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MELiSSA

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TECHNICAL NOTE 39.1

Towards a dynamic model of the MELiSSA loop

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CONTENT

T.N. 39.1: Towards a dynamic model of the MELiSSA loop

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Introduction

Before simulating the dynamic behaviour of the whole MELiSSA loop, two points must be clarified:

- the state of the art of the dynamic models of all elements of the loop
- the flow design of the loop

For the first point, all the current models developed in the frame of the MELiSSA project will be reviewed. Biological, physical and hydrodynamics characteristics of each compartment will be presented. This will give a complete overview of the system and show the main weak points that must be studied and solved in the future. An homogeneous structure is chosen for the expression of the model of each compartment..

The loop design is an important point to define for the dynamic simulation. Special attention must be paid to the description of the flow rates and of the compartments dimensions. A way for the calculation of characteristic time constants in the loop are also proposed.

I Dynamic mass balance equations describing the MELiSSA compartments

The mass balance model (stoichiometric equations) of each compartment of MELiSSA was used to perform mass balanced simulations of the complete loop (TN 32.3), which are representatives of a steady-state situation. In order to perform simulations of the loop in dynamic conditions, this mass balance model must be completed by the addition of accumulation terms and the modelling of the hydrodynamics of the compartments and of the links between the compartments.

An approach for the modelling of biological processes has been presented for the modelling of the nitrifying column. It is based on the mechanistical description of the process as proposed by Noorman (1991) and can be subdivided into 4 steps:

1- mass balance description (stoichiometric equations) of the process
2- kinetics laws
3- hydrodynamic laws and description of the process
4- economic aspect

The first step was already studied, even if some improvement would be made on the liquefying compartment, accordingly to future experimental results.
Kinetics models were developed for the Spirulina and *Rs. Rubrum* growth in a photobioreactor by Cornet (TN19.1; TN 19.2 and TN 23.4) and for *Ns. europaea* and *Nb. winogradskyi* (TN 27.1). The basis of a biological kinetic model for the liquefying compartment was proposed in TN 39.3.
The biological processes of the MELiSSA loop (compartments I to IV) are continuous processes. An overview of the modelling of the hydrodynamics of the biological and chemical processes was given in TN 27.1. It described the two ideal behaviours: the perfectly stirred tank reactor and the plug-flow reactor. The dynamics of the crew compartment, and of the higher plant compartment that could be associated to the four biological compartments of MELiSSA, are sequential, depending on the activity of the crew (working periods, eating...) or on the growth phases for the plants (seeding, harvesting, day/night periods).

The purpose of this chapter is to present the basis of the dynamical model for each compartment of the MELiSSA loop. Most of these models have been already developed or previously proposed. Some of them (compartment IV and compartment II) are included in the first global simulator for the loop control developed by ADERSA (TN 28.3; TN 35.1).

For simplicity, all compartments will be described in an homogeneous form:

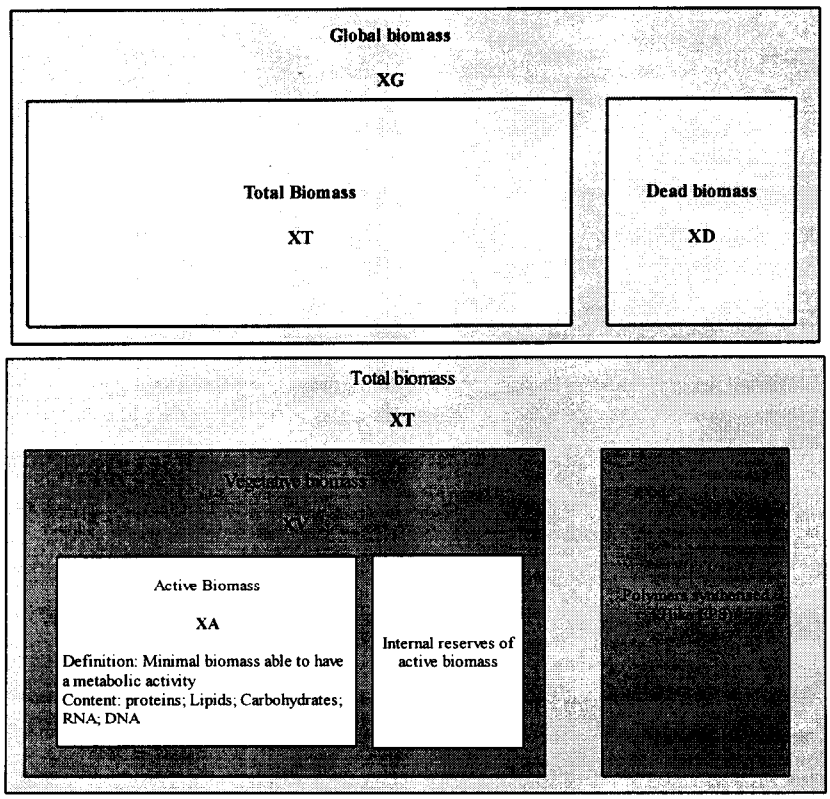
- the mass balanced description of reactions (i.e. the stoichiometric equations) which is already used in ProSim simulations of MELiSSA
- the biological models, giving the growth rate, the consumption/production rate laws for the organisms
- the dynamic of the reactor (behaviour and hydrodynamic)

All models established for dynamic simulations of the compartments will be reviewed with the parameters values obtained and validated or those assumed.

I.1 Notations

I.1.1 Description of the biomass

As biomass is a complex compound, the definition of a standard notation, able to represent all aspects of its variable composition was required. The notation for biomass is mainly taken from the representation of Cornet (TN 19.2).



As at the present time in all models, the presence of intracellular reserve is included in the biomass description used in biosynthesis stoichiometric equations, no differences are made between XA and XV (XA=XV). In models, the biomass is often called X, as XA=XV=XT=X.

For the nitrifying process where the biomass exists in a fixed and in a free form, differences can be made by calling X-F the fixed biomass and X-L the biomass free in the liquid phase.

The biomass decay can be important for some processes and can then be sometime taken into account. The dead biomass (called XD) has the same chemical composition of the vegetative biomass but is not active. The dead biomass can be lysed and then the metabolites released can be used as substrates.

I.1.2 Common nomenclature

A common nomenclature was chosen for the description of the different models. But some of them involved specific parameters which are not listed here.

$C_{Si}^{n}\big|_{P}$: Concentration of compound Si in the phase P (liquid=L; gas=G; biofilm/solid=B) of reactor n ($mol.L^{-1}$).

Simplified expression: $C_{Si}^{n} = C_{Si}^{n}\big|_{L}$

$C_{Si}^{*n}\big|_{L}$: Saturation concentration of a gaseous compound Si in the liquid phase in reactor n ($mol.L^{-1}$)

F: Liquid flow rate ($L.h^{-1}$)

F_r: Recycled liquid flow rate ($L.h^{-1}$)

G: Gas flow rate ($L.h^{-1}$)

G_r: Recycled gas flow rate ($L.h^{-1}$)

I_{si}: Inhibition constant of compound Si ($mol.L^{-1}$)

KS_{Si} : Affinity constant for compound Si ($mol.L^{-1}$)

KA_{Si}: Acid-base equilibrium constant of compound Si

K_La: Gas-Liquid volumetric transfer coefficient (h^{-1}) . It is in fact specific of one compound.

k_{Si}: Partition coefficient of a compound Si between the gas and the liquid phases

k_D: decay rate (h^{-1})

r_X^n : Growth rate in reactor n ($g.L^{-1}.h^{-1}$).

V_L: Liquid volume (L)

V_G: Gas volume (L)

y_{Si}^{n} : Gas fraction of compound Si in the reactor n

$Y_{X/Si}$: Biomass yield for compound Si (g biomass.mol^{-1})

$\phi_{Si}^{n}\big|_{LB}$: Transfer rate between the liquid phase and the biofilm or the biomass for the compound Si in the reactor n. ($mol.L.h^{-1}$)

$\phi_{Si}^{n}\big|_{GL}$: Transfer rate between the gas phase and the liquid phase for the compound Si in the reactor n ($mol.L.h^{-1}$)

$\phi_{Si}^{n}\big|_{REAC}$: reactionnal term relative to compound Si in reactor n ($mol.L.h^{-1}$)

μ^n : Specific growth rate in reactor n (h^{-1})

μ_{max} : Maximum specific growth rate (h^{-1})

I.2 Compartment I - Liquefying

Description of the process

An overview of the degradation steps performed by the liquefying compartment, as well as a review of the past experiments led on this compartment was presented in TN39.3. These first studies concerned only the batch process. Stoichiometric equations were proposed for the representation of the multi-step process of anaerobic degradation in TN 39.3. In this first approach, the mass balanced model was chosen flexible enough to be adaptable to the process results.

Mass balanced model

The principle of the model is summarized in figure 1. The stoichiometric coefficients of the related equations were established in TN 39.3. If the number and the coefficients of the equations could be changed with the future studies of the compartment, the approach of the problem will probably stay unchanged.

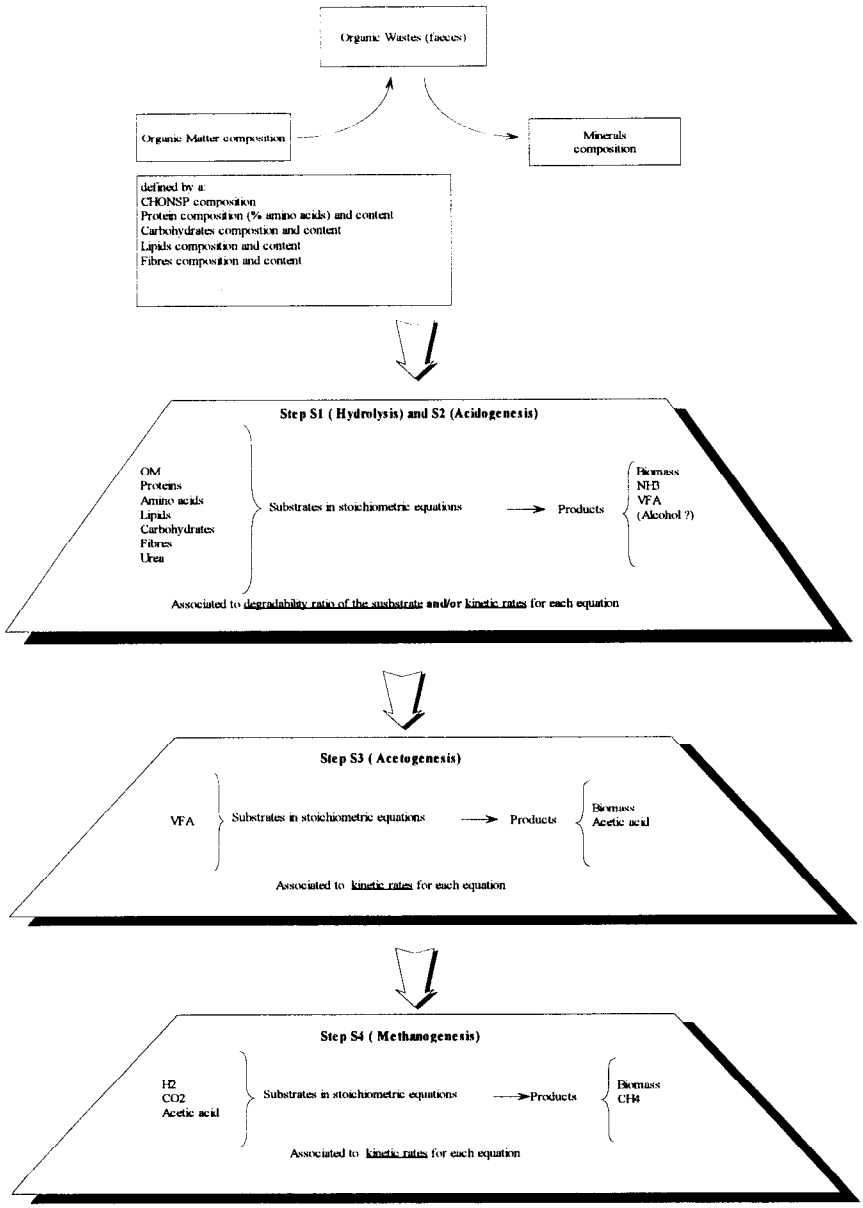


Figure 1: Principle of the representation for the anaerobic biodegradation in compartment I.

As it was noted in TN 39.3, the most delicate points in this approach are:

- the description of steps S1 and S2
- the determination of the yield between anabolism (biomass synthesis) and catabolism (substrate degradation). For this point, some results are available in the literature, and some stoichiometric equations can be found for steps S3 and S4.

The current stoichiometric equations established in TN 39.3 are reported in table 1. It must be kept in mind that they are subject to more or less important changes.

	Step 1: hydrolysis of organic matter	
1-1	$Urea + H_2O \longrightarrow CO_2 + 2\,NH_3$	% degradation
1-2	$[CHONS]_{proteins} + H_2O \longrightarrow [CHONP]_{poolAA}$	% degradation
1-3	$[CHONS]_{carbohydrates} + H_2O \longrightarrow [CHONP]_{oses}$	% degradation
1-4	$[CHONS]_{fibres} + H_2O \longrightarrow [CHONP]$	% degradation

	Step 2: acidogenesis (assimilation)	
2-1	$[CHONS]_{poolAA} + 0.4729\,H_2O \Downarrow$ $0.01\,[CHONSP]_{Bio\_1} + 0.12704\,CH_3COOH + 0.012535\,C_2H_5COOH + 0.01515\,C_3H_7COOH + 0.00757\,C_3H_7COOH_{[isobutyrate]} + 0.01254\,C_4H_9COOH + 0.017729\,C_4H_9COOH_{[isovalerate]} + 0.01773\,C_5H_{11}COOH + 0.00989\,C_5H_{11}COOH_{[isocaproate]} + 0.25275\,CO_2 + 0.34064\,H_2 + 0.16936NH_3 + 0.00635\,H_2SO_4$	Kinetic law
2-2	$1.0833\,[CHO]_{oses} + 0.1\,NH_3 \longrightarrow 0.1\,[CHONSP]_{Bio\_2} + 0.6667CH3COOH + 0.6667\,CO_2 + 0.9\,H_2O$	Kinetic law
2-3	$1.0833\,[CHO]_{oses} + 0.1\,NH_3 \longrightarrow 0.1\,[CHONSP]_{Bio\_3} + C3H7COOH + 2\,CO_2 + 2\,H_2 + 0.3\,H_2O$	Kinetic law
2-4	$1.0833\,[CHO]_{oses} + 0.1\,NH_3 \longrightarrow 0.1\,[CHONSP]_{Bio\_4} + 3\,CH3COOH + 0.3\,H_2O$	Kinetic law
2-5	$[CHON]_{lipids} + 0.1\,NH_3 + 0.575\,H_2O \longrightarrow 0.1\,[CHONSP]_{Bio\_5} + 0.875\,H_2 + 0.5\,CH_3COOH$	Kinetic law

	Step 3: acetogenesis	
3-1	$C_2H_5COOH + 1.85\,H_2O + 0.05\,NH_3 \longrightarrow 0.05\,[CHONSP]_{Bio\_6} + CO_2 + 3\,H_2 + 0.875\,CH_3COOH$	Kinetic law
3-2	$C_3H_7COOH + 1.85\,H_2O + 0.05\,NH_3 \longrightarrow 0.05\,[CHONSP]_{Bio\_7} + 2\,H_2 + 1.875\,CH_3COOH$	Kinetic law
3-3	$C_3H_7COOH_{[Isoburate]} + 3.85\,H_2O + 0.05\,NH_3 \longrightarrow 0.05\,[CHONSP]_{Bio\_8} + 2\,CO_2 + 6\,H_2 + 0.875\,CH_3COOH$	Kinetic law
3-4	$C_4H_9COOH + 3.85\,H_2O + 0.05\,NH_3 \longrightarrow 0.05\,[CHONSP]_{Bio\_9} + CO_2 + 5\,H_2 + 1.875\,CH_3COOH$	Kinetic law
3-5	$C_4H_9COOH_{[Isovalerate]} + 3.85\,H_2O + 0.05\,NH_3 \longrightarrow 0.05\,[CHONSP]_{Bio\_10} + CO_2 + 5\,H_2 + 1.875\,CH_3COOH$	Kinetic law
3-6	$C_5H_{11}COOH + 3.85\,H_2O + 0.05\,NH_3 \longrightarrow 0.05\,[CHONSP]_{Bio\_11} + 4\,H_2 + 2.875\,CH_3COOH$	Kinetic law
3-7	$C_5H_{11}COOH_{[Isocaproate]} + 5.85\,H_2O + 0.05\,NH_3 \longrightarrow 0.05\,[CHONSP]_{Bio\_12} + 2\,CO_2 + 8\,H_2 + 1.875\,CH_3COOH$	Kinetic law

	Step 4: methanogenesis	
4-1	$CH_3COOH + 0.022\,NH_3 \longrightarrow 0.022\,[CHONSP]_{Bio\_13} + 0.945\,CO_2 + 0.945\,CH_4 + 0.066\,H_2O$	Kinetic law
4-2	$0.5\,CO_2 + 1.8909\,H_2 + 0.0109\,NH_3 \longrightarrow 0.0109\,[CHONSP]_{Bio\_14} + 0.4452\,CH_4 + 0.978\,H_2O$	Kinetic law

Table 1: Equations and their associated laws for dynamic modelling of the anaerobic biodegradation.

$[CHONSP]_{proteins}=CH_{1.56828}O_{0.3063}N_{0.2693}S_{0.00635}$
$[CHONSP]_{poolAA}=CH_{1.9800}O_{0.5122}N_{0.2693}S_{0.00635}$
$[CHONSP]_{Carbohydrates}=CH_{1.6667}O_{0.8333}$
$[CHONSP]_{Lipids}=CH_2O_{0.125}$
$[CHONSP]_{oses}=C_6H_{12}O_6$
$[CHONSP]_{Bio}=C_5H_7O_2N$

Even if the process will be designed in order to avoid methane production, it will be necessary to conserve the equations for the step 4 as there is no evidence that the methanogenic bacteria are absent of autochtonous inoculum, and that in favourable conditions the methanogenesis activity cannot start again.

Biological kinetic model

The biological kinetic model described in TN 39.3 and used as the basis for the dynamic simulations of anaerobic degradation in batch process condition can be used:

$$\begin{cases} r_X = \mu . X - k_D . X \\ r_{XD} = k_D . X \\ r_{Si} = \dfrac{-1}{Y_{X/Si}} \mu X \end{cases}$$

$$K_{I-k} = 1 + \frac{C_k}{I_k}$$

$$\mu = \mu_{max} \prod_k \frac{C_k}{(Ks_k + C_k)} \frac{1}{K_{I-k}}$$

The yields $Y_{X/Si}$ are calculated from the stoichiometric equations. The kinetic parameters used in first simulations presented in TN 39.3 are taken from the literature and are reported in table 2.

Dynamic of the reactor

Design

A schematic design of the reactor facilities in compartment I in continuous conditions was proposed in TN 39.3 and is reported in figure 2.

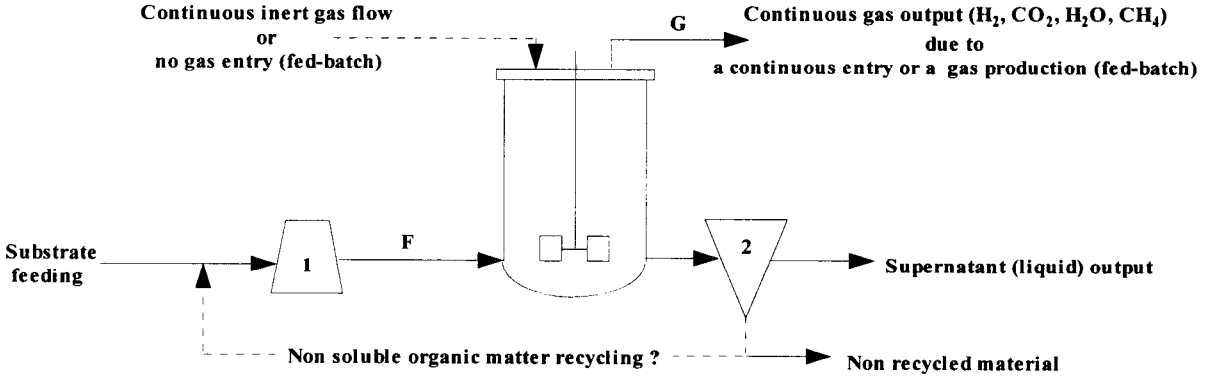


Figure 2: Proposed design for the reactor. Dashed lines are for possible flows.
[1] is a pre-treatment process (or post-treatment if there is recycling).
[2] is the separation process for recycling and/or liquid output of the reactor. It is evident that at least a value of the efficiency of these processes must be known for their integration in a dynamic model.

The feeding of the reactor was sequential in batch experiments. The organic matter produced by the crew (faeces) is not continuously produced. To have a continuous feeding of the reactor, a storage tank or "buffer reactor" are required. The modelling of these pre-treatment processes and their influence on the quality of the substrates must be considered in the modelling of the loop.
At the present time, the design for the process is not completely defined and then the model cannot be definitively established. In a first approach, it is assumed that the reactor has a perfectly mixed behaviour and that the liquid (organic waste) feeding is continuous. This point could be discussed.

Hydrodynamic equations for the reactor in continuous conditions (not including pre and post treatment)

$$V_L \cdot \frac{dC_{Si}\big|_L}{dt} = F.C_{Si}^{in}\big|_L - F.C_{Si}\big|_L + V_L.\phi_{Si}\big|_{GL} + V_L.\phi_{Si}\big|_{Reac}$$

$$V_G \cdot \frac{dC_{Si}\big|_G}{dt} = G.C_{Si}^{in}\big|_G - G.C_{Si}\big|_G - V_L.\phi_{Si}\big|_{GL}$$

It must be outlined that in this model, the flow rates (gas and liquid) were assumed to be the same at outputs and at inputs (the net gas production is neglected compared to the entry flow rate). As the reactor is probably an important gas producer, this assumption must be tested. The possibility of accumulation of matter in the reactor has to be considered too. It is then probable that the basic expression for the dynamic behaviour of the reactor as given above will be changed in the future.

Another set of hydrodynamic equations can be proposed if we consider that there is no gas feeding on the reactor. In such a case the gas prduction can must be taken into account as it is responsible of the output gas flow rate.

Hydrodynamic equations for the reactor in fed-batch conditions for the gas (not including pre and post treatment)

$$V_L \cdot \frac{dC_{Si}\big|_L}{dt} = F.C_{Si}^{in}\big|_L - F.C_{Si}\big|_L + V_L.\phi_{Si}\big|_{GL} + V_L.\phi_{Si}\big|_{Reac}$$

$$V_G \cdot \frac{dC_{Si}\big|_G}{dt} = -G.C_{Si}\big|_G - V_L.\phi_{Si}\big|_{GL}$$

$$G = \sum_{Si} \frac{R.T}{P.V_G} \frac{dC_{Si}\big|_G}{dt}$$

It must be kept in mind that this set of equations is stated asssuming that the liquid volume V_L and that the gas volume V_G remain constant throughout the whole process. It is also assumed that the total gas pressure P is constant (i.e gas does not accumulate).

Eq. 1-1	Complete hydrolysis of the degradable part		
Eq. 1-2	Complete hydrolysis of the degradable part		
Eq. 1-3	Complete hydrolysis of the degradable part		
Eq. 1-4	Complete hydrolysis of the degradable part		
Eq. 2-1	KS=0.001 mol/l (Pool AA)		μ_m=0.2 h^{-1} k_D=0.01 h^{-1}
Eq. 2-2	KS=0.0033 mol/l (osides) KS=0.0002 mol/l (NH3)		μ_m=0.2 h^{-1} k_D=0.01 h^{-1}
Eq. 2-3	KS=0.0033 mol/l (osides) KS=0.0002 mol/l (NH3)		μ_m=0.2 h^{-1} k_D=0.01 h^{-1}
Eq. 2-4	KS=0.0033 mol/l (osides) KS=0.0002 mol/l (NH3)		μ_m=0.2 h^{-1} k_D=0.01 h^{-1}
Eq. 2-5	KS=0.001 mol/l (Lipids) KS=0.0002 mol/l (NH3)		μ_m=0.2 h^{-1} k_D=0.01 h^{-1}
Eq. 3-1	KS=0.004 mol/l (propionate) KS=0.0002 mol/l (NH3)	KI=0.016 mol/l (acetate) KI=10^{-6} mol/l (H2)	μ_m=0.02 h^{-1} k_D=0.001 h^{-1}
Eq. 3-2	KS=0.002 mol/l (butyrate) KS=0.0002 mol/l (NH3)	KI=0.012 mol/l (acetate) KI=10^{-6} mol/l (H2)	μ_m=0.02 h^{-1} k_D=0.001 h^{-1}
Eq. 3-3	KS=0.002 mol/l (isobutyrate) KS=0.0002 mol/l (NH3)	KI=0.01 mol/l (acetate) KI=10^{-6} mol/l (H2)	μ_m=0.02 h^{-1} k_D=0.001 h^{-1}
Eq. 3-4	KS=0.002 mol/l (valerate) KS=0.0002 mol/l (NH3)	KI=0.01 mol/l (acetate) KI=10^{-6} mol/l (H2)	μ_m=0.02 h^{-1} k_D=0.001 h^{-1}
Eq. 3-5	KS=0.002 mol/l (isovalerate) KS=0.0002 mol/l (NH3)	KI=0.01 mol/l (acetate) KI=10^{-6} mol/l (H2)	μ_m=0.02 h^{-1} k_D=0.001 h^{-1}
Eq. 3-6	KS=0.002 mol/l (caproate) KS=0.0002 mol/l (NH3)	KI=0.01 mol/l (acetate) KI=10^{-6} mol/l (H2)	μ_m=0.02 h^{-1} k_D=0.001 h^{-1}
Eq. 3-7	KS=0.002 mol/l (isocaproate) KS=0.0002 mol/l (NH3)	KI=0.01 mol/l (acetate) KI=10^{-6} mol/l (H2)	μ_m=0.02 h^{-1} k_D=0.001 h^{-1}
Eq. 4-1	KS=0.002 mol/l (acetate) KS=0.0002 mol/l (NH3)	KI=0.0153 mol/l (NH3)	μ_m=0.02 h^{-1} k_D=0.001 h^{-1}
Eq. 4-2	KS=0.002 mol/l (CO2) KS=0.0002 mol/l (NH3) KS=10^{-6} mol/l (H2)		μ_m=0.06 h^{-1} k_D=0.003 h^{-1}

Table 2: Parameters values for the biological model of compartment I (Notes: all values are taken from the literature).

I.3 Compartment II - Photoheterotrophic

Description of the process

This is an anaerobic compartment. It is recieves gas (elimination of H_2?) and liquid (elimination of VFA and remaining organic matter) outputs from the first compartment. The mass balanced model and the biological model for light limitation have been presented respectively in TN 23.3 and TN 23.4. Most of the data used for the modelling are taken from Albiol (1994). The strain selected for heterotrophic growth is *Rs. rubrum*.

The control law developed from the light limitation model is used to control the biomass production. But it is important to notice that the objective of the compartment is not to produce biomass but to assimilate VFA. Of course by controlling the biomass production the assimilation of VFA is controlled too, but they are not necessarily completely exhausted. Further studies are then required to assess the working conditions of the compartment.

Mass balanced model

Stoichiometric equations have been established for the growth on several carbon sources. It must be noted that the biomass composition used in these stoichiometries was always the same. It was based on a biomass obtained in non limiting growth conditions on acetate: 48.9% proteins; 12.13% carbohydrates; 13.53% lipids; 3.73% DNA; 8.40% RNA; 1.30% glycogen and 5% PHB.

It is probable that the biomass composition, mainly the reserve content (glycogen; PHB), can change with growth conditions. The equations obtained in TN 23.3 are reported in table 3.

Carbon source	
Acetic acid	$Acetic\ acid + 0.3876\ NH_3 + 0.0282\ H_3PO_4 + 0.0062\ H_2SO_4 \downarrow 1.8505\ CH_{1.5951}O_{0.3699}N_{0.2094}S_{0.0034}P_{0.0152} + 0.1495\ CO_2 + 1.1540\ H_2O$
Propionic acid	$\text{Pr}opionic\ acid + 0.6782\ NH_3 + 0.0493\ H_3PO_4 + 0.0102\ H_2SO_4 + 0.2383\ CO_2 \downarrow 3.2383\ CH_{1.5951}O_{0.3699}N_{0.2094}S_{0.0034}P_{0.0152} + 2.5195\ H_2O$
Butyric acid	$\text{B}utyric\ acid + 0.9689\ NH_3 + 0.0704\ H_3PO_4 + 0.0156\ H_2SO_4 + 0.6261\ CO_2 \downarrow 4.6261\ CH_{1.5951}O_{0.3699}N_{0.2094}S_{0.0034}P_{0.0152} + 1.8850\ H_2O$
Lactic acid	$\text{L}actic\ acid + 0.5813\ NH_3 + 0.0422\ H_3PO_4 + 0.0093\ H_2SO_4 \downarrow 2.7757\ CH_{1.5951}O_{0.3699}N_{0.2094}S_{0.0034}P_{0.0152} + 1.7310\ H_2O + 0.2243\ CO_2$

Table 3: Stoichiometric equations for *Rs. rubrum* on various carbon sources.

Biological kinetic model

A model for the photoheterotrophic growth of *Rs. rubrum* in light limiting conditions has been established by Cornet in TN 23.4. This model is based upon the model developed for *Sp. platensis* (cf. I.4). The model parameters for *Rs. rubrum* have been identified (table 4) from experimental results reported by Albiol (1994).

It can be assumed that the light parameters identified (Ea, Es, J_{min}) are only characteristic of the micro-organism and are independent on the growth conditions, especially of the carbon (or other substrates) sources.

Model for radiant light energy available versus the radius of the reactor

$$\frac{4\pi J}{F_R} = \frac{R}{r}\frac{2\cosh\left(\frac{\delta r}{R}\right)}{\cosh(\delta)+\alpha\sinh(\delta)}$$

$$\alpha = \sqrt{\frac{Ea}{Ea+Es}} \qquad \delta = (Ea+Es).Cx.\alpha.R$$

the solutions of the following equation (R_2' and R_2) gives the working illuminated radius

$$\frac{r}{R}\frac{2\cosh\left(\frac{\delta r}{R}\right)}{\cosh(\delta)+\alpha\sinh(\delta)} - \frac{4\pi J_{\min}}{F_R} = 0$$

Mean volumetric growth rate (light limitation)

$$\langle r_X \rangle = \langle \mu \rangle.\gamma.C_X$$

$$\gamma = \frac{R_2'^2}{R^2} + \frac{(R^2 - R_2^2)}{R^2}$$

$$\langle \mu' \rangle = \frac{1}{\pi.(R_2'^2 + R^2 - R_2^2)}\left[\int_0^{R_2'} 2\pi r \mu'_m \frac{4.\pi.J}{K_J + 4.\pi.J}dr + \int_{R_2}^{R} 2.\pi.r.\mu'_m \frac{4.\pi.J}{K_J + 4.\pi.J}dr\right]$$

Mean consumption/production rate

$$\langle r_{Si} \rangle = \frac{1}{Y_{X/Si}}\langle \mu \rangle.\gamma.C_X$$

This model was established for light limitation only. It does not include substrate limitation nor decay of the biomass. A more complete model taking into account this phenomenon can be written, but at the present time there is no value for the parameters that could be involved in such a model, and the model itself (based on Monod equation) is not validated:

$$\langle r_X \rangle = \langle \mu \rangle.\gamma.C_X.\prod_{Si}\frac{C_{Si}}{\left(KS_{Si} + C_{Si}\right)\left(1 + \frac{C_{Si}}{I_{Si}}\right)} - k_D.C_X$$

$$\langle r_{XD} \rangle = k_D.C_X$$

$$\langle r_{Si} \rangle = \frac{1}{Y_{X/Si}} \langle \mu \rangle . \gamma . C_X . \prod_{Si} \frac{C_{Si}}{\left(KS_{Si} + CSi \right) \left(1 + \frac{C_{Si}}{I_{Si}} \right)}$$

These Monod based equations are more simple than those established for *Spirulina*. It is probable that it is a too important simplification, and a more complex model may be necessary to describe variation of the biomass in limiting condition as for *Spirulina* (cf. I.5).

Light limitation parameters	Ea=220 m^2/kg biomass for 350-750 nm Es=480 m^2/kg biomass for 350-750 nm $4\pi J_{min}$=1 W/m^2
Growth on acetate	μmax=0.17 h^{-1} K_J=7 W/m^2 KS_{si}=unknown I_{si}=unknown k_D= unknown
Growth on other substrates	Data not yet obtained

Table 4: Parameter for the biological kinetic model of *Rs. rubrum*.

Dynamic of the reactor

Design

The photobioreactor used for compartment II is represented in figure 3. It can be assumed to be a perfectly mixed tank reactor with one input and one output for gas and for liquid streams.

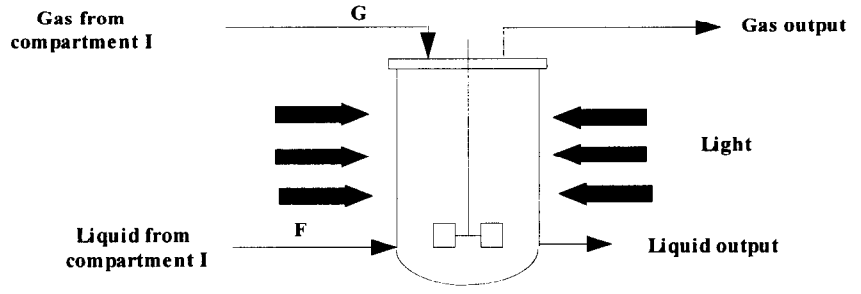


Figure 3: Schematic representation of the photobioreactor for compartment II

The reactor operates in continuous conditions. Liquid and gas are coming from the previous compartment I. Then flow rates are roughly fixed by the behaviour of the first compartment. There is at the present time no details upon the possible step for the link between the two compartments (dilution of liquid flow; "buffer tanks" to control the flow rate). Then as for the first compartment, the hydrodynamic equations proposed concern only the mass balance on the photobioreactor.

Hydrodynamic equations for the reactor (not including pre and post treatment)

$$V_L \cdot \frac{dC_{Si}\big|_L}{dt} = F.C_{Si}^{in}\big|_L - F.C_{Si}\big|_L + V_L.\phi_{Si}\big|_{GL} + V_L.\phi_{Si}\big|_{Reac}$$

$$V_G \cdot \frac{dC_{Si}\big|_G}{dt} = G.C_{Si}^{in}\big|_G - G.C_{Si}\big|_G - V_L.\phi_{Si}\big|_{GL}$$

I.4 Compartment III - Nitrifying

Description of the process

The process selected for the nitrifying compartment is a column packed with polystyrene beads on which the biomass is attached. The column is colonised by a coculture of *Nitrosomonas europea* and *Nitrobacter winogradskyi*.

The objective of this compartment is the oxidation of ammonia to nitrate. On the contrary of the two first compartments, the process is aerobic. In principle, the liquid input is free of organic matter and the growth occurs in autotrophic conditions. The links between the outputs of the compartment II and the inputs of the compartment III will be probably one critical point (filtration of the liquid; entry of oxygen from another point of the loop, probably lower flow rates on the column than the outputs flow rates from compartment II).

Mass balanced model

The bases and the assumptions used to establish the stoichiometric equations were presented in TN 23.2 and TN 32.1. Both equations for the growth in autotrophic and in heterotrophic conditions exist, but for the growth in presence of organic matter some points remain to be studied It is still necessary to describe growth in presence of organic matter and to compare with experiments. The organic matter coming from the previous compartment II of MELiSSA is mainly composed of VFA not assimilated by *Rs. rubrum*. Only stoichiometric equations for the growth in autotrophic condition are presented here (table 5).

Contrary to the other stoichiometric equations, a difference is made between the equation representing growth and the equation for maintenance. In fact maintenance is, in autotrophy, the main reaction for the oxidation of ammonia and nitrite.

Nitrosomonas	
Biosynthesis	Maintenance
$CO_2 + 4.3652\,O_2 + 0.0041\,H_2SO_4 + 0.0136\,H_3PO_4 + 3.8400\,NH_3 \rightarrow CH_{1.6097}O_{0.3777}N_{0.2107}S_{0.0041}P_{0.0136} + 3.1649\,H_2O + 3.6292\,[NO_2^- + H^+]$	$1.5\,O_2 + NH_3 \rightarrow H_2O + [NO_2^- + H^+]$
Nitrobacter	
Biosynthesis	Maintenance
$CO_2 + 6.8413\,O_2 + 0.0041\,H_2SO_4 + 0.0136\,H_3PO_4 + 0.2107\,NH_3 + 15.8398\,[NO_2^- + H^+] \rightarrow CH_{1.6097}O_{0.3777}N_{0.2107}S_{0.0041}P_{0.0136} + 0.4643\,H_2O + 15.8398\,[NO_3^- + H^+]$	$0.5\,O_2 + [NO_2^- + H^+] \rightarrow [NO_3^- + H^+]$

Table 5: Stoichiometric equations for the oxidation of NH_3 by *Nitrosomonas* and the oxidation of nitrite by *Nitrobacter*.

Biological kinetic model

The model of Beeftink has been used. This model was also used in the development of model for nitrification in an air lift reactor with biomass entrapped in carrageenan beads. The details of the model are reported in TN 27.1 and TN 32.2. The complete expression of the model

equation is presented below. A difference is made between free and fixed biomass and each species (*Nitrosomonas* and *Nitrobacter*) is treated separately.

$$r_X^{Ns-Nb} = \mu^{Ns-Nb}.C_X^{Ns-Nb}\big|_B - Y_{X/Smt}^{Ns-Nb}.m^{Ns-Nb}.\left(\frac{\mu^{Ns-Nb}}{\mu_{\max}^{Ns-Nb}} - 1\right).C_X^{Ns-Nb}\big|_B \text{ with}$$

$$\mu^{Ns-Nb} = \mu_{\max}^{Ns-Nb} \frac{C_{Si}^n\big|_B}{\left(C_{Si}^n\big|_B + KS_{Si}^{Ns-Nb}\right)\left(1 + \frac{C_{Si}^n\big|_B}{I_{Si}}\right)}$$

where Ns-Nb means *Nitrosomonas* or *Nitrobacter*

The biomass released in the liquid from the biofilm on the beads is represented by:

$r_{X-L}^{Ns \text{ or Nb free biomass}} = K_{wo} r_X^{Ns-Nb}$ if r_X^{Ns-Nb} is ≥ 0.

$r_{X-L}^{Ns \text{ or Nb free biomass}} = 0.$ if r_X^{Ns-Nb} is < 0.

The consumption/production rates of substrates are expressed by the following relations:

$$r_{Si}^{Ns-Nb} = \frac{1}{Y_{X/Si}^{Ns-Nb}} \mu^{Ns-Nb}.C_X^{Ns-Nb}\big|_B + \frac{1}{Y_{Smt/Si}^{Ns-Nb}} m^{Ns-Nb}.C_X^{Ns-Nb}\big|_B$$

The apparition of the so-called Dead biomass (XD) follows the law

$$r_{XD}^{Ns-Nb} = Y_{X/Smt}^{Ns-Nb}.m^{Ns-Nb}.\left(\frac{\mu^{Ns-Nb}}{\mu_{\max}^{Ns-Nb}} - 1\right).C_X^{Ns-Nb}\big|_B$$

Note: maintenance is independent of substrates and of their possible limitation or exhaustion. To include substrate limitation for maintenance in calculations, it is necessary:

- to skip the maintenance term if oxygen, ammonia or nitrite (for Nitrobacter) are limiting.

- or to introduce a michaelian type limitation (S/(Ks+S)) with a lower Ks than growth kinetics (10^{-8} mol/l)

The description and the current setting values of the parameters involved in the biological model are taken from the literature and are reported in table 6.

It can be noticed that the introduction of maintenance in the growth rate law is equivalent to the introduction of a decay term. The dead biomass had to be considered in the checking of the mass balance of the system, but has not yet be introduced in the Nitrisim dynamic model. This dead biomass (XD) is taken into account in the simplified dynamic model developed by Leclerc (TN 35.2).

			Reference	Remarks
Growth rates				
μ_{max}^{Ns}	$5.7\ 10^{-2}\ h^{-1}$		[TN 27.2]	mean values calculated
μ_{max}^{Nb}	$3.6\ 10^{-2}\ h^{-1}$		[TN 27.2]	from several
m^{Ns}	$3.38\ 10^{-3}$ mol NH_3.g biomass^{-1}.h^{-1}		[TN 27.2]	continuous cultures
m^{Nb}	$7.92\ 10^{-3}$ mol NO_2^-.g biomass^{-1}.h^{-1}		[TN 27.2]	
Limiting substrate [Si]	K_{Si}^{Ns}	K_{Si}^{Nb}		
NH_3	$6.625\ 10^{-5}$ mol/l	-	[TN 27.2]	Model parameter
NO_2^-	-	$3.6\ 10^{-4}$ mol/l	[TN 27.2]	values for a fixed bed
O_2	$5.05\ 10^{-6}$ mol/l	$1.7\ 10^{-5}$ mol/l	[TN 27.2]	of carragenan beads
HCO_3^-	10^{-8} mol/l	10^{-8} mol /l		no carbon limitation
HPO_4^{2-}	10^{-8} mol/l	10^{-8} mol /l		no phosphate limitation
SO_4^{2-}	10^{-8} mol/l	10^{-8} mol /l		no sulphur limitation
Other (non limiting)	0.	0.		
Inhibitory substrate Si	I_{Si}^{Ns}	I_{Si}^{Nb}		
NO_2^-	-	0.159	[TN 27.3]	
NO_3^-	-	0.188	[TN 27.3]	
Others (no inhibition)	10^{10}	10^{10}		

Table 6: Parameters for the biological models of the growth of *Nitrosomonas* and *Nitrobacter*.

Dynamic behavior of the reactor

Design

The nitrifying compartment is a complex 3 phases system (liquid-gas-solid). Two phases are circulating (liquid and solid) and the third is fixed (on beads). In order to have a model flexible enough to fit any hydrodynamic situation (from a perfectly mixed tank to a plug flow reactor), a model based on a N-tanks in series with back-mixing flows between the tanks was chosen (figure 4). In any case the column is slipped into 3 parts: part A for the bottom; part B for the fixed bed and part C for the top. Some improvements remain to do with this model, mainly to fix hydrodynamic parameters (number of tanks; back-mixing).

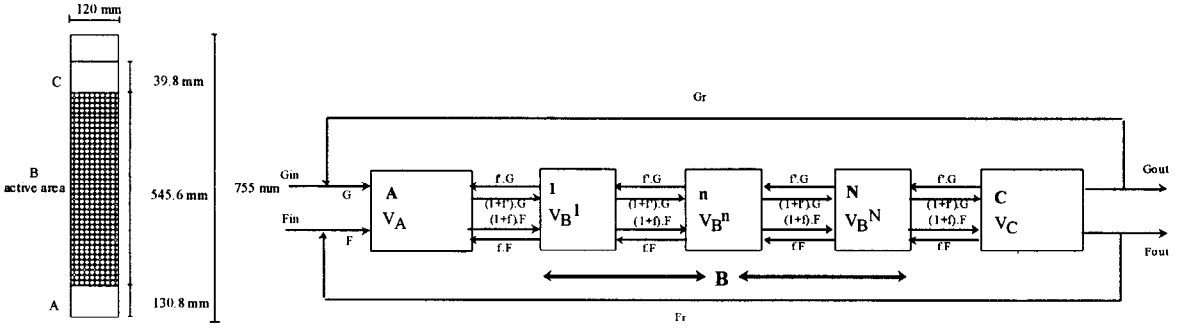


Figure 4: Schematic representations of the nitrifying column.

Hydrodynamic equations

Part A

$$\frac{\varepsilon_L}{\varepsilon} V_A \frac{dC_{Si}^A|_L}{dt} = F_{in}.C_{Si}^{in}|_L + F_r.C_{Si}^{out}|_L - (f+1).F.C_{Si}^A|_L + f.F.C_{Si}^1|_L + \frac{\varepsilon_L}{\varepsilon} V_A.\phi_{Si}^A|_{GL}$$

$$\frac{\varepsilon_G}{\varepsilon} V_A \frac{dC_{Si}^A|_G}{dt} = G_{in}.C_{Si}^{in}|_G + G_r.C_{Si}^{out}|_G - (f'+1).G.C_{Si}^A|_G + f'.G.C_{Si}^1|_G - \frac{\varepsilon_1}{\varepsilon} V_A.\phi_{Si}^A|_{GL}$$

Part B (fixed bed)

$$\varepsilon_L.V_B^n.\frac{dC_{Si}^n|_L}{dt} = (1+f).F.C_{Si}^{n-1}|_L + f.F.C_{Si}^{n+1}|_L - (f+1).F.C_{Si}^n|_L - f.F.C_{Si}^n|_L + \varepsilon_L.V_B^n.\phi_{Si}^n|_{GL} + \varepsilon_L.V_B^n.\phi_{Si}^n|_{LB}$$

$$\varepsilon_G.V_B^n.\frac{dC_{Si}^n|_G}{dt} = (1+f').G.C_{Si}^{n-1}|_G + f'.G.C_{Si}^{n+1}|_G - (f'+1).G.C_{Si}^n|_G - f'.G.C_{Si}^n|_G - \varepsilon_L.V_B^n.\phi_{Si}^n|_{GL}$$

$$\frac{dC_X^n|_B}{dt} = \phi_{Xi}^n|_{LB}$$

Part C

$$\frac{\varepsilon_L}{\varepsilon} V_C \frac{dC_{Si}^C|_L}{dt} = (f+1).F.C_{Si}^N|_L - f.F.C_{Si}^C|_L - F_r.C_{Si}^C|_L - F_{out}.C_{Si}^C|_L + \frac{\varepsilon_L}{\varepsilon} V_C.\phi_{Si}^C|_{GL}$$

$$\frac{\varepsilon_G}{\varepsilon} V_C \frac{dC_{Si}^C|_G}{dt} = (f'+1).G.C_{Si}^N|_G - f'.G.C_{Si}^C|_G - G_r.C_{Si}^C|_G - G_{out}.C_{Si}^C|_G - \frac{\varepsilon_G}{\varepsilon} V_C.\phi_{Si}^C|_{GL}$$

n is the number of the tank, 1<n<N, $\phi_{Si}^n|_{GL}$ the gas-liquid transfer term (mol/unit volume. unit time) and $\phi_{Si}^n|_{LB}$ the liquid-biofilm transfer term (mol/unit volume. unit time). In absence of mass transfer limitation in the biofilm, $\phi_{Si}^n|_{LB} = \phi_{Si}^n|_{Reac}$.

I.5 Compartment IV - Photosynthetic

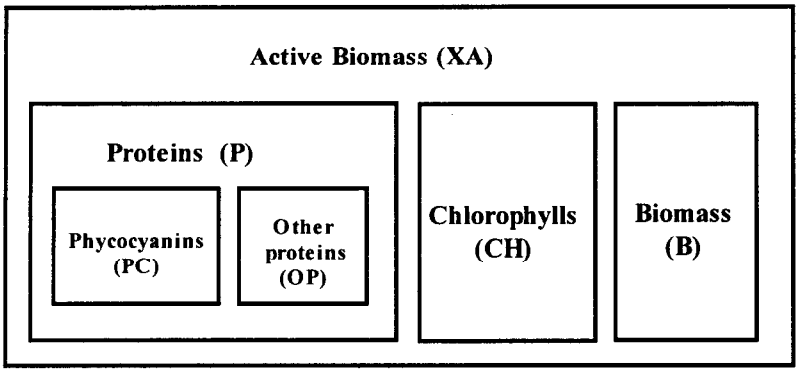
Description of the process

The photosynthetic compartment is composed of a photobioreactor. Its principal objective is the production of edible biomass. The process operates in autotrophic conditions and is linked with the liquid output of compartment III. The photobioreactor is also able to regenerate the atmosphere by consuming CO_2 and producing O_2. The gas input and output of the compartment are then more or less closely linked with the gas fluxes of the other compartments.

First continuous experiments were led with stirred tank reactors. Stoichiometric equations and a dynamic model for the growth in light limiting, P limiting and S limiting conditions has been developed by Cornet. Most of the details concerning the model of the photosynthetic compartment can be found in TN 19.1 and 19.2.

The non-structured model developed by Cornet (TN 19.2) will be reviewed here.

In its biomass definition, Cornet divided the active biomass (XA) into several elemental constituents:



Mass balanced model

Two stoichiometric equations were written to describe the growth of *Spirulina platensis*: one to achieve the active biomass synthesis and one for the synthesis of an exopolysaccharide (EPS) (table 7).

Carbon source	
Biomass synthesis	$CO_2 + 0.1921\ HNO_3 + 0.0063\ H_3PO_4 + 0.0052\ H_2SO_4 + 1.3794H2O \rightarrow CH_{1.566}O_{0.405}N_{0.192}S_{0.0054}P_{0.0063} + 1.437\ O_2$
EPS synthesis	$CO_2 + 0.015\ H_2SO_4 + 2.22\ H_2O \rightarrow CH_{1.650}O_{0.950}S_{0.015} + 0.96\ O_2$

Table 7: Mass balanced equations for the growth of *Spirulina platensis*

Biological kinetic model

A dynamic model for the growth of *Spirulina platensis* in light limiting condition was established by Cornet (TN 19.2). It takes into account the variation of the production of EPS in light limiting condition as well as the variation of the active biomass and the vegetative biomass composition in mineral limiting conditions.

Model for radiant light energy available versus the radius of the reactor

$$\frac{4\pi J}{F_R} = \frac{R}{r}\frac{2\cosh\left(\frac{\delta r}{R}\right)}{\cosh(\delta)+\alpha\sinh(\delta)}$$

$$\alpha = \sqrt{\frac{Ea.(C_{PC}+C_{CH})}{Ea.(C_{PC}+C_{CH})+Es.C_{XV}}}$$

$$\delta = R.\sqrt{Ea.(C_{PC}+C_{CH})\left[Ea.(C_{PC}+C_{CH})+Es.C_{XV}\right]}$$

C_{PC} is the concentrations of Phycocyanins (contained in XA)
C_{CH} is the concentrations of Chlorophylls(contained in XA)
XV is the vegetative biomass.

The solutions of the following equation (R_2' and R_2) gives the working illuminated radius

$$\frac{r}{R}\frac{2\cosh\left(\frac{\delta r}{R}\right)}{\cosh(\delta)+\alpha\sinh(\delta)} - \frac{4\pi J_{\min}}{F_R} = 0$$

Mean volumetric growth rate (light limitation) with respect to Phycocyanins

$$\langle R_X \rangle = \langle \mu' \rangle . \gamma . C_{PC}$$

$$\gamma = \frac{R_2'^2}{R^2} + \frac{(R^2 - R_2^2)}{R^2}$$

$$\langle \mu' \rangle = \frac{1}{\pi.(R_2'^2 + R^2 - R_2^2)}\left[\int_0^{R_2'} 2\pi r \mu'_m \frac{4.\pi.J}{K_J + 4.\pi.J} dr + \int_{R_2}^{R} 2.\pi.r.\mu'_m \frac{4.\pi.J}{K_J + 4.\pi.J} dr\right]$$

Mean volumetric rate of EPS biosysnthesis (light limitation) with respect to Phycocyanins

$$\langle R_{EPS} \rangle = \langle \mu'^{EPS} \rangle . \gamma . C_{PC}$$

$$\langle \mu'^{EPS} \rangle = \frac{1}{\pi.\left(R_2'^2 + R^2 - R_2^2\right)}\left[\int_0^{R_2'} 2\pi r \mu'^{EPS}_m \frac{4.\pi.J}{K_J + 4.\pi.J} dr + \int_{R_2}^{R} 2.\pi.r.\mu'^{EPS}_m \frac{4.\pi.J}{K_J + 4.\pi.J} dr\right]$$

Kinetic equations

$$\langle r_{XT} \rangle = \langle R_{XA} \rangle + \langle R_{EPS} \rangle$$

$$\langle r_{XA} \rangle = \langle R_{XA} \rangle \frac{C_{NO3}}{KS_{NO3} + C_{NO3}} \cdot \frac{C_{SO4}}{KS_{SO4} + C_{SO4}}$$

$$\langle r_{XV} \rangle = \langle R_{XA} \rangle \cdot \left[\frac{C_{NO3}}{KS_{NO3} + C_{NO3}} \cdot \frac{C_{SO4}}{KS_{SO4} + C_{SO4}} + \frac{C_{PC}}{KS_{PC} + C_{PC}} \left(\frac{KS_{NO3}}{KS_{NO3} + C_{NO3}} + \frac{KS_{SO4}}{KS_{SO4} + C_{SO4}} \right) \right]$$

$$\langle r_{EPS} \rangle = \langle r_{XT} \rangle - \langle r_{XVS} \rangle$$

$$\langle r_{CH} \rangle = z_{CH} \cdot \langle r_{XA} \rangle$$

$$\langle r_{PC} \rangle = z_{PC} \cdot \langle R_{XA} \rangle \cdot \left[\frac{C_{NO3}}{KS_{NO3} + C_{NO3}} \cdot \frac{C_{SO4}}{KS_{SO4} + C_{SO4}} - \left(\frac{KS_{NO3}}{KS_{NO3} + C_{NO3}} + \frac{KS_{SO4}}{KS_{SO4} + C_{SO4}} \right) \right]$$

$$\langle r_{P} \rangle = z_{P} \cdot \langle R_{XA} \rangle \cdot \left[\frac{C_{NO3}}{KS_{NO3} + C_{NO3}} \cdot \frac{C_{SO4}}{KS_{SO4} + C_{SO4}} - q \cdot \left(\frac{KS_{SO4}}{KS_{SO4} + C_{SO4}} \right) \right]$$

$$\langle r_{Si} \rangle = \frac{-1}{Y_{X/Si}} \langle r_{XA} \rangle + \frac{-1}{Y_{EPS/Si}} \langle R_{EPS} \rangle \frac{C_{NO3}}{KS_{NO3} + C_{NO3}} \cdot \frac{C_{SO4}}{KS_{SO4} + C_{SO4}}$$

The carbon limitation (from CO_2 gas) is difficult to model. The addition of a classical Monod term to the previous kinetic equations failed. The variation of the active biomass in carbon limiting conditions suggests a more complicated model.
Changes in the model are then attempted for the introduction of the carbon limitation in the future. Nevertheless, in its present form the model is able to describe the growth of *Spirulina* in mineral and light limiting conditions.

Light limitation parameters	Ea=872 m^2/kg biomass Es=200 m^2/kg biomass $4\pi J_{min}$=1 W/m^2
Autotrophic growth model parameters	μ'_m=0.45 h^{-1} μ^{EPS}_m=1.852 h^{-1} K_J=20 W/m^2 K^{EPS}_J=750 W/m^2 KS_{NO3}= 5.3 10^{-3} kg/m^3 KS_{SO4}= 2.5 10^{-4} kg/m^3 KS_{PC}= 0.06 kg/m^3 q=0.55 Zp=0.684 Zpc=0.162 Zch=0.01

Table 8: Parameter values for the biological model of the growth of *Spirulina platensis*.

Dynamic of the reactor

Design

The photobioreactor used for compartment IV is represented in figure 5. It was in the first experiments a cylindrical stirred tank or a rectangular reactor. An air lift photobioreactor was built at UAB laboratory for the growth of *Spirulina platensis*. The hydrodynamic behaviour of the air lift has not yet be studied and then as a first approximation a perfectly stirred tank behaviour will be assumed.

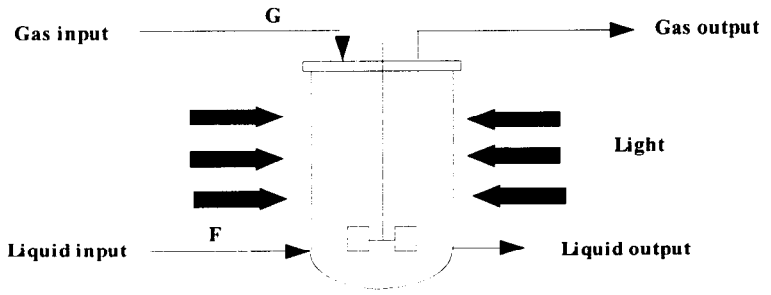
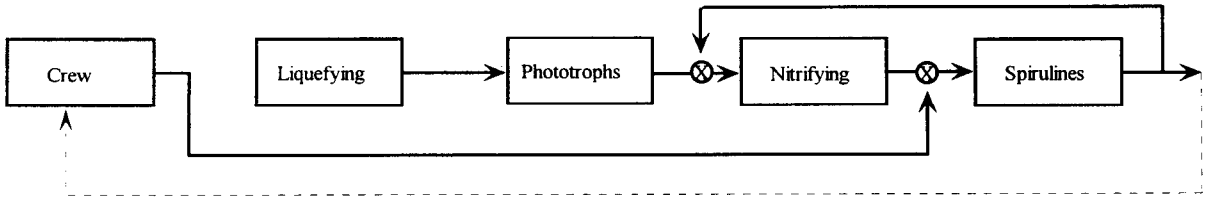
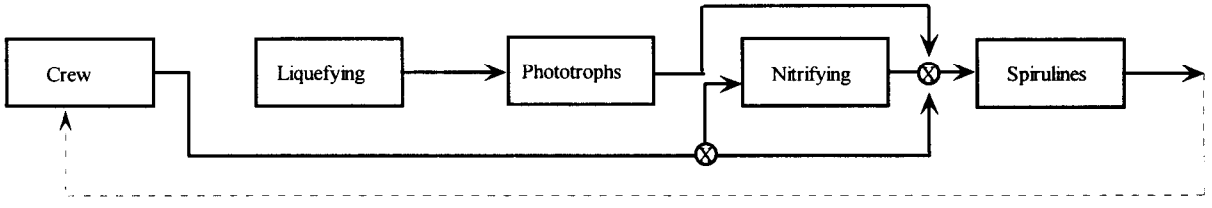


Figure 5: Schematic representation of the photobioreactor for compartment IV

The reactor operates in autotrophic continuous conditions. The liquid input comes normally from the nitrifying compartment, providing the culture with mineral sources (NO_3^- , S compounds and P compounds).
For the gas phase, the scheme established in the first study of the complete loop control (TN 28.3) illustrates that the link with the other compartments can be complex:



This representation is that used in ProSim simulations. The links between the nitrifying and the photosynthetic compartments can be modified and other configurations can be adopted. So, the nitrifying compartment can also be fed by the crew atmosphere:



Hydrodynamic equations

$$V_L \cdot \frac{dC_{Si}\big|_L}{dt} = F.C_{Si}^{in}\big|_L - F.C_{Si}\big|_L + V_L.\phi_{Si}\big|_{GL} + V_L.\phi_{Si}\big|_{Reac}$$

$$V_G \cdot \frac{dC_{Si}\big|_G}{dt} = G.C_{Si}^{in}\big|_G - G.C_{Si}\big|_G - V_L.\phi_{Si}\big|_{GL}$$

I.6 Compartment V - Crew

Description of the process

The crew modelling is one critical point in the modelling of a complete and a closed MELiSSA loop, as the wastes produced are substrates for all MELiSSA compartments. Moreover, as the activity (i.e. the outputs) of the crew is variable among several days, a realistic dynamic model representative of these variations is required in order to determine the ability of the loop to adapt its behaviour to these variations.

In ProSim simulations, the crew was modelled:

- by a variable stoichiometric equation (function of the food quality consumed).
- by assuming a mean constant flow rate for the consumption of food and the production of waste (faeces; urea; CO2; water), based on a mean activity calculated for one day (figure 7a).
- by assuming no accumulation (no mass variation) in the compartment.

Of course, faeces, urea or water are not continuously produced, and if CO_2 is continuously produced, its production depend on the activity of the crew (peak of CO_2). If the mass balanced model developed for ProSim simulation of the loop can be conserved, the feeding periods of the crew, the profile for CO_2 production and waste production are not defined (figure 7b).

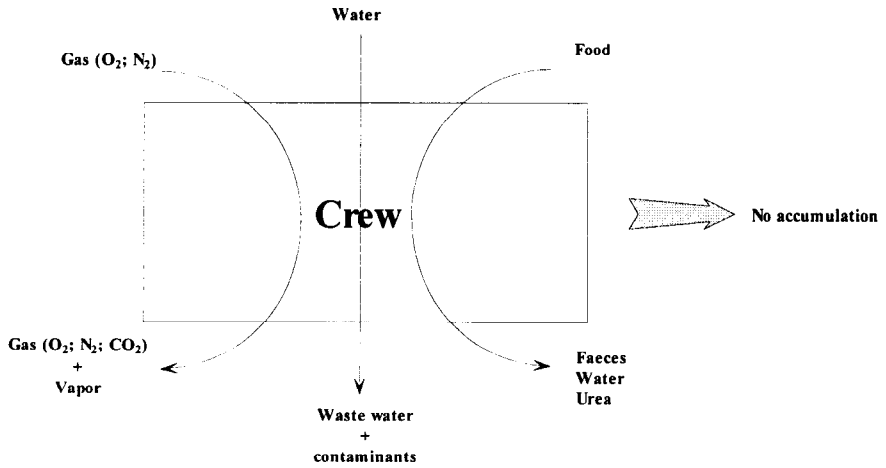


Figure 7a: Schematic representation of the crew compartment assuming an average continuous feeding of the compartment (ProSim representation).

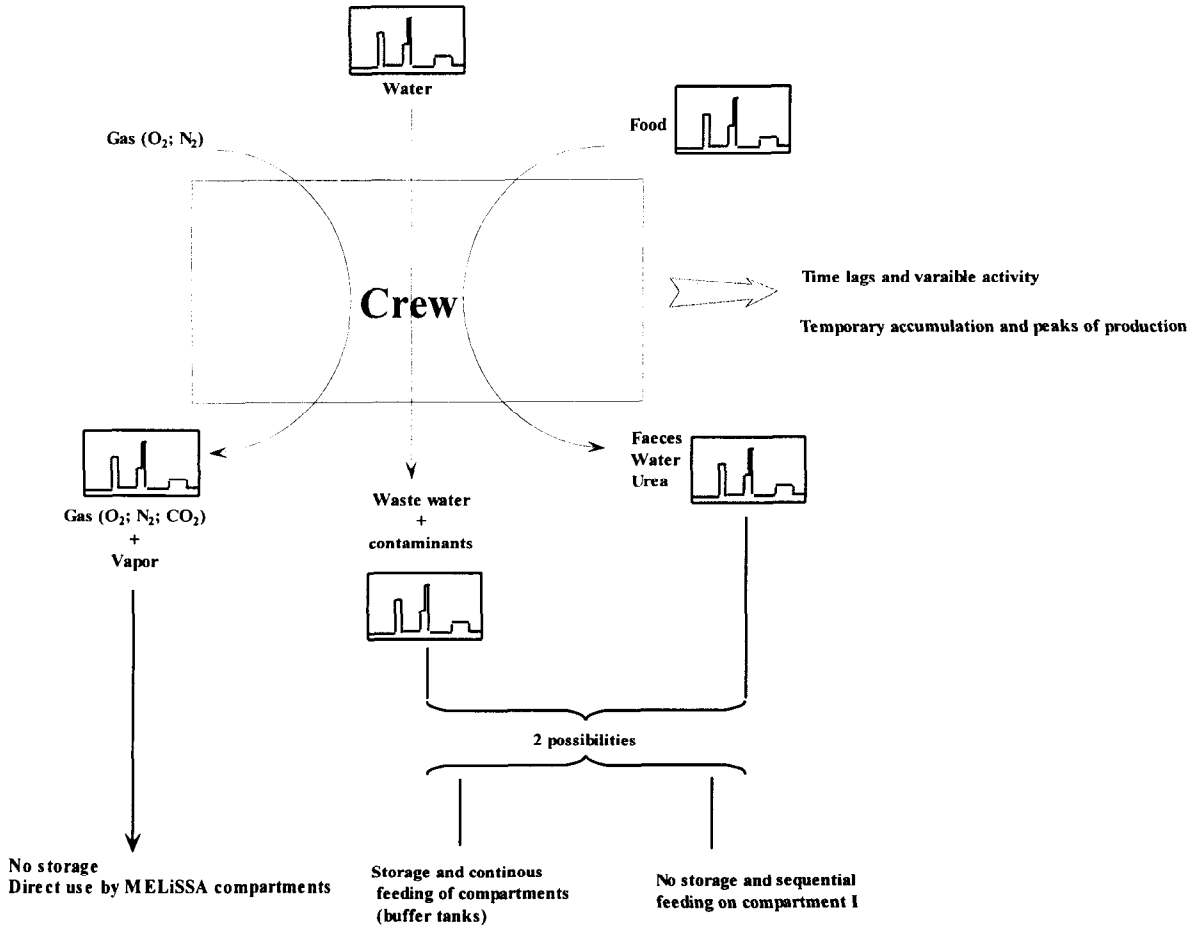


Figure 7b: Schematic representation of the dynamic of the crew compartment .

Mass balanced model

The mass balanced model developed is an average represention of the crew activity. It can be used in a first attempt to estimate the quantity of waste that the loop must treat.
The model is based upon a variable stoichiometric equation:

$$[CHONSP]_{food} + O_2$$
$$\Downarrow$$
$$[CHONSP]_{faeces} + CO_2 + H_2O + H_2SO_4 + H_3PO_4 + NH_3 + VFA + Urea$$

For the calculation of the 9 stoichiometric coefficients, the following assumptions were made:

- the fraction of proteins in faeces is fixed as well as their elemental composition
- the fraction of lipids in faeces is fixed as well as their elemental composition
- the quantity of ammonia produced is fixed
- the fraction of carbohydrate in the faeces is calculated taking into account the non digestible part from plants (fibres) (figure 7c)
- the oxygen consumption is calculated from the available energy given by the food (TN17.3).

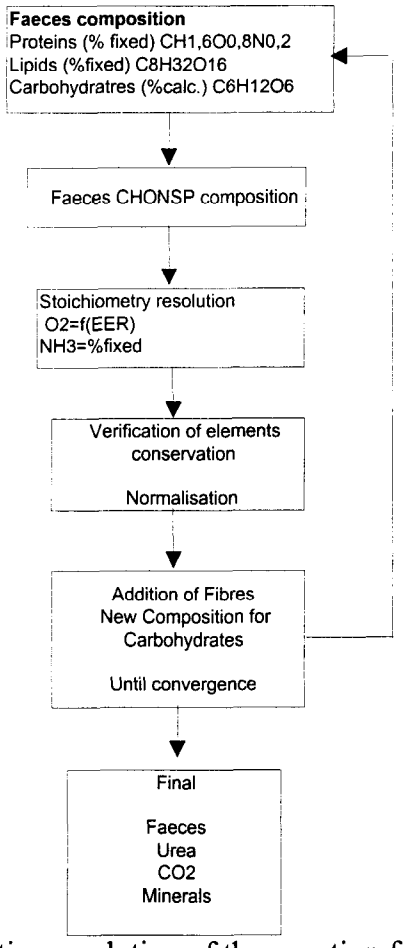


Figure 7c: Principle of the iterative resolution of the equation for the crew, taking into account the variable composition of the food into fibres (non digestible part of the food).

Dynamic modelling of the activity of the crew

At the present time a dynamic model for the crew has not been studied for the MELiSSA project. In the objective of a dynamic modelling of the whole loop, such a model will be required. Some models can probably be found in the literature as it exists models and software for the simulation of LSS (ECOSIM) and of the nutritional behaviour of crews (Perez et al., 1991; Eckart, 1994).

I.7 Compartment HPC

Description of the process

As for the crew, the HPC can not be considered as a "continuous" process" as it exists several phases (seeding, harvesting...) in the crop production. A first plant selection was made in TN 32.2 when a HPC was added to MELiSSA in mass balance simulation.
A more detailed analysis of higher plant cultivation in closed chambers and selection as a part of a Life Support System is reported by Cloutier and Dixon in TN 40.1 and 40.2.

Mass balanced model

The stoichiometric equations of each of the plant selected in a first approach (TN 32.2) are assumed to be composed of an edible (digestible + dietary fibre) and an inedible (waste) part. Considering the observations reported in TN 40.2, where plants grown in fields, and chambers are compared, some improvement for the plant composition could be made, but at the present time this update was not made. The stoichiometric equations reviewed here were established for ProSim simulation in TN 32.2.

The general form of the stoichiometric equations is:

$$CO_2 + NH_3 + HNO_3 + H_2SO_4 + H_2O$$

$$\Downarrow$$

$$O_2 + [CHONS]_{digestible} + [CHONS]_{fibre} + [CHONS]_{waste}$$

The elemental composition for the 3 parts of the 8 plants used, as well as the stoichiometric coefficients are reported in table 9.

Composition of the HPC

The description and the design of the HPC is a critical point. One composition of the HPC, based upon a menu adapted to several nutritional constraints for the crew was proposed inTN 32.2. Some improvement could be made accordingly to cultures constraints due to plants (Biomass Production Chamber, required production area, required maintenance, harvesting periods) in order to define an optimal compartment.

Table 5: Stoichiometric coefficients for the representation of the growth of the plants

	Digestible part						Fibre				CO2	H2O	NH3	HNO3	O2	H2SO4
	Coeff	C	H	O	N	S	Coeff	C	H	O						
Tomato	1	1	1,7928	0,8004	0,0546	0,0005	0,4040	1	1,6560	0,8280	-1,4040	-1,1799	-0,0232	-0,0313	1,4744	-0,0005
Rice	1	1	1,6650	0,7546	0,0257	0,0006	0,0335	1	1,6667	0,8333	-1,0335	-0,8360	-0,0109	-0,0147	1,0836	-0,0006
Lettuce	1	1	1,7107	0,4464	0,1348	0,0019	0,5016	1	1,6537	0,8268	-1,5016	-1,1435	-0,0019	-0,0774	1,7627	-0,0019
Potato	1	1	1,6492	0,7750	0,0335	0,0006	0,1413	1	1,6513	0,8257	-1,1413	-0,9097	-0,0142	-0,0192	1,1803	-0,0006
Soybean	1	1	1,6878	0,2952	0,1321	0,0035	0,2022	1	1,6000	0,8000	-1,2022	-0,8799	-0,0562	-0,0758	1,5344	-0,0035
Spinach	1	1	1,6406	0,2835	0,1870	0,0088	0,4215	1	1,6467	0,8233	-1,4215	-0,9855	-0,0796	-0,1074	1,7777	-0,0088
Onion	1	1	1,8113	0,7510	0,0742	0,0010	0,4183	1	1,6560	0,8280	-1,4183	-1,1823	-0,0316	-0,0426	1,5266	-0,0010
Wheat	1	1	1,6548	0,7215	0,0430	0,0012	0,1320	1	1,6667	0,8333	-1,1320	-0,8963	-0,0183	-0,0247	1,2039	-0,0012

	Waste						CO2	H2O	NH3	HNO3	O2	H2SO4
	Coeff	C	H	O	N	S						
Tomato	1	1	1,43	0,62	0,017	0,007	-1	-0,6923	-0,0072	-0,0098	1,0648	-0,0070
Rice	1	1	1,43	0,62	0,017	0,007	-1	-0,6923	-0,0072	-0,0098	1,0648	-0,0070
Lettuce	1	1	1,43	0,62	0,017	0,007	-1	-0,6923	-0,0072	-0,0098	1,0648	-0,0070
Potato	1	1	1,43	0,62	0,017	0,007	-1	-0,6923	-0,0072	-0,0098	1,0648	-0,0070
Soybean	1	1	1,43	0,62	0,017	0,007	-1	-0,6923	-0,0072	-0,0098	1,0648	-0,0070
Spinach	1	1	1,43	0,62	0,017	0,007	-1	-0,6923	-0,0072	-0,0098	1,0648	-0,0070
Onion	1	1	1,43	0,62	0,017	0,007	-1	-0,6923	-0,0072	-0,0098	1,0648	-0,0070
Wheat	1	1	1,43	0,62	0,017	0,007	-1	-0,6923	-0,0072	-0,0098	1,0648	-0,0070

Dynamic model for crop culture and growth

No dynamic models were currently developed in the MELiSSA project for the HPC compartment. Nevertheless it exists a lot of projects for using the higher plants as an element of a biological life support system. As an example, a dynamic model for lettuce has been developed for ECOSIM, and some other are available for wheat. The main points studied concern evapotranspiration and the influence of light and CO_2 concentration.
It must be kept in mind that plant cultivation is not a continuous process, as several periods can be distinguished: seeding-planting, growing, harvesting.

One important point for the integration of the HPC in the Biological Life Support System is the recycling of mineral elements of the system necessary to generate the nutrient solution (hydroponics growth) for the plants. For ProSim mass balance simulations this aspect was skipped and it was assumed that solutions coming from MELiSSA compartments and containing the elements required for the growth of plants can be directly used. A study of the element recycled (N ,K, Fe, Mo...) in a vegetable supplying system with a treatment of waste by wet oxidation was led by Akitoshi et al (1994). They conclude to the necessity of a mineral input of 2 kg/man per crop cycle (30-56 days).

I.8 Physico-chemical equilibria and transfer terms

In the models, several phases are considered (liquid, gas, biomass, solid) between which exist dynamic exchanges.
Gas-liquid equilibrium is important in processes where the liquid phase is the most important phase (biological reactor). In compartments such as the crew compartment or the HPC compartment, the equilibrium between liquid and gas is more difficult (impossible) to describe, as it doesn't exist a real liquid phase. In such cases, the exchanges with the gas phase are reduced to respiration, transpiration and evapotranspiration.

I.8.1 Perspiration and transpiration of the crew

One of the most "pure" water-containing products of life is condensate of crew respiration products derived from breathing and through the skin (perspiration). Atmospheric moisture condensate amounts to approximately 45% (1.1 - 1.7 kg water /man.day) of the total mass of water collected from the crew (Samsonov et al., 1991).

The quantity of water lost by respiration will equal:
Mass flow of air passing through the lungs x (Air leaving moisture - Air entering moisture)

This can be approximated by noting that the body losses 10% of its metabolic heat output (equivalent to the energy demand, EER) via respiration: $\frac{0.1\ .\ \text{EER (in kcal.day}^{-1})}{576\ (\text{kcal.kg}^{-1})}$
The evolution of EER as a function of the activity of the crew during a day can be found (Life Support and Habitability Manual), and then an estimation of water produced by breathing can be estimated using the previous relation.

The estimation of the amount of water produced by perspiration seems more difficult to determined. The minimum loss in a comfortable environment is 1kg per day. It must be noted that the water lost by respiration is approximately 0.5kg per day. At the present time no law was found in literature to describe the losses by perspiration.

I.8.2 Biological reactions and hydrodynamic equations

The term representing the exchanges between the biological phase and the liquid phase in the biological reactor is noted $\phi_{Si}^{n}\big|_{REAC}$.
Assuming no transfer limitation between the two phases leads to:

$$\phi_{Si}^{n}\big|_{REAC} = r_{Si} \text{ or } r_X$$

In the case of the nitrifying column, this assumption is not always justified (because of a possible transfer limitation in the fixed biofilm) (TN 32.1).

I.8.3 Ionic forms and pH equilibrium

pH and ionic forms of a compound are an important element, as well in mass balance model as in the dynamic model. In the mass balance model, the pH equilibrium was introduced for the gas-liquid equilibrium by modifying the partition coefficients of the compounds concerned.

In dynamic models it seems more realistic to directly consider in the different reactions involved in a process, both the ionic and the non ionic forms. This requires:

1- to define the acid-base equilibrium constant for each compound, and then calculate the partition of a compounds in each of its ionic/non ionic forms
2- to translate the stoichiometric equations in a ionic form (i.e., the carbon dioxide is not assimilated as CO_2 but as HCO_3^-). This can be made by replacing:

CO_2: $HCO_3^- + H^+ \longrightarrow H_2O$ or $HCO_3^- \longrightarrow OH^-$

H_2SO_4: $SO_4^{2-} + 2H^+ \longrightarrow .$

H_3PO_4: $HPO_4^{2-} + 2H^+ \longrightarrow .$

It must be noticed that usually the pH of a reactor is maintained by the addition of an acid or of a base. The volume quantities added of base and acid used to maintain the pH are rarely included in dynamic models as the volumes added are generally low.
In a first study for the complete loop (TN 28.3) the control of volume of reactors was taken into account. For a closed system the additions for pH control may perhaps play a role in the control of volumes. Another point is that these additions can constitute a non negligible mass addition to the system. These aspects were pourly studied as there is no estimation of the requirements for maintaining the pH of the reactors.

I.8.4 Gas-liquid mass transfer

The gas liquid equilibrium is an important aspect to take into account in dynamic modelling of bioreactors.
In ProSim mass balance simulations, only thermodynamic equilibrium is taken into account, what is equivalent to assume an infinite K_La value. It must be noted that if a cooler is added to the gas output, water is condensed and return to the reactor. A cooler is an apparatus that must be added to the reactor model described previously.
For most of the compounds in the MELiSSA loop, the partition coefficients have been already determined in TN 23.1. These coefficients are characteristic of the thermodynamic equilibrium of each compound. The dynamic of the transfer from the gaseous compounds to the liquid phase can be expressed by:

$$\phi_{Si}^n\big|_{GL} = K_L a\big|_{Si} \cdot (C_{Si}^{*n}\big|_L - C_{Si}^n\big|_L)$$

On a numerical point of view, the gas-liquid transfer dynamic can be a limiting step in the numerical treatment of the biological models. The simplification of models, based on Laplace transformed equations, developed by Leclercq (TN 35.2) could be a useful way to skip such problems.

I.9 Other unit operations to consider (pre and post treatments)

All the previous models reviewed concerned the "core" of the processes involved, i.e. the biologically active part of the compartments.

It could be necessary in a dynamic model of the loop to include other operations such as external entries, cooling, separations, physico-chemical treatments of fluxes and lag between compartments. An example of possible operations to take into account is presented in figure 8.

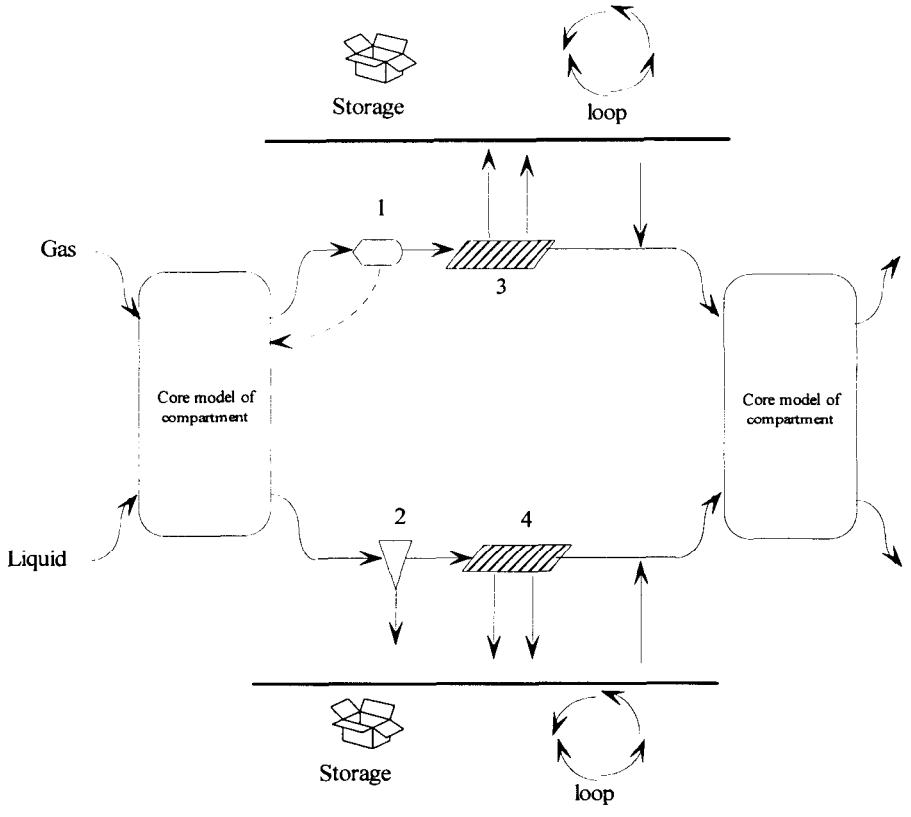


Figure 8: Operation between two biological reactors. 1: cooler; 2: harvesting; 3-4 separations/filtrations. Outputs and inputs fluxes are from other part of the loop or from stocking area.

II Loop description, constraints, time constants and sizing of the system

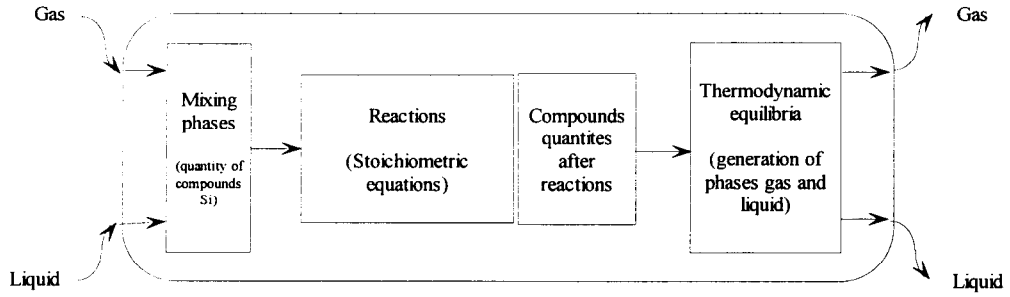
A first structure for the loop was established with Fulget in TN 28.3. In this first complete loop study for control, a loop structure and a compartment structure were defined, as well as the manipulated and the controlled variable on each compartment. It must be noted that operation between compartment for gas and liquid (figure 8) were not included in this first study (excepted harvesting of biomass).

This section will study the global design of the loop, the design of compartments and the links between compartment. A procedure for the building of the dynamic model for the loop is also proposed.

II.1 Loop and compartments design for dynamic modelling

II.1.1 Compartments design

In mass balance modelling (ProSim simulation), the modelling of compartment (i.e. the core model of figure 8) is described by the following scheme:



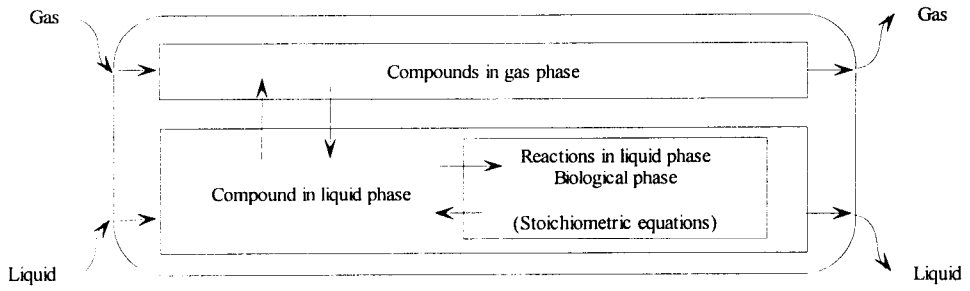
It is important to notes that in the models reviewed in section I:

- volumes were assumed to be constant in the dynamic models previously described (the assumption can be discussed), what leads to a simplified system of equation. In the first global loop dynamic modelling of ADERSA (TN28.3) the modelling of the compartments was the same, excepted that the volume variations of the reactor was taken into account. In such a case, the global expression of the dynamic equations take the form:

$$\begin{cases} \dfrac{d(V.C_{Si})}{dt} = F_{in}.C_{Si}^{in} - F_{out}.C_{Si} + V.\phi_{Si} \\ \dfrac{dV}{dt} = F_{in} - F_{out} \end{cases}$$

- dynamic transfer between gas and liquid phases is considered in the reviewed equations, what is not the case in the first global dynamic model (as in ProSim simulations), where only thermodynamic equilibrium is considered. It must be outlined that taking into account mass transfer dynamics can slighty increase the computationnal requirements.

This last remark leads to consider the model (core model) as slightly different from the previous one:



II.1.2 Open/closed loop design

A structure for the loop including 3 step level of control was established in TN 28.3. The structure for the modelling of MELiSSA+HPC, presented in TN 32.3, is a more complex description including treatment operations on fluxes (as gas divider) and a more complete definition for the crew and the constraints associated to it. The complete flowsheet of the loop including gas, water and food management units is given in figure 9. This figure shows that a lot of operations have been introduced between the compartments for the distribution inside the loop of gas, liquid and biomass fluxes.

One of the lessons learned from the loop design and the mass balance calculations was that it is easier to make first an uncoupled open representation of the loop, then progressively to link compartments together, then to check if they can work properly and at the end to close the loop with specific constraints.

The dynamic modelling of the Nitrifying-Photosynthetic compartments system seems to be an interesting preliminary study for the dynamic modelling of the complete loop.

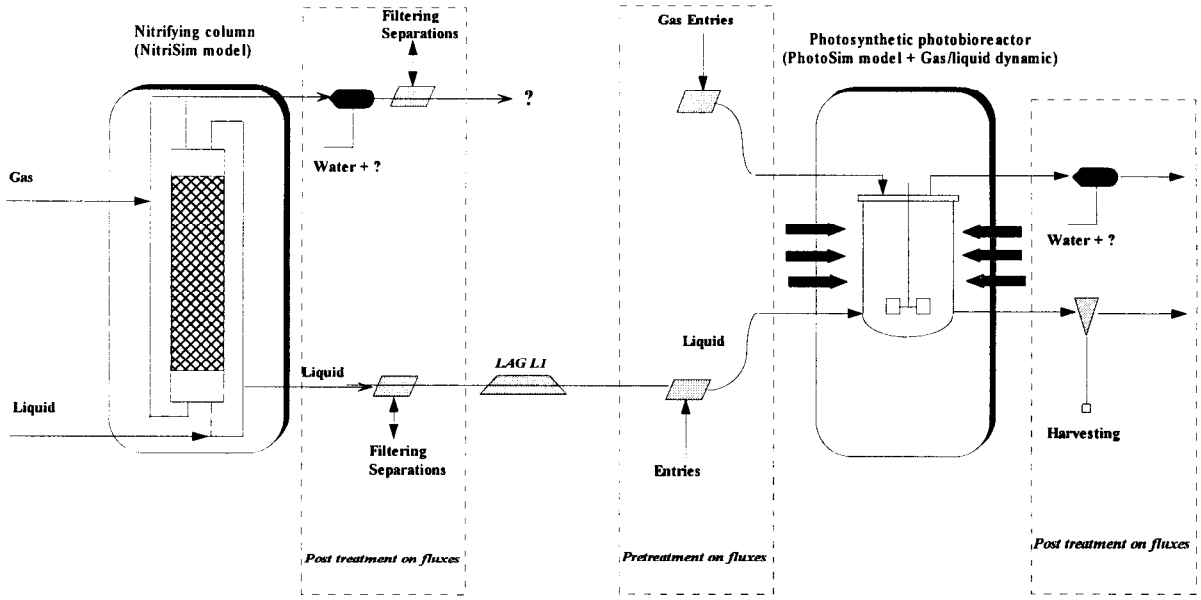


Figure 10: Nitrifying + Photosynthetic reactor - linking for dynamic modelling. In this representation there is no links between gas fluxes for the compartment. This point remains to be discussed.

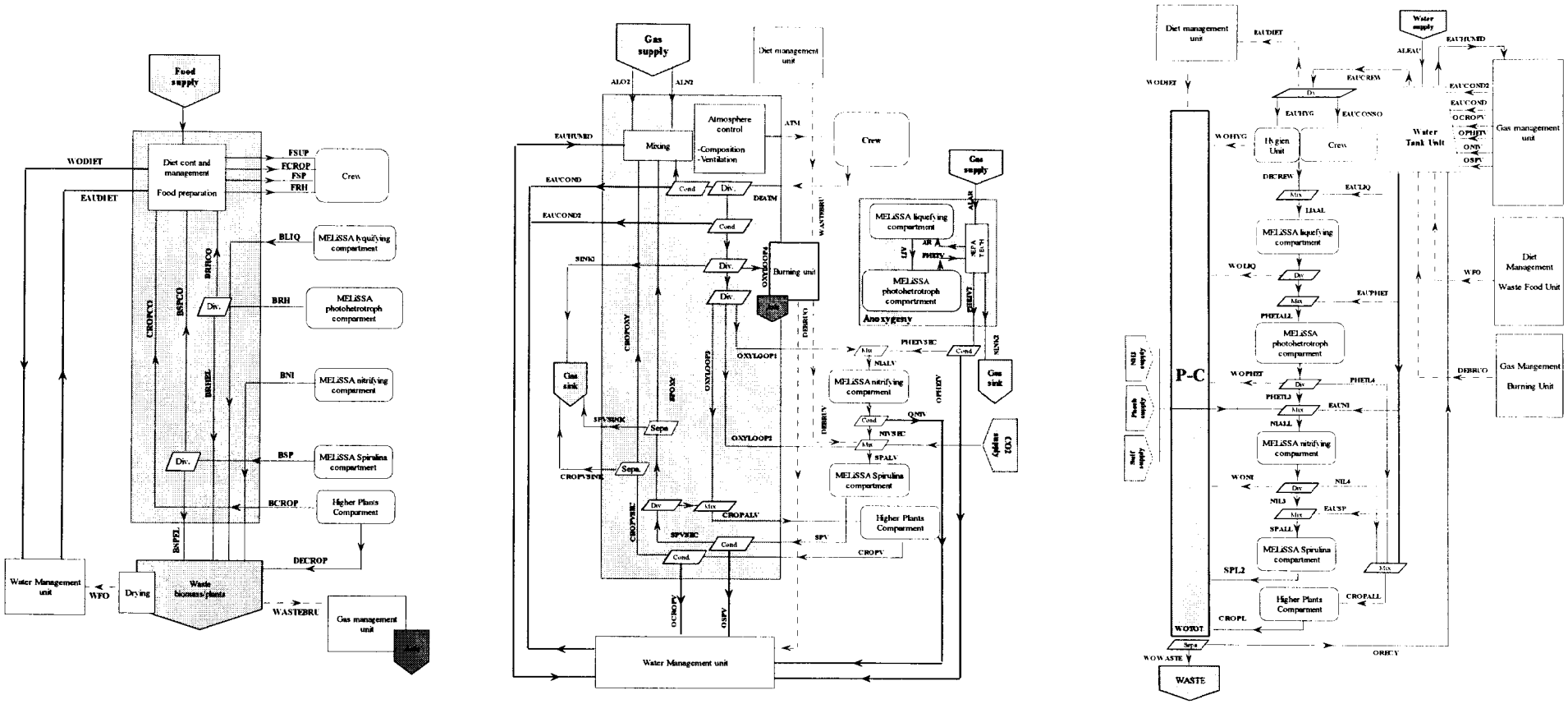


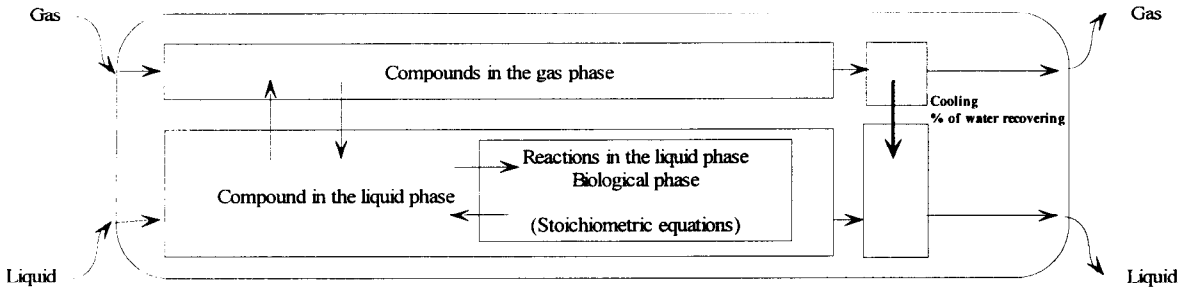
Figure 10: Overview of the detailed flow-sheet of the MELiSSA+HPC loop.

For reliability, the system is divided into biomass fluxes, gas fluxes and liquid fluxes. Cond;: condenser (cooler); Sepa.:separator; Div.: fluxes divider.; Mix.:mixing.

The models for the core of the compartments were reviewed in section I. It must be outlined that at the present time the PhotoSim model doesn't include the gas-liquid transfer hydrodynamic. Between the reactors several operations must be considered:

- Post operations on output fluxes from the bioreactors: cooler on gas output, biomass harvesting on liquid output, and filtering, separation/division of the fluxes.
- Pre operations on inputs to the bioreactors: mainly addition of other fluxes to create a required input on the reactor.

On a practical point of view it seems better to introduce the gas cooler directly in the core model of the reactor. This will avoid to introduce a backward flux from the gas output to the bioreactor. The scheme for the reactor modelling became then:



The cooling can be included in the dynamic model of the reactor by recalculating the output compositions of gas and liquid considering a recovering efficiencies of the cooler (i.e. the quantity of water condensed). The maximum gas fraction of water (saturation) is about 3%. Then fraction of the other compounds in gas is only slightly modified. For compounds in liquid phase no recalculation of the composition of the phase is needed in principle as the volume effect of vaporised water can be neglected in a first approximation.

The biomass harvesting is an important aspect of post treatment for the photoheterotrophic and the photosynthetic compartments. Several biomass harvester for the Spirulina compartment were studied by Vernerey et al. (TN 37.30). Even if some aspects as the effects EPS or PHB content of the biomass are still to be investigated, a biomass harvester based on the succession of two separation units (a disk stack centrifuge and a tangential filtration) was selected as the more efficient continuous system. The global system characteristics (water yield: 75-80%; solid yield >95%; Separation efficiency > 95%) can be used as the parameters for the definition of a "black-box" model of a biomass harvester both in the ProSim based model and in a dynamic model for the loop. If a dynamic model for the biomass harvester exists, it is yet not established, and in a first approximation a time lag is probably sufficient.

In figure 9, it can be remarked that as it is attempted to have only few biomass in liquid output of the nitrifying column, a simple filtering unit is considered to remove free biomass and other solids (dead biomass?). The biomass recovered at this point is not recycled in the loop as an edible biomass and can be treated as an organic waste.

The other post operation that can be introduced concerned the division of fluxes (for example a part of the nitrate is used for the HPC, what required to divide the liquid output of the

nitrifying into one input for Spirulina and one input for HPC). It not yet necessary to consider such problem in the preliminary link of Nitrifying and photosynthetic compartment.

Pre-operations on a compartment would be mainly mixing operations of gas and liquid from storage (lacks of compounds) or from other part of the loop. For the photosynthetic compartment it is probable that the flow rates (both gas and liquid) coming from the nitrifying compartment will be lower than those used as input on the Spirulina compartment.

In dynamic modelling of the system, the lag between output of a compartment to the input to the other one must be taken into account. The lag can be estimated assuming a plug flow inside tubes linking the compartments (cf. II.2).

II.1.3 Constraints and variables for the compartments and the whole loop

In mass balance loop modelling

In mass balance simulations the main constraints applied on the system concerned (TN 32.3):

- the crew (nutritional constraints, habitability constraints).
- the gas fluxes, which are set up in order to avoid the drying of reactor by the way of gas/liquid thermodynamic equilibrium.

Some variables are fixed (such as the conversion efficiency of a key element in each compartment), some are used as parameter to modify the loop behaviour and recycling efficiencies (rate of recycled biomass called Y and Z, quantity of wastes oxidised, light on photobioreactors, presence of an HPC), and some other are controlled in order to close the loop and to minimise the entries (entry of ammonia and minerals, entry of food and water).

Variables of compartments and of the loop

For the global loop control strategy (TN 28.3) a review of the manipulated and of the controlled variables for the compartments was established (table 10). It must be noted that for this firts global loop analysis, the addition of processes between compartments were not considered. If pre or post operations are required for the compartment, the manipulated and the controlled variables listed in table 10 could be modified.

Liquefying compartment		Rhodobacter compartment		Nitrifying compartment		Spirulina compartment	
MV	CV	MV	CV	MV	CV	MV	CV
exogen water flow	volume	exogen water flow	volume	exogen water flow	volume	exogen water flow	volume
output flow	dilution rate	output flow	dilution rate	output flow	dilution rate	output flow	dilution rate
	acetate/CO2	light power	VFA/Urea	exogen O2 flow	pO2	light power	dissolved CO2
	NH3		biomass	total gas flow	Nitrate	Incoming CO2 flow	biomass

Table 10: Manipulated variables (MV) and Controlled variables (CV) for compartments of MELiSSA. (Global loop control strategy - TN 28.3).

Classification of variables into manipulated, controlled or frozen classes is important for the control of the loop. Such distinctions are not made in dynamics models of compartments. Nevertheless it can be noted that some variables were frozen in actually developed models. They are:

- the volumes. In the hydrodynamic expression presented in section I, volumes are implicitly considered as constant in bioreactors. It is assumed that volume variations (mainly from water vaporisation) are sufficiently low to be neglected. If this assumption is not used, the hydrodynamic model must be modified in order to take in account the volume variations as described in section II.1.1.
- the physical parameters, pH and temperature, are assumed to be controlled and set to a constant value. It must be noted that for pH the volume addition of base or acid is neglected.

The conversion efficiency that is fixed in mass balance model is dependant on the biological reactions rate and of the dynamic of the reactors in the dynamical models. This frozen variable of the mass balance model is "free" in the dynamical model.

One important point for the dynamic modelling of the loop is the definition of sizes (volume, surfaces) and the setting points values for flow rates. The two aspects are closely linked as the mean residence time inside reactors is an important characteristic of their working efficiency. An estimation for the volume and the surface of the MELiSSA compartment was made from the results obtained with mass balance simulations, assuming a mean conversion rate for each compartment (table 11). But it is important to notice that the flow rate in such a simulation was not adapted to the hydrodynamic characteristics of the compartments (i.e. mean residences time are not always respected).

Compartment	Yield used for calculation	Volume or surface of compartment
Liquefying	Organic load: 4g dry/l.day **	30 l
Photoautotrophic	Production: 2880 dry g/m^3.day	26 l
Nitrifying	Ammonia load: 1.6 kg/m^3.day	6 l
Photosynthetic	Production: 1440 dry g/m^3.day	55 l
HPC	Yield (in g dry edible/m^2.day)	33 m^2
Tomato	18	
Rice	4	
Lettuce	6	
Potato	33	
Soybean	15	
Spinach	21	
Onion	22.5	
Wheat	33	

Table 11: Estimation of the dimension for MELiSSA compartment for 1 person (design of the loop described in TN 32.3).
** For this value for the liquefying compartment, it is assumed that the degradation efficiency is 100%. It must also be noted that for the calculation of the volume, the urea is assimilated to OM.

II.1.4 Conclusion - Main points to keep in mind

As for the mass balance simulations, the building of the flow-sheet (i.e. links between compartments) is a complex problem and it is strongly recommended to act step by step by linking compartments one after one. The first step will be to build a dynamic model for the system including the Nitrifying compartment and the photosynthetic compartment. This will be also the first step of the physical construction of the loop.
A structure for the representation of each bioreactor was proposed, in accordance to the dynamic models developed in section I.
Between each compartment, several operations must be taken into account, which can be probably represented by a black box with an efficiency factor (for separation or harvesting process) and a time lag (cf II.2). The detailed flow-sheet of the loop established for the mass balance simulations (figure 9) can be a tool to determine what kind of operations are required between compartments.

The variables for the control of the compartments have been already defined (table 11). Nevertheless it must outlined that the present dynamical models (section I) are established assuming no volume variations. For the processes themselves, pH and temperature are frozen. The constraints and the manipulated variables used in mass balance simulations would be probably conserved in the dynamic model of the complete loop, as the structure previously established (figure 9) can be used as a basis for the dynamic modelling.

The last point for the dynamic modelling will be the sizing of each compartment, as well as the definition of the ranging values for their input/output flow rates in order to maintain their optimal performances.

II.2 Estimating the time constants

This section will provide relations for the calculation of time constants in bioreactor (compartment), between compartments and in the loop.

II.2.1 Time constants: in a compartment

The characteristic time constants taking place in a bioreactor are reported in table 12. For the crew and the HPC compartments, other time constants must be considered such as:

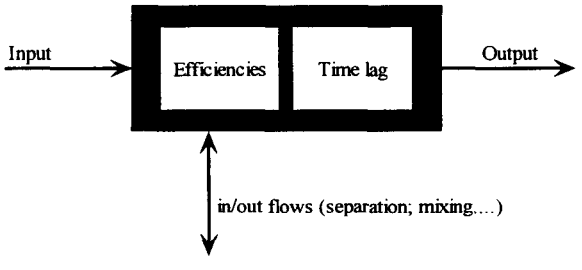
- the cyclic activity of the crew
- the culture periods of the plants (planting, seeding, harvesting)
- the photoperiods for the plants

Process	time constant	
Gas-liquid mass transfer	$t_{kla} = \frac{1}{K_L a}$	
Mean liquid residence time	$t_L = \frac{V_L}{F_{in}}$	
Mean gas residence time	$t_G = \frac{V_G}{G_{in}}$	
Substrate consumption	$t_{Si} = \frac{C_{Si}^{in}}{r_{Si}^{max}}$	
Biomass growth	$t_X = \frac{1}{\mu_{max}}$	h: heat transfer coefficient A:exchange area
Heat transfer	$t_{HT} = \frac{V\rho Cp}{hA}$	Cp: specific heat $\Delta T_{cooling}$: temperature variation for cooling
Heat production	$t_{HP} = \frac{\rho Cp \Delta T_{cooling}}{r_{Hm} + r_{HS}}$	ρ: density r_{HM}; r_{HS} heat production rates

Table 12: time constants for different processes taking place in a bioreactor. (Reuss and Bajpai, 1991)

II.2.2 Time constants between compartments

The most simple way to represent intermediate operations between compartments is to use a "black box" model which is characterised by an efficiency factor (for separation/harvesting process for example) and a mean time lag relative to the process:



The lag due to the flow through tubes between compartments can be estimated considering a plug flow behaviour by:

$$t_{lag} = \frac{\text{length of the tube}}{\text{mean velocity of the fluid}}$$

II.2.3 Residence time for the loop

The calculation of time constants for the whole loop is simple for single processes or if the loop is open.

For the open loop, the mean residence time of fluids (gas, liquid) and elements (C,H,O,N,S,P) in the whole system can be estimated by the sum of mean residence time on each compartment and the time lags between compartments.

It is more complicated for the closed loop. For liquid and gas, using an inert compound as tracer in the dynamic model will allow to determine mean residence times (as it is usually done to model RTD in bioreactors).
The calculation of a residence time for elements in the closed loop ($t_{Closed\ RT\text{-}Element}$) can be estimated considering the residence time (from the crew to the HPC and photosynthetic compartment) in the open loop ($t_{Open\ RT\text{-}Element}$) and the recycling efficiency ($Recy\%_{Element}$) of the loop for the element:

$$t_{ClosedRT-Element} = \frac{t_{OpenRT-Element}}{100 - Recy\%_{Element}}$$

It can be noted that the cyclic behaviour of the crew and of the HPC could perhaps induce a cyclic behaviour for the whole loop.

II.3 Some calculations for the couplig of Nitrifying and Photosynthetic compartments

As can be seen in table 11, volumes estimated on the basis of ProSim calculation for the MELiSSA+HPC loop are closed to the volume of the actual pilot reactors developped at UAB Laboratory:

- 6 liters for the nitrifying column (8 liters for the pilot)
- 55 liters for the photobioreactor (70 liters for the pilot)

For the nitrifying column, this volume is calculated for a load of 1.6 kg/m^3.day, in order to produce about 0.63 mol/day of nitrate. It must be noted that only 60% of this production is used in for the photosynthtic reactor (the other 40% are used to feed the HPC).

For the *Spirulina* compartment the volume is calculated assuming a production yield of 1440 dry g/m^3.day, in order to produce about 79 g of dry biomass/day. (biomass composed of EPS+active biomass)

Some characterisitcs for the coupling of the two last MELiSSA compartments are reported in table 13, according to key values (NH_3 oxydation and biomass production) calculated for steady state simulations of the MELiSSA+HPC system.

The values presented in table 13 for the physical characteristics of the reactors are taken from the description of experiments that were performed with these reactors in the past. In a proposed scheme for the coupling of compartment III and compartment IV (figure 10), liquid

output of the nitrifying compartment is linked to the liquid input of the photosynthetic compartment. It will be then better to configure the system in order to use for the two reactors liquid flow rates of the same order of magnitude (i.e. to increase the flow rate of the nitrifying reactor and/or to decrease the liquid flow rate of the photosynthetic reactor). The models NitriSim and PhotoSim can help to determine what kind of fluxes would be the best for the system.

Nitrifying column		**Photosynthetic reactor**	
	Physical characteristics		
K_La (for O2)	51 h^{-1}	K_La	300 h-1
Input Gas	1.8 l/h	Input Gas	3000 l/h
Recirculated Gas	178.2 l/h		
Input/output Liquid	0.168 l/h	Input/output Liquid	1.5 l/h
Recirculated Liquid	1.1 l/h		
Liquid Volume	3.9 l	Liquid Volume	56 l (80% of total)
Total Volume	8.1 l	Total Volume	70 l
		Illuminated liquid volume	-

	Requirement (from ProSim simulations)		
Production required	0.63 mol Nitrate/day	Production required	79 g dry biomass/day

	Calculated characteristics		
NH3 input required	0.15 mol NH_3/l	Biomass	
NH3 load required	1.07 kg NH_3/m^3.day	concentration required	2.2 g dry biomass/l

	Time constants		
Gas/Liquid mass transfer	0.02 h	Gas/Liquid mass transfer	0.0033 h
Mean Liquid RTD	23.2 h	Mean Liquid RTD	37.3 h
Mean Gas RTD	2.3 h	Mean Gas RTD	0.005 h
Biomass growth (Ns)	17.5 h	Biomass growth	
Biomass growth (Nb)	27.7 h	(without EPS)	2.2 h

Table 13: Some characteristic of the couple Nitrifying compartment-Photosynthetic compartment.

In principle it is possible to apply the calculated NH_3 load on the current nitrifying pilot column. It is also possible to have a biomass concentration of 2.2 g/l and a productivity of 1440 g/m^3.day for the photobioreactor.

We must notice that the other requirements on each reactor (O_2, CO_2, mineral feeding) must also be checked.

Conclusion

The current state of the art of a dynamic model for the MELiSSA system was presented. The main next step in the study of the model will be:

- for the liquefying compartment, the development and the validation of a model for the compartment , accordingly to the last experiments in continuous conditions.
- for the photoheterotrophic compartment, the completion of the actual light limiting model for the growth of *Rs. rubrum* with the use of different carbon substrates.
- for the nitrifying compartment, the validation of the model which is under study. It msut be also be established a model taking int account the mixotrophic nitrification (nitrification in presence of organic matter), with the remaining organic products of the previous photoheterotrophic compartment. The organic acids that seems the less degraded by the photoheterotrophic compartment seem to be C5 and C6 acids.
- for the crew and the HPC; only stoichiometric equations are available. They are only a mean representation of the periodic and cyclic dynamic behavior of the compartment. A more complete dynamic model must be developed for this compartment in order to perform a dynamic simulation of the whole loop.

The models developed represent the core of the compartments. The integration of a compartment (bioreactor) in the loop is associated to other operations on fluxes (harvesting, mixing, filtering) which must be identified and taken into account. The previous experience acquired with the development of the loop design for mass balance simulation can help to defined interrelations between the MELiSSA compartments. It is better to work step by step by linking compartment one after one until to obtain an open loop and then only to close the loop.

The first step is the coupling of the nitrifying and of the photosynthetic compartments. It is then important to prepare this coupling by coupling their respectives dynamic models (NitriSim and PhotoSim).

One of the key point for dynamic simulation will be the determination of coherent flow rate for the fluxes and of adapted dimension for the compartments in order to have optimal efficiencies for the reactor and to have a loop able to maintain habitability constraints

The time constants can be sorted into 3 classes: for the processes themselves, between the compartments and for the whole loop. As they are mainly function of the flow rates this constants can not be calculated yet.

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