DYNAMICS

All reactors are operated as continuous bioreactors. Thus, for the biphasic compounds, two dynamic equations can be established:

- For the gas phase:

$$V_G \cdot \frac{da_i}{dt} = G_{in} \cdot a_i^{in} - G_{out} \cdot a_i + V_L \cdot \boldsymbol{f}_i \quad (9)$$

- For the liquid phase:

$$V_L \cdot \frac{db_i}{dt} = F_{in} \cdot b_i^{in} - F_{out} \cdot b_i - V_L \cdot \boldsymbol{f}_i + r_i \quad (10)$$

For monophasic compounds, only one equation is needed:

$$V_L \cdot \frac{db_i}{dt} = F_{in} \cdot b_i^{in} - F_{out} \cdot b_i + r_i \qquad (11)$$

The temperatures and pH used in equations (2) to (8) are fixed at the respective reactor values.

3   SIMULATIONS

3.1   CONTROL EXAMPLE

The following simulation refers to the photoautotrophic compartment. The function of this compartment is the transformation of CO_2 to O_2, by means of photosynthesis and to produce food for the crew. It is meant to work in parallel with the Higher Plants Compartment, to enforce the O_2 production as well as to increase overall reliability of compartment IV.

This example shows how to obtain the desired O_2 production rate, which is directly related to the production rate of biomass [4]. The biomass production rate mainly depends on the light flux and the active biomass concentration, so these two inputs are needed for the controller.

Thus, the controller needs two inputs from the reactor, the concentration of biomass and the liquid flow (the later is needed because the reactor is working as continuous culture reactor), while it can only tune the light flux. The control system employs a predictive control strategy [5,6]. It makes use of a moderate complex algorithm to predict the results a few time steps ahead. The control algorithm was developed by ADERSA[2] in C code, and imported into EcosimPro by means of an external function. The schematic is shown on figure 2.
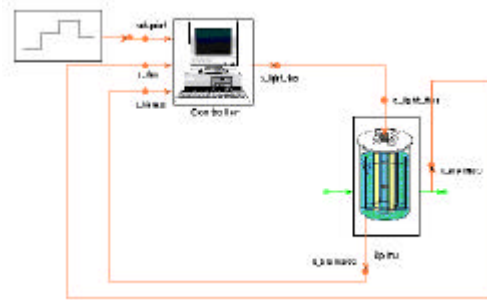

Figure 2. Control Schematic

As the light flux is constricted by an upper and lower limit, certain biomass concentration on the reactor has to be achieved in a first step to ensure that the set point can be obtained within the limits. In a second step, keeping this concentration constant, the control modifies the light flux until it attains the correct value for the biomass production rate.

Biomass production rate, active biomass concentration and the light flux are shown in figures 3, 4 and 5 respectively.
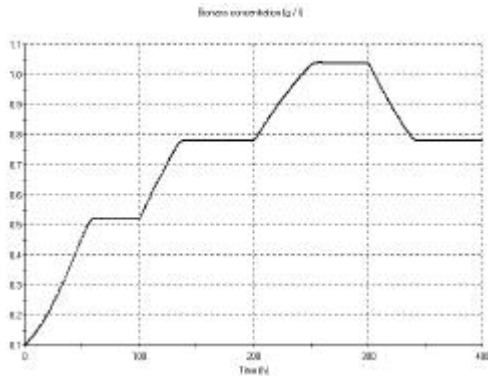

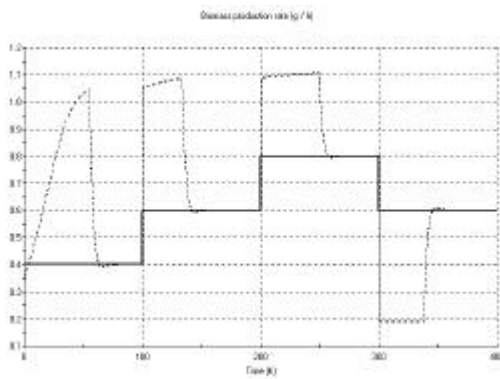Figure 3. Biomass Production Rate

Figure 4. Active Biomass Concentration (dotted: real production rate, straight: production rate set points)
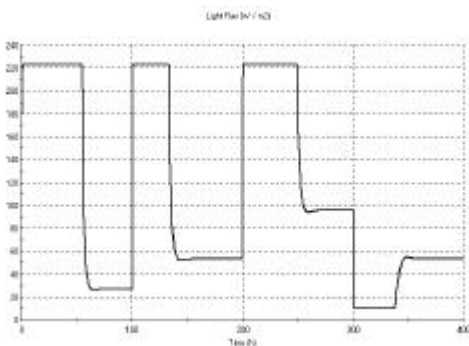

Figure 5. Light Flux

As the previous figures indicate, EcosimPro is able to correctly simulate the behaviour of a photo-bioreactor with a predictive control strategy.

3.2 pH ANALYSIS

Although photo-bioreactors work at a constant pH value, the case of pH evolution must be simulated as well to prepare for possible non-nominal operational states.

A detailed pH analysis can be added to the model by introducing a detailed description of all the acid - base equilibriums, as well as the definition of the OH^- and H^+ concentrations on the liquid phase, and their creation rates on the reactions block. In addition, water has to be considered as well, and consider an algebraic variable defining the rate of the dissociation reaction:

$$H_2O \xrightarrow{\ rH_2O\ } OH^- + H^+$$
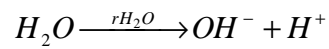
This algebraic variable is used to break the High Index problem that arrives because of the well-known constriction.

$$[OH^-] \cdot [H^+] = k_w \qquad (12)$$

The goal of this simulation is to enable a comparison between the predicted results of the model with real testing in the lab. This will lead to the evaluation of the differences on the bacteria behaviour when pH increases. The experiment will be conducted in a badge culture (no circulating liquid flow) with no control in the pH. Results are shown on figures 6 and 7.
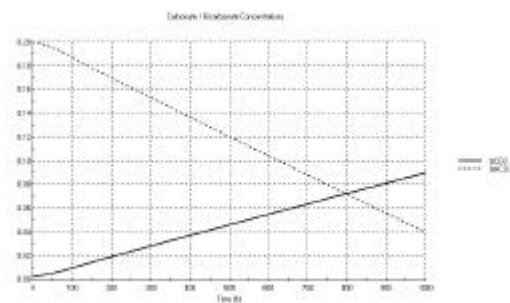

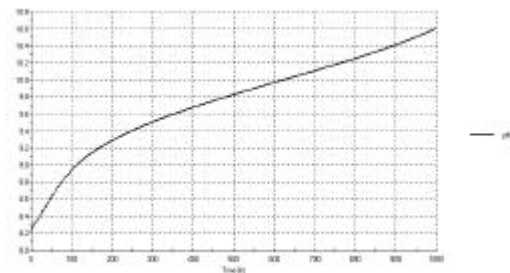Figure 6. Carbonate – Bicarbonate concentration

Figure 7. pH Evolution.

As the experiment has not been carried out yet, no conclusion about the simulation quality can be made. However, the results obtained are roughly the theoretically expected.

3.3 CLOSED LOOP

Main features of the loop model are:

- Liquid stream is continuous within the compartments I, II, III and IV (not the consumer)
- Gas stream is sub-divided. The lower part (Compartments I and II) has to be considered separately because the processes taking part on these compartments are anaerobic.

Figure 8 represents the whole loop, where one finds the following inputs and outputs:

Inputs
- Faeces and Urea to the compartment I.
- Minerals to the compartment. I

Outputs
- Biomass from the compartments II, III, and IV.
- Minerals at the output of the Compartment IV
- Non-degraded fatty acids at the output of Compartment II.

In the simulation, minerals had to be removed from compartment IV and added into compartment I because they were not entirely consumed by the microbes in compartments II, III and IV.
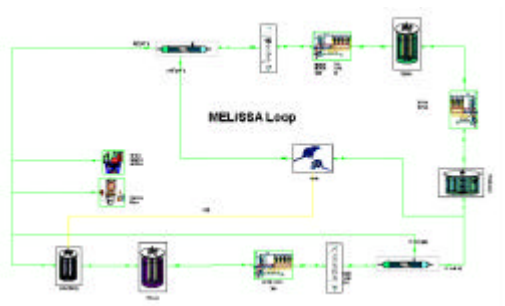

Figure 8. MELiSSA Loop

Subsequent parameters can be modified in the simulation:

- The rate of human daily wastes introduced in the Liquefying compartment.
- The number of rats in the consumer compartment.

- The light fluxes on Compartments II and IV.

In order to reach a proper steady state solution, we can modify these parameters, taking into account the limits on the light fluxes, and the following requirements:

- The predicted degradation of fatty acids has to be better than or equal to 99.5 %.
- The concentrations of CO_2 and O_2 at the consumer compartment have to be (molar fraction):
  O_2: 21 %
  CO_2: 0.3%

Results have been obtained with a required relative tolerance (REL_ERROR_NL) of 10^{-5}, and are shown in table 1, where:

b: Concentration in liquid phase
a: Concentration in gaseous phase
r: Production rate (consumption if negative)
FR: Light Flux
deg[Ac]: Rate of degradation of fatty acids
err: Relative error on the mass balance
XA: Active biomass

Table 1. Closed Loop Steady State Results

Compartment	Variable	Value	Units
I	r[O2]	0.0	mol / h
II	r[O2]	0.0	mol / h
III	r[O2]	- 0.0145	mol / h
IV	r[O2]	0.0835	mol / h
V	r[O2]	- 0.0688	mol / h
I	r[CO2]	0.0054	mol / h
II	r[CO2]	0.0002	mol / h
III	r[CO2]	- 0.0145	mol / h
IV	r[CO2]	- 0.0638	mol / h
V	r[CO2]	0.06	mol / h
II	b[XA]	0.083	g / l
III	b[XA]	0.011	g / l
IV	b[XA]	1.37	g / l
II	r[XA]	0.064	g / h
IV	r[XA]	1.583	g / h
II	FR	202.0	W / m^2
IV	FR	2.8	W / m^2
II	deg[Ac]	99.62	%
V	a[O2]	0.21	mol/mol
V	a[CO2]	0.003	mol/mol
All	err[C]	4.6 10^{-14}	--
All	err[H]	1.1 10^{-5}	--
All	err[O]	1.6 10^{-5}	--
All	err[N]	4.8 10^{-7}	--
All	err[P]	4.1 10^{-8}	--
All	err[S]	1.6 10^{-5}	--

The results in table 1 show that both requirements (gas composition in compartment V and acetic acid degradation rate in compartment II) are met.

4 MATLAB vs. ECOSIMPRO

In order to validate the library and its results, a comparison between two identical models in Matlab / Simulink and EcosimPro have been performed. The Matlab / Simulink model has been successfully used by the MELiSSA partners for years and a great confidence in correctness of the models has been established. The comparison has been done with an open loop simulation including compartments II, III and IV. Figures 9 and 10 show Simulink and EcosimPro model respectively.
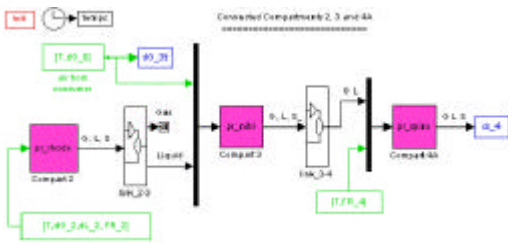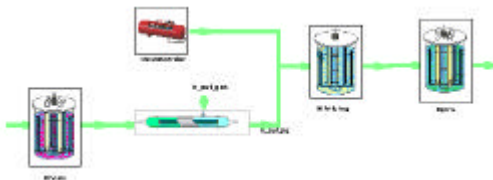

Figure 9. Simulink Model

Figure 10. EcosimPro Model

The simulation investigates the transient behaviour between two steady states. The transient is caused by a light flux step in the compartment II. The comparison examines the differences between numerical results obtained with EcosimPro and Matlab / Simulink, as well as the CPU time.

4.1 NUMERICAL RESULTS

Figure 10 shows the relative differences on the concentrations of different compounds between Matlab / Simulink and EcosimPro solution, calculated throughout all the simulation.
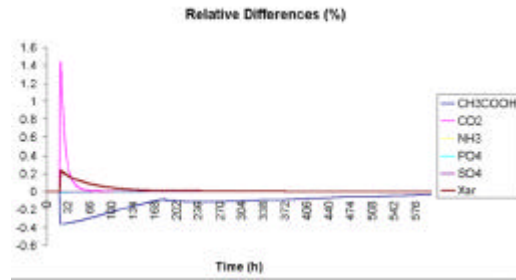

Figure 11. Relative differences in Compartment II

Although the differences are not significant (the maximum difference is 1.5 %) the importance relies on the fact that they increase when any discontinuity takes place. This can be noted in figure 11, where the two discontinuities on the simulation (the light flux step at t = 20 h, and a different one, due to compartment II, at t   180 h) can be perfectly allocated by the peaks on the relative difference between the two solutions.

The explanation of these differences is not a discrepancy in the model because the initial state and the model dynamics are exactly the same. In order to detect which simulation obtained better results, a mass balance check has been completed. The mass balance check was based on verifying the number of atoms of different classes (C, H, O, N, S, P) entering the reactor is the same as the number of atoms leaving it, plus possibly an instantaneous increase inside the tank.

This is, checking that the following quantity:

$$Dif_i = \sum_{j \in biphasic} h_{in} . Ga_j \cdot St_i^j + \sum_{j \in all} h_{in} . Lb_j \cdot St_i^j -$$
$$- \sum_{j \in all} h_{out} . Lb_j \cdot St_i^j - \sum_{j \in biphasic} h_{out} . Ga_j \cdot St_i^j - \tag{13}$$
$$- V_L \cdot \sum_{j \in all} b_j^` \cdot St_i^j - V_G \cdot \sum_{j \in biphasic} a_j^` \cdot St_i^j$$

is zero during the simulation, where "i" represents the different atomic species (C, H, O, N, S, P).

This calculation makes sense if and only if the stoechiometric coefficients of the reactions are consistent for both simulations. As the stoechiometry for carbon is well defined for all reactions, it has been selected for the mass balance check. The results for EcosimPro and Matlab / Simulink simulations are plotted in figures 12 to 17.
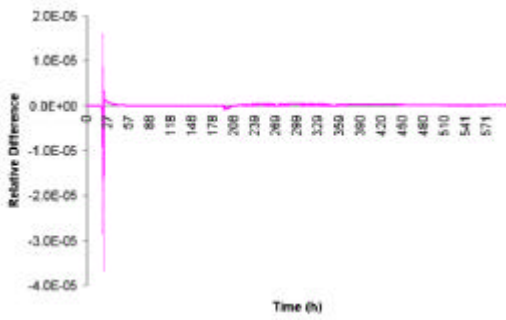
Figure 12. Carbon mass balance in Compartment II (Matlab / Simulink)
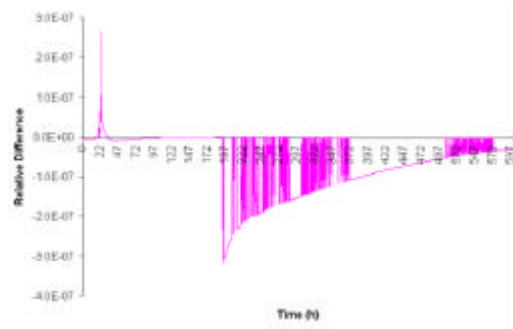

Figure 13. Carbon mass balance in Compartment II (EcosimPro)

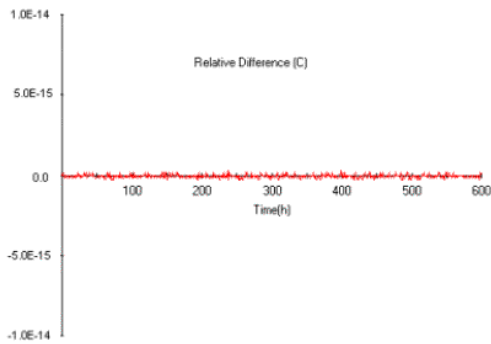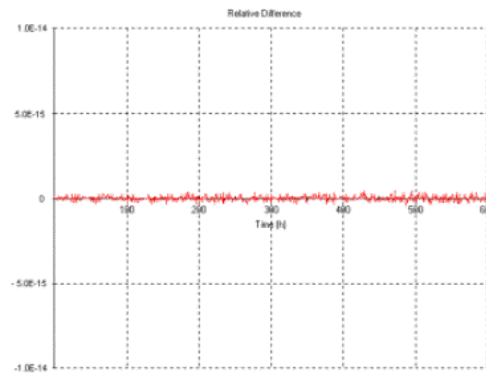Figure 14. Carbon mass balance in Compartment III (Matlab / Simulink)

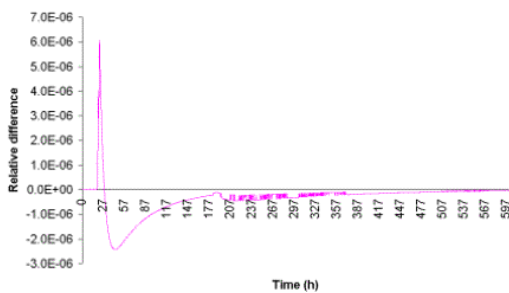Figure 15. Carbon mass balance in Compartment III (EcosimPro)

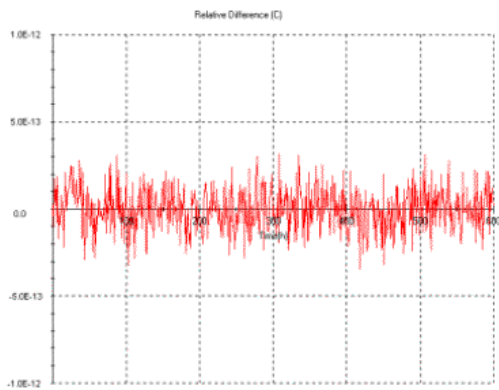Figure 16. Carbon mass balance in Compartment IV (Matlab / Simulink)

Figure 17. Carbon mass balance in compartment IV (EcosimPro)

As it can be seen, the carbon mass balance is imbalanced in Matlab / Simulink model at both discontinuities, while EcosimPro does not exhibit sensitive behaviour at the step changes.

4.2   CPU PERFORMANCE

A comparison dealing with the performance of both simulations in terms of CPU time has been made. The processor used was a Pentium III at 1.0 GHz.

Table 2 shows the CPU time for both simulations for different relative tolerances:

Table 2. CPU Time

Relative Tolerance	Matlab CPU Time (s)	EcosimPro CPU Time (s)
10^{-4}	9.72	0.77
10^{-5}	9.89	0.89
10^{-6}	10.27	1.09
10^{-7}	10.33	1.42
10^{-8}	12.69	1.64
10^{-9}	14.56	1.98
10^{-10}	205.42	2.47

As the results indicate, EcosimPro needs less CPU time than Matlab / Simulink to execute the simulations.

5   CONCLUSIONS

The investigations suggest that EcosimPro is suitable for modelling biochemical processes. The investigations included the implementation of a predictive control strategies developed in external code, and a steady state evaluation of the closed loop.

Furthermore, EcosimPro's numerical performance was compared to Matlab / Simulink's performance. The results indicate that EcosimPro handles discrete events in a more satisfying approach than Matlab / Simulink. In addition, EcosimPro's integrator (DDASSL sparse) seemed to perform more efficiently than Matlab's (ode15s).

However, the comparison between Matlab / Simulink and EcosimPro is in an initial state. No final conclusion can be made on which software package is more suitable to simulate bio-regenerative life support systems.

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