

# ADERSA

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## MELISSA

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## TECHNICAL NOTE : 54.4

Overall strategy for the interfacing of the HPC  
to the MELISSA loop  
Phase II : closing the loop with HPC

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Draft

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<b>ESA-ESTEC</b>	<b>MELISSA - Technical Note 54.4</b> <b>Overall strategy for the interfacing of the HPC to the MELISSA loop – Phase II</b>		October 2001
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Abbreviations or notations:

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AcOH : Acetic acid  
 CH : chlorophyll  
 CO<sub>2</sub> : carbon dioxide (gaseous or solvated)  
 EPS : exopolysaccharide  
 HPC : Higher Plant Chamber  
 NH<sub>3</sub> : ammonia (gaseous or solvated)  
 NO<sub>2</sub> : nitrite ion  
 NO<sub>3</sub> : nitrate ion  
 N<sub>s</sub> : Nitrosomonas  
 N<sub>b</sub> : Nitrobacter  
 PC : phycocyanin  
 XA : Spirulina active biomass  
 XV : Spirulina vegetative biomass

Note :

In a figure, a graph ij is located by its row i and its column j.

The fundamental MELISSA loop is composed of the Consumer, Liquefying, Rhodobacter, Nitrifying and Spirulina compartments.

The extended loop is the fundamental one completed with the HPC.

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# 1. INTRODUCTION

During the meetings at Toulouse (July 2000) and Guelph (May 2001), it has been decided to close the MELISSA loop in order to demonstrate that it was able to furnish oxygen to a team of a few rats and to produce food from human wastes that are introduced into the liquefying compartment. This food will have two main origin : the Spirulina (and perhaps the Rhodobacter) and the edible part of the plants coming from the HPC.

In the previous Technical Note on the subject, TN 54.3, the study has been done on the fundamental loop composed of the Liquefying, Rhodobacter, Nitrifying and Spirulina compartments (compartments 1 to 4A) only, without HPC. It showed then that, on the one hand, the closing of the gas loop is possible without addition of any compound, and on the other hand, the closing of the liquid loop is also possible under the condition of adding NO<sub>3</sub> (1 molar % of NH<sub>3</sub> produced by Liquefying).

In the present study, the HPC, which is assumed to produce 20 % of the diet of 1 man, is interfaced to the fundamental loop.

As in TN 54.3, the proposed strategy is validated on a simulator which is as complete as possible at the moment and whose limitations are listed hereafter. The study, whose results strongly depend on the present models, shows that the closing of the gas and water loops are possible under conditions. It must be considered as a first attempt to quantify the problem.

## 2. DESCRIPTION OF THE SIMULATOR

### 2.1. Limitations

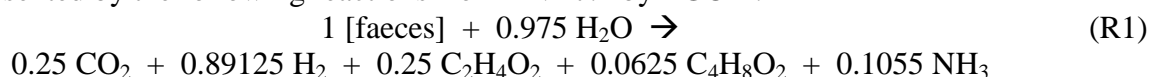
Due to different degree of achievement in the modelling of the compartments, the simulator is composed of both static and dynamic models : the Consumer and Liquefying are static and the other (Rhodobacter, Nitrifying and Spirulina) are dynamic and they are used in steady state. The HPC is a peculiar case : the chemical reactions have an average constant rate (the state of development of the plants is skipped) but the interactions between the gas and liquid phases are dynamic.

1\_ The Consumer compartment, which is considered from the gaseous aspect only, is simply represented by a consumption rate of O<sub>2</sub> and a production rate of CO<sub>2</sub>. In the examples given hereafter, these data are (according to TN 47.3 by UAB) :

- O<sub>2</sub> consumption = 4.45 10<sup>-2</sup> mol/h/rat;
- CO<sub>2</sub> production = 4 10<sup>-2</sup> mol/h/rat.

So the consumer compartment is a source of carbon and a sink of oxygen.

2\_ The degradation of faeces and urea that occurs in the Liquefying compartment is total and represented by the following reactions from TN 17.1 by LGCB :



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As the wastes do not contain sulphate nor phosphate, these substrates are added at the input of the Liquefying compartment.

3\_ The Rhodobacter compartment is simulated according to the latest version of the first principles model of TN 45.1 by LGCB : the only source of carbon is the acetic acid. In order to fit this constraint, all the butyric acid produced by the present Liquefying is transformed into acetic acid according to the following global balanced chemical equation :



The oxygen requested by this equation is produced by Spirulina and HPC.

4\_ The model of the nitrifying column is limited to TN 27.1 and TN 27.2 by LGCB and does not take into account :

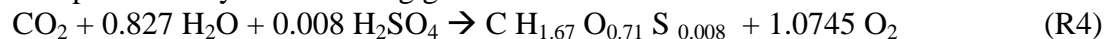
- the inhibitory effect of  $NO_2^-$  and  $NO_3^-$  on the Nitrobacter growth (introduced in TN 27.3);
- the biofilm diffusion model (introduced in TN 27.3) ;
- the metabolism and growth of Nitrosomonas and Nitrobacter in presence of organic matter (introduced in TN 32.1). The heterotrophic model is not necessary as the Rhodobacter is supposed to transform 99.5 % of the acetate (at least in the present simulation).

5\_ The Spirulina compartment is simulated according to the first principles model of TN 19.1 and 19.2 (Version 1, issues 0 and 1, January 1997) by LGCB. A Monod term for the phosphate

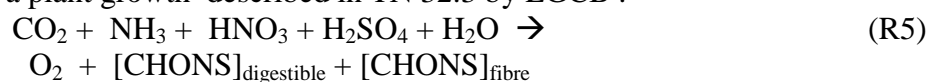
$\frac{C_p}{K_p + C_p}$  has been added in the production rates of the active biomass (XA), of the

phycocyanin (PC) and of the vegetative biomass (XV) in order to limit the kinetics when the phosphate concentration is going to zero (detail in TN 54.2 annex A3.1.2.).

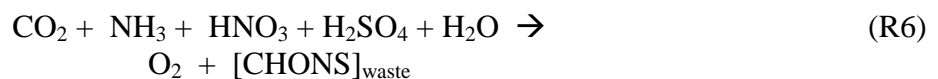
As an additional information to the TN 19.1 and 19.2, it is mentioned that the synthesis of glycogen is represented by the following global chemical reaction :



6\_ The Higher Plants Chamber (figure 1) is simulated according to the global, complete chemical equations of a plant growth described in TN 32.3 by LGCB :



and



whose stoichiometric coefficients are given in TN 32.3 table 15.

The HPC is supposed to produce the plants at a constant rate to fit the menu proposed in this TN. The growth rates of the plants are extracted from the table 17c and recalled hereafter :

Plants	Waste (dry g/day)	Edible (dry g/day)
Tomato	32.97	3.45
Rice	82.71	69.06
Lettuce	1.77	2.07
Potato	63.34	126.79

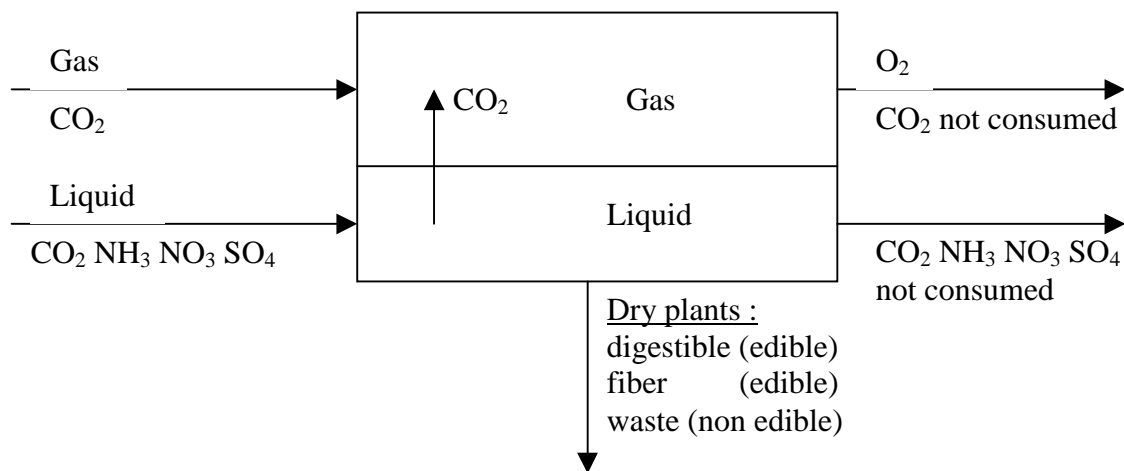
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Soybean	3.85	6.91
Spinach	10.88	6.91
Onion	10.90	6.91
Wheat	315.93	207.17
Total	522.35	429.27

**Table 1 : Growth rates of the plants of HPC for the diet of 1 man**

The simulated HPC can produce a variable ratio of the diet of 1 man. The HPC is simulated dynamically at steady state, taking into account

- the gas/liquid equilibria of O<sub>2</sub>, CO<sub>2</sub> and NH<sub>3</sub>,
- the dissociation of these compounds in the liquid phase,
- the pH and temperature.



**Figure 1 : Scheme of the Higher Plants Chamber**

## 2.2. Sizing of the compartments of the simulator

The Consumer and the Liquefying compartments, which are reduced to mere chemical reactions, have no volume.

The volume of the Rhodobacter compartment is fixed to its minimum (9 l) to allow the transformation of all the acetate produced by the wastes.

The size of the nitrifying column is reviewed in order to allow a good oxidation of ammonia into nitrate with a very low production of nitrite as it is explained in annex A4.2 of TN 54.2. Given the value of KLa in the simulator (51 h<sup>-1</sup>) the volume of the fixed bed is determined to 17.5 litres (the load is 0.3 gN/m<sup>3</sup>/day).

The volume of the Spirulina compartment is set to 77 litres, as it is in the pilot at UAB.

The volume of gas and liquid of the HPC are set arbitrarily to 40 m<sup>3</sup> and 100 litres, respectively.

## 2.3. Connections between compartments of the simulator

### 2.3.1. Gaseous circuit

Air is recirculating successively from the Consumer to the Nitrifying, the Spirulina, the HPC and then back to the Consumer. At HPC output, the NH<sub>3</sub> Gas is supposed to be captured to

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avoid ammonia in the air of the Consumer and sent into the liquid stream to respect the mass conservation of the whole process. For Rhodo too, the CO<sub>2</sub> and NH<sub>3</sub> present in the inert gas is captured and sent into the liquid stream. The oxygen needed for oxidation of H<sub>2</sub> and for transformation of butyric acid into acetic acid in Lique is extracted from the air circuit so that the mass balance of the whole process is fulfilled.

### 2.3.2. Liquid circuit

The stream of water is recirculating through the 5 compartments : Lique, Rhodo, Nitri, Spiru and HPC. A part of the main liquid stream is derived at output of Rhodo so that not to oxidise the NH<sub>3</sub> necessary to the HPC. All the biomass outgoing from Rhodo and Spiru is removed as dry matter while the biomass produced by Nitri is fixed. The crop extracted from HPC is assumed dry too. The human wastes (faeces and urea) are introduced continuously at the input of Lique as dry matter.

The water produced or consumed by the biochemical reactions is neglected and the one coming from evapotranspiration of plants is injected back into the main stream of water.

These circuits are represented in the figure 2.

## 2.4. Input and output of the loop

The input is composed of

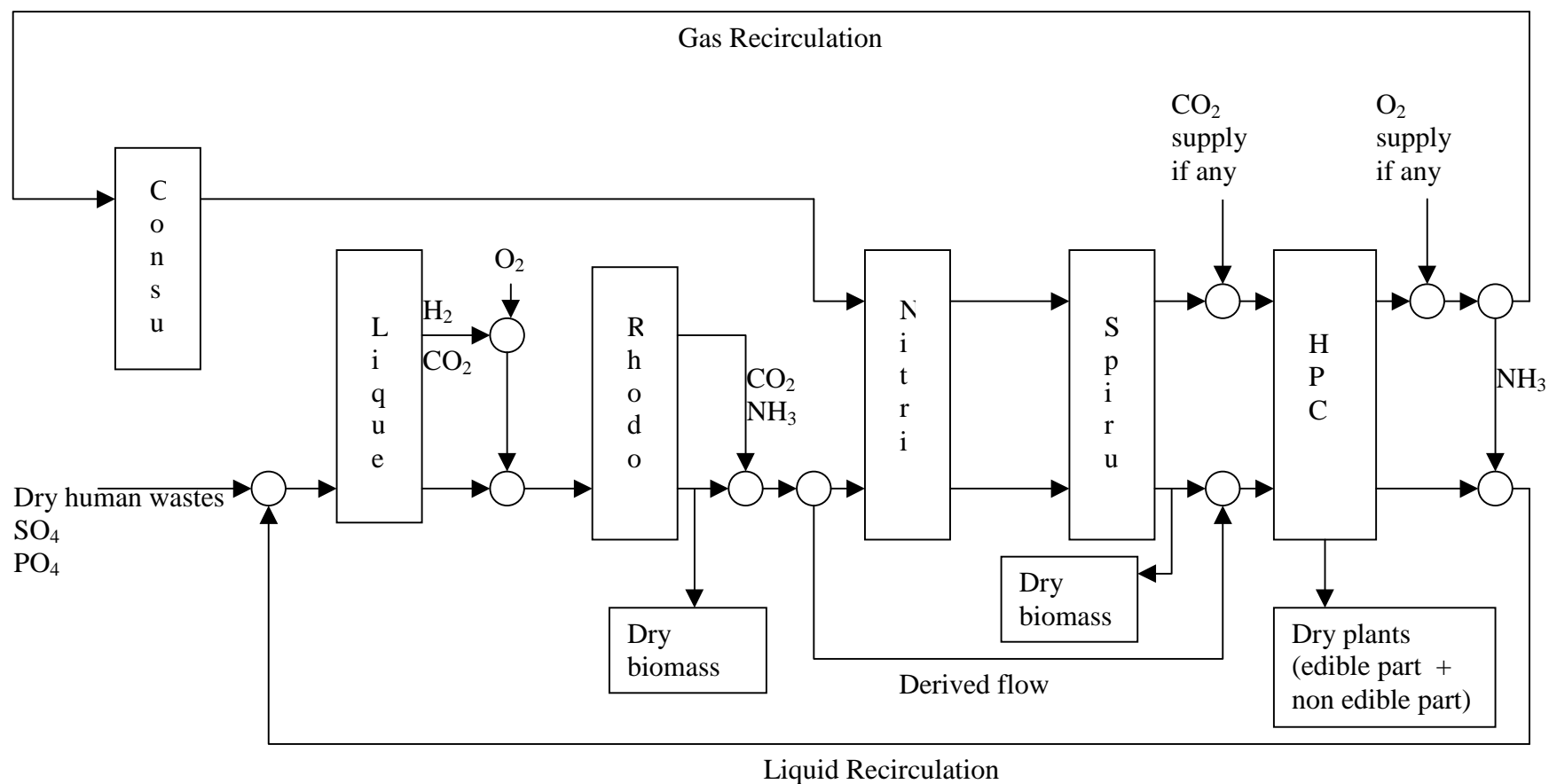
- dry human wastes (faeces and urea);
- SO<sub>4</sub> and PO<sub>4</sub> added in the liquid circuit;
- O<sub>2</sub> or CO<sub>2</sub> (depending of type of closing) in the gaseous circuit;
- carbon rejected in the carbonic gas of the rats.

The output is composed of

- dry biomass;
- dry plants;
- oxygen absorbed by the rats.

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**Figure 2 : Gas and Liquid connections between compartments**

*One remembers that the consumption of gaseous  $O_2$  in the Liquefying compartment is not physically possible; but, in the simulator, it is needed by the transformation of  $H_2$  and butyric acid, as explained above, in order to fulfil the mass balance of the whole process.*

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### 3. METHOD OF SOLUTION

#### 3.1. Introduction

The general approach is to consider each of the chemical compounds and its variation rates (production or consumption) in each of the compartments.

The principle of the method is based on the fact that the loop of a compound can be closed only and only if the sum of its variation rates is zero. It is obvious that this condition cannot be fulfilled for all the compounds simultaneously and that the first step is to choose which ones are the best candidates.

Under this consideration, H<sub>2</sub>O is discarded because it is easy to add (or remove) H<sub>2</sub>O into (or from) the mean liquid stream. So are SO<sub>4</sub> and PO<sub>4</sub> because they are not components (not yet in this simulator) of the human wastes.

The solids too, as biomass or waste part of the plants, are not considered because their transformation (in the Liquefying compartment or a burner for example) is not yet modelled.

Of course it will be checked if the by-products, as nitrite, or the partly transformed compounds, as acetate, accumulate or not in the loop.

So the main compounds whose closing is studied here are : O<sub>2</sub>, CO<sub>2</sub>, NH<sub>3</sub> and NO<sub>3</sub>.

#### 3.2. The variables of the problem

In order to have the most global approach, the variables are :

- n : number of rats in the Consumer compartment
- y : production of active biomass XA in Spiru (mol/h)
- v : input rate of human wastes in Liquefying compartment
- ρ : ratio of the diet for 1 man produced by HPC

#### Remarks :

- Although the ratio of the diet produced by HPC, ρ, has been fixed to 20 % at the meetings in Toulouse and Guelph, it is considered as a variable to increase the degree of freedom of the problem during the study.
- The production of active biomass of Spirulina, y, is equivalent to the light flux.
- The production of biomass of Rhodobacter is bound to the input rate of waste v in order to transform all the acetate coming from the Lique compartment. Then it is not a variable.

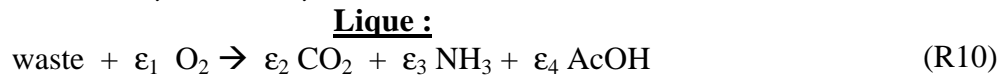
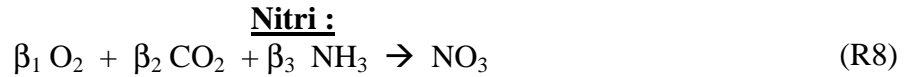
#### 3.3. Chemical equations binding the variations of the main compounds

The following chemical equations are stoichiometric but not completely balanced as they are reduced to the only compounds implied in the problem. They globally represent the steady state behaviour of a compartment around a functioning point on which the stoichiometric coefficients depend. For example, in the case of Spiru, the stoichiometric coefficients α<sub>1</sub>, α<sub>2</sub>, and α<sub>3</sub> cannot be explicitly given but they are computed by the simulator. The equation (R7) does not make appear the other biomass (G and EPS) because XA is the only key element for the determination of the light flux. The same approach is done for the other compartments.

#### Spiru :



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Remark :

In this study the compound ‘waste’ is composed of  $9.5 \cdot 10^{-2}$  mol of faeces and  $1.036 \cdot 10^{-1}$  mol of urea (TN 35.1).

### 3.4. Parameters of the Consumer compartment and of the HPC

The behaviours of these 2 compartments are described by means of the following parameters which represent the variation rates of the involved compounds:

- $r_{01}$  : O<sub>2</sub> consumption rate of 1 rat (negative value; mol/h)
- $r_{02}$  : CO<sub>2</sub> production rate of 1 rat (positive value; mol/h)
- $r_{51}$  : O<sub>2</sub> production rate of HPC for 100 % diet (positive value; mol/h)
- $r_{52}$  : CO<sub>2</sub> consumption rate of HPC for 100 % diet (negative value; mol/h)
- $r_{53}$  : NH<sub>3</sub> consumption rate of HPC for 100 % diet (negative value; mol/h)
- $r_{54}$  : NO<sub>3</sub> consumption rate of HPC for 100 % diet (negative value; mol/h)
- $r_{55}$  : SO<sub>4</sub> consumption rate of HPC for 100 % diet (negative value; mol/h)
- $r_{56}$  : PO<sub>4</sub> consumption rate of HPC for 100 % diet (negative value; mol/h)

### 3.5. General system of equations

The necessary and sufficient condition for closing the loop of a compound j whose steady state variation rate in a compartment i is  $v_{ij}$  :

$$v_{ij} = 0 \quad (1)$$

For each compartment, the variations rates (algebraic values) of the main involved compounds are gathered in the tables 2 and 3 where  $\xi = \varepsilon_3 - \varepsilon_4 \cdot \frac{\gamma_1}{\gamma_2}$ .

	O <sub>2</sub> variation rate (mol/h)	CO <sub>2</sub> variation rate (mol/h)
<b>Consu</b>	$r_{01} \cdot n$	$r_{02} \cdot n$
<b>Lique</b>	$\varepsilon_1 \cdot v$ (*)	$\varepsilon_2 \cdot v$
<b>Rhodo</b>	0	$-\frac{1}{\gamma_2} \cdot \varepsilon_4 \cdot v$
<b>Nitri</b>	$-\frac{\beta_1}{\beta_3} \cdot (\xi \cdot v + r_{53} \cdot \rho)$	$-\frac{\beta_2}{\beta_3} \cdot (\xi \cdot v + r_{53} \cdot \rho)$
<b>Spiru</b>	$\frac{1}{\alpha_3} \cdot y$	$\frac{\alpha_1}{\alpha_3} \cdot y$
<b>HPC</b>	$r_{51} \cdot \rho$	$r_{52} \cdot \rho$

(\*) : One remembers that the consumption of gaseous  $O_2$  in the Liquefying compartment is not physically possible; but, in the simulator, it is needed by the transformation of  $H_2$  and butyric acid, as explained above, in order to fulfil the mass balance of the whole process.

**Table 2 :  $O_2$  and  $CO_2$  variation rates of the process**

	<b><math>NH_3</math> variation rate (mol/h)</b>	<b><math>NO_3</math> variation rate (mol/h)</b>
<b>Consu</b>	0	0
<b>Lique</b>	$\varepsilon_3 \cdot v$	0
<b>Rhodo</b>	$-\frac{\gamma_1}{\gamma_2} \cdot \varepsilon_4 \cdot v$	0
<b>Nitri</b>	$-\beta_3 \cdot \left( \frac{\alpha_2}{\alpha_3} \cdot y + r_{54} \cdot \rho \right)$	$-\left( \frac{\alpha_2}{\alpha_3} \cdot y + r_{54} \cdot \rho \right)$
<b>Spiru</b>	0	$\frac{\alpha_2}{\alpha_3} \cdot y$
<b>HPC</b>	$r_{53} \cdot \rho$	$r_{54} \cdot \rho$

**Table 3 :  $NH_3$  and  $NO_3$  variation rates of the process**

When the global relation (1) is applied to each of the compound  $O_2$ ,  $CO_2$ ,  $NH_3$  and  $NO_3$ , it implies the 3 following equations :

$$r_{01} \cdot n + \left( \varepsilon_1 - \frac{\beta_1}{\beta_3} \cdot \xi \right) \cdot v + \frac{1}{\alpha_3} \cdot y + \left( r_{51} - \frac{\beta_1}{\beta_3} \cdot r_{53} \right) \cdot \rho = 0 \quad (2)$$

$$r_{02} \cdot n + \left( \varepsilon_2 - \frac{1}{\gamma_2} \cdot \varepsilon_4 - \frac{\beta_2}{\beta_3} \cdot \xi \right) \cdot v + \frac{\alpha_1}{\alpha_3} \cdot y + \left( r_{52} - \frac{\beta_2}{\beta_3} \cdot r_{53} \right) \cdot \rho = 0 \quad (3)$$

$$\xi \cdot v - \beta_3 \frac{\alpha_2}{\alpha_3} \cdot y + (r_{53} - \beta_3 \cdot r_{54}) \cdot \rho = 0 \quad (4)$$

The relation (4) represents the closing of N (nitrogen) globally under its  $NH_3$  and  $NO_3$  forms.

From this set of equations, four possible closings are investigated :

- closing of  $O_2$ ,  $CO_2$  and  $NH_3/NO_3$ .
- closing of  $O_2$  and  $CO_2$ .
- closing of  $O_2$  and  $NH_3/NO_3$ .
- closing of  $CO_2$  and  $NH_3/NO_3$ .

## 4. STUDY OF DIFFERENT WAYS OF CLOSING

### 4.1. Closing $O_2$ , $CO_2$ and $NH_3/NO_3$

In that case the 4 variables  $n$ ,  $v$ ,  $y$  and  $\rho$  are bound by the 3 equations (2), (3) and (4). Considering that the production of biomass XA can vary between its minimum (0 g/h) and its maximum (1.1 g/h), the ranges of the other variables, computed by (2), (3) and (4), are :

$$0 \leq n \leq 1.1$$

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$$0 \leq v \leq .14$$

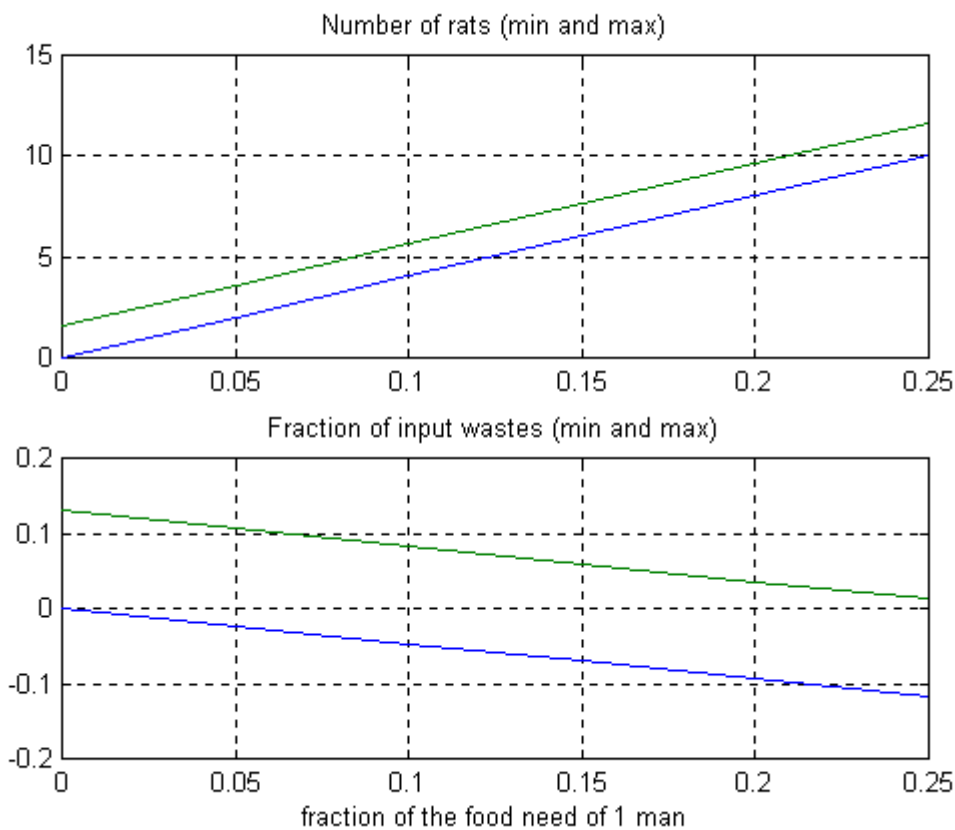
$$-.01 \leq \rho \leq 0$$

So, the existence domain of  $\rho$  is negative which is physically impossible. It means that the simultaneous closing of  $O_2$ ,  $CO_2$  and  $NH_3/NO_3$  is also impossible, in the case of the present simulator. Of course a simulator with another model a Liquefying could give a complete different result.

#### 4.2. Closing $O_2$ and $CO_2$

In that case the 4 variables  $n$ ,  $v$ ,  $y$  and  $\rho$  are bound by the 2 equations (2) and (3).

Considering now not only the variation range of  $y$  but also the variation range of  $\rho$  between 0 and 0.25 (a domain that contains the choice of 20 %), the ranges of the other variables  $n$  and  $v$  are plotted in the figure 2.



**Figure 2 : Domain of  $n$  and  $v$  for closing of  $O_2$  and  $CO_2$**

It is recalled here that, in meetings in Toulouse and Guelph, it was expected that the HPC would produce 20 % of the diet of 1 man and that the team would be composed of 3 rats. The figure 2 shows that, if the HPC is required to produce 20 % of the diet of 1 man, the number of rats should be between 8 and 9.5, the fraction of input wastes between 0 and 3 %. On the other side, if the number of rats is fixed to 3, the HPC has to produce between 3 and 7.5 % of the diet, the fraction of input wastes should be between 0 and 11 %.

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In these 2 approaches, either the max input wastes flow (3 %) is too low, either the max fraction of diet produced by HPC (7.5 %) is too low. So it can be concluded that the experiment of closing O<sub>2</sub> and CO<sub>2</sub> simultaneously is not interesting.

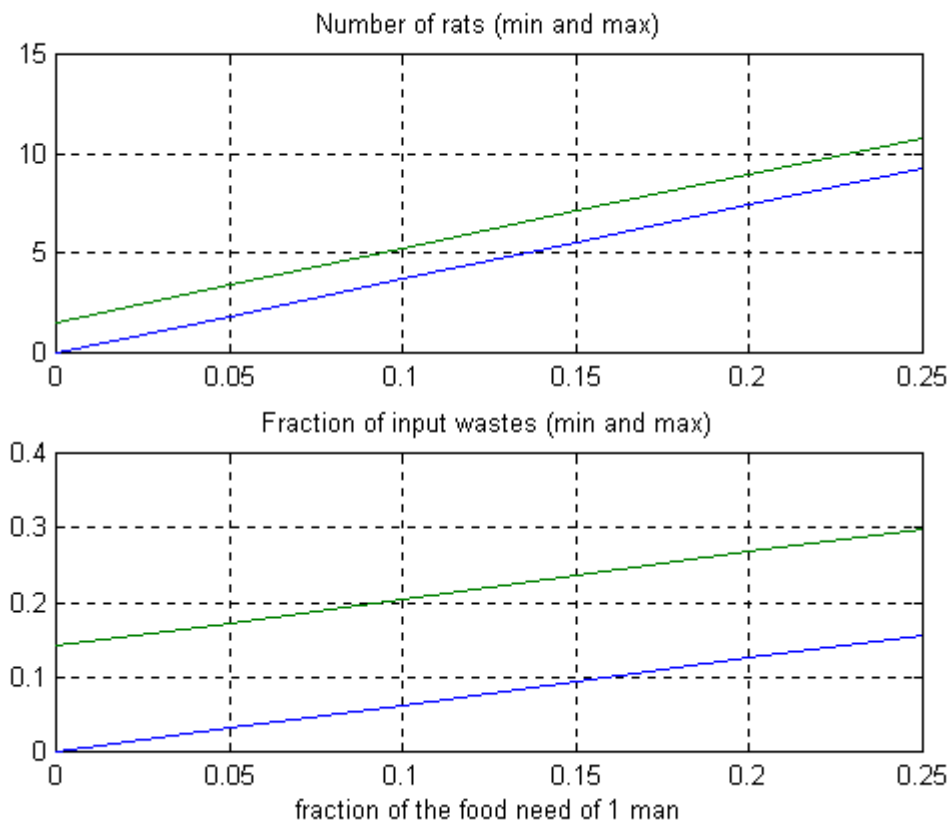
Remark :

When there is no HPC in the MELISSA loop (then the fraction of the diet for 1 man is zero), according to the figure 2 the number of rats should be between 0 and 1.6, the fraction of input wastes between 0 and 13.5 %. These conditions have been fulfilled in TN54.3 where the study is done without HPC. In fact the present study includes the previous one of TN 54.3 .

**4.3. Closing O<sub>2</sub> and NH<sub>3</sub>/NO<sub>3</sub>**

In that case the 4 variables n, v, y and ρ are bound by the 2 equations (2) and (4).

Considering as previously the variation ranges of y and ρ, the ranges of the other variables n and v are plotted in the figure 3.



**Figure 3 : Domain of n and v for closing of O<sub>2</sub> and NH<sub>3</sub>/NO<sub>3</sub>**

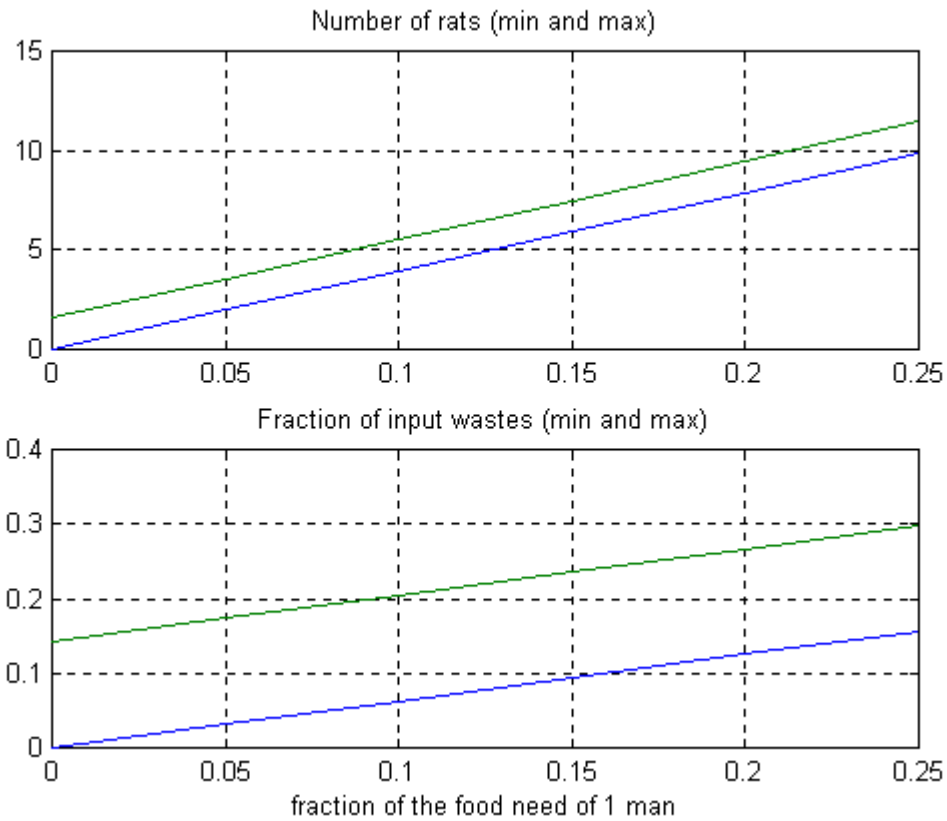
The figure 3 shows that, if the HPC is required to produce 20 % of the diet of 1 man, the number of rats should be between 7.5 and 9, the fraction of input wastes between 13 and 27 %.

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#### 4.4. Closing CO<sub>2</sub> and NH<sub>3</sub>/NO<sub>3</sub>

In that case the 4 variables n, v, y and ρ are bound by the 2 equations (3) and (4).

Considering as previously the variation ranges of y and ρ, the ranges of the other variables n and v are plotted in the figure 4.



**Figure 4 : Domain of n and v for closing of CO<sub>2</sub> and NH<sub>3</sub>/NO<sub>3</sub>**

The figure 4 shows that, if the HPC is required to produce 20 % of the diet of 1 man, the number of rats should be between 8 and 9.5, the fraction of input wastes between 13 and 27 %.

#### 4.5. Conclusion

The closing of O<sub>2</sub>, CO<sub>2</sub>, NH<sub>3</sub> and NO<sub>3</sub> is impossible simultaneously.

The closing of O<sub>2</sub> and CO<sub>2</sub> presents little interest because too low proportions of HPC and human wastes will be involved in the experiment.

Only the closing of O<sub>2</sub> and NH<sub>3</sub>/NO<sub>3</sub> or the closing of CO<sub>2</sub> and NH<sub>3</sub>/NO<sub>3</sub> can be proposed. They are more investigated and compared hereafter.

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## 5. EXAMPLES OF CLOSING

### 5.1. Introduction

The 2 types of closing (first O<sub>2</sub> and NH<sub>3</sub>/NO<sub>3</sub> and then CO<sub>2</sub> and NH<sub>3</sub>/NO<sub>3</sub>) are simulated on the global simulator described in section 2. The number of rats is the same in the 2 cases : 8.5, value that is the middle of the common domain of existence (between 8 and 9). The HPC produces 20 % of the diet of 1 man. When a substrate lacks because it is not in sufficient quantity in the input wastes, it is supplied so that the gas and liquid loops can be closed at steady state.

The main parameters of the process are :

- $r_{01} = 4.45 \cdot 10^{-2}$  mol/h/rat : O<sub>2</sub> consumption for 1 rat (TN 47.3 by UAB);
- $r_{02} = 4 \cdot 10^{-2}$  mol/h/rat : CO<sub>2</sub> production for 1 rat (TN 47.3 by UAB);
- $q = 0.77$  l/h : re-circulating liquid flow rate;
- $q' = 1.8$  l/h : re-circulating air flow rate;
- molar fraction of O<sub>2</sub> in the air at the Consumer input : .21;
- molar fraction of CO<sub>2</sub> in the air at the Consumer input : .003;
- molar concentration of NH<sub>3</sub> (total form in liquid) at the HPC output :  $3 \cdot 10^{-4}$ ;
- molar concentration of NO<sub>3</sub> at the HPC output :  $2 \cdot 10^{-3}$ ;
- molar concentration of SO<sub>4</sub> and PO<sub>4</sub> at the HPC output :  $1 \cdot 10^{-3}$ ;
- input rate of 1 man wastes :  $\frac{9.5 \cdot 10^{-3}}{3}$  mol/h of faeces +  $\frac{1.036 \cdot 10^{-1}}{3}$  mol/h of urea (TN 35.1).

The other parameters are detailed in annex (initialisation Matlab files : i\_sim\_0.m, i\_sim\_1.m, i\_sim\_2.m, i\_sim\_3.m , i\_sim\_4.m and i\_sim\_5.m).

As the coefficients  $\alpha$ ,  $\beta$ ,  $\gamma$  and  $\varepsilon$  of the equations (2) to (4) are non linear depending on the concentration of the substrates, the solution of the system is obtained through an iterative algorithm, as in TN 54.3.

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## 5.2. Results

The results of the 2 simulations are gathered in the table 2.

The main features :

- HPC produces the main part of O<sub>2</sub> : 85 or 90 % depending of the type of closing;
- correlatively HPC consumes the main part of CO<sub>2</sub> : 87 or 92 %;
- in the case of closing of O<sub>2</sub>, 5 % of the total consumption of CO<sub>2</sub> has to be injected at input of the HPC;
- in the case of closing of CO<sub>2</sub>, 5 % of the total consumption of O<sub>2</sub> has to be injected at input of the consumer compartment;

	<b>closing O<sub>2</sub> and NH<sub>3</sub>/NO<sub>3</sub></b>	<b>closing CO<sub>2</sub> and NH<sub>3</sub>/NO<sub>3</sub></b>
<b>Number of rats</b>	<b>8.5</b>	<b>8.5</b>
<b>Input rate of man wastes (ratio of 1 man)</b>	<b>.23</b>	<b>.19</b>
<b>O<sub>2</sub> consumption in Consu (mol/h)</b>	<b>.378</b>	<b>.378</b>
<b>O<sub>2</sub> consumption in Nitri (mol/h)</b>	<b>.021</b>	<b>.016</b>
<b>O<sub>2</sub> production in Spiru (mol/h)</b>	<b>.062</b>	<b>.036</b>
<b>O<sub>2</sub> production in HPC (mol/h)</b>	<b>.340</b>	<b>.340</b>
<b>CO<sub>2</sub> production in Consu (mol/h)</b>	<b>.340</b>	<b>.340</b>
<b>CO<sub>2</sub> production in Lique (mol/h)</b>	<b>.010</b>	<b>.008</b>
<b>CO<sub>2</sub> consumption in Spiru (mol/h)</b>	<b>.047</b>	<b>.026</b>
<b>CO<sub>2</sub> consumption in HPC (mol/h)</b>	<b>.320</b>	<b>.320</b>
<b>Supply of CO<sub>2</sub> (mol/h)</b>	<b>.019</b>	<b>0</b>
<b>Supply of O<sub>2</sub> (mol/h)</b>	<b>0</b>	<b>.021</b>
<b>Production of biomass Rhodo (dry g/h)</b>	<b>0.12</b>	<b>0.10</b>
<b>Production of biomass Spiru : XA+G+EPS (dry g/h)</b>	<b>2.12</b>	<b>1.27</b>
<b>Production of higher plants (dry g/h)</b>	<b>3.58</b>	<b>3.58</b>
<b>Light flux for Rhodo (W/m<sup>2</sup>)</b>	<b>400</b>	<b>320</b>
<b>Light flux for Spiru (W/m<sup>2</sup>)</b>	<b>107</b>	<b>40</b>
<b>Ratio of the main liquid flow going through Nitri and Spiru</b>	<b>.78</b>	<b>.73</b>
<b>NO<sub>2</sub> in the loop (mol/l)</b>	<b>1.4 10<sup>-4</sup></b>	<b>1.4 10<sup>-4</sup></b>
<b>Acetate (all forms) at output of Rhodo (mol/l)</b>	<b>1.8 10<sup>-5</sup></b>	<b>1.5 10<sup>-5</sup></b>
<b>Conversion yield of NH<sub>3</sub> into NO<sub>3</sub> in Nitri</b>	<b>.957</b>	<b>.957</b>

Table 2 : Comparison of the 2 types of closing

## 6. CONCLUSION

The study has established a tool and a method to determine the domain of existence of the variables of the problem : number of rats, ratio of input human wastes and ratio of diet

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produced by the HPC. The method is general and the results will be improved each time a better knowledge of the process is acquired.

Two examples illustrate the way to determine the conditions that make possible the closing of the gas and liquid loops in the present state of the project. Their results are surprising compared to which was expected at the meeting in Toulouse : when the HPC is required to produce 20 % of the diet of 1 man, the team has to be composed of about 8 rats (compared to 3 or 4 expected) and the ratio of input wastes of 1 man is only about 20 % (compared to the 100 % expected).

Of course these results strongly depend on the mean composition of the wastes and on the modelling of the Liquefying compartment. Any modification will imply new results.

On the basis of the results of TN 54.3 and 54.4, the successive steps to close the whole loop could be :

- first, with all the compartments connected except HPC, the experiment is in fact a replay of Biorat by closing the gas loop alone with 1 rat;
- then the liquid loop is closed too;
- at the end the HPC is connected. Depending on the state of development of the plants, the rats are added in sufficient quantity to consume the O<sub>2</sub> produced by HPC. The ratio of input wastes is tuned.

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## 8. ANNEX (Software)

### 6.1. Closing the Gas and Liquid loops – Resolution of the system

```

%*****
%      Connected compartments 0,1,2,3,4A and 4B (numbered 5 here)      *
%      Version 3.0      October 2001                                  *
%                                                                    *
%      i_sim.m      Initialization of the simulation                  *
%                  of the extended MELISSA loop (with HPC)          *
%                                                                    *
%*****

clear all
global ind_2u ind_2v ind_3u rKdis_2 rKdis_3
global VM_0 Gin_0
global Gin_1 Fin_1 NG1_1 NG_1 NL_1 Kdis_1 rKdis_1 Yp_lp
global Gin_2 Fin_2 NG_2 NL_2 NO_2 vNB_2 vNM_2 VL_2 Yx1_2 Kdis_2 KSSO4_2 ...
    A2_2 B2_2 GG1_2 GG2_2 ...
    FRmin_2 FRmax_2 fI_2 RT_2 Ea_2 Es_2 muM_2 KJ_2 EpsJ_2 q_rhod_2 zmin_I_2
global Gin_3 Fin_3 NL_3 NG_3 NS_3 NB_3 NX_3 NO_3 NI_3 NV_3 ...
    Ae_3 Be_3 Ce_3 De_3 E_3 WX_3 WYG_3 WYL_3 ...
    iO2_3 iCO2_3 iNH3_3 iNO2_3 iSub_3 iXNs_3 iXNb_3 iXag_3 ...
    Klns_3 Klnb_3 KmNs_3 KmNb_3 mumax_3 maint_3 Yx_3 Yx1_3 Yml_3 ...
    RL_3 indG_3 indL_3 Kdis_3
global Fin_4 NG_4 NL_4 NO_4 vNB_4 vNM_4 VL_4 Yx1_4 Kdis_4 ...
    A2_4 B2_4 GG1_4 GG2_4 ...
    FRmin_4 FRmax_4 FRmaxc_4 fI_4 zPC_4 zCH_4 ...
    RT_4 Ea_4 Es_4 muM_4 muEPS_4 Kj_4 KJeps_4 Fmin_4 zmin_I_4 ...
    KSNO3_4 KSSO4_4 KSP04_4 KSPC_4
global Gin_5 Fin_5 NG_5 NL_5 NS_5 VG_5 VL_5 Yx1e_5 Yx1w_5 Kdis_5 ...
    Diete_5 Dietw_5 A2_5 B2_5 ind_3u5
global idisp

% Initializing global parameters
% =====
idisp=0; % flag to display intermediate variables (if equal to 1)
istudy=1;% flag to look for the existence interval of 'nRat' and 'nMan' (if equal to 1)
lambda = 0*.1; % relaxation coefficient
niter=10; % number of iterations
% Type of closed loop
% =====
typloop = 1;      titre = 'Closed loop for O2 and CO2';
typloop = 2;      titre = 'Closed loop for O2 , CO2 and NH3';
typloop = 3;      titre = 'Closed loop for O2 and NH3/NO3';
typloop = 4;      titre = 'Closed loop for CO2 and NH3/NO3';
% Initializing parameters versus the type of closed loop
% =====
if typloop == 1
    nRat = 5.5; % number of rats in the consumer compartment
    nMan = .08; % ratio of 1 man_waste at input of the liquefying compartment
    cXA0_4 = 2; % (g/l) Value of biomass at starting of the iterative procedure
    cover_p=.10; % possible choice of 'cover'
                % Recall:HPC has to furnish 20 % of the need of 1 man (Toulouse and Guelph
meeting)
    share2 = .6; % sharing ratio of liquid at output of compart 2 (Rhodo) towards Nitri
elseif typloop == 2
    nRat = 1; % number of rats in the consumer compartment
    nMan = .1; % ratio of 1 man_waste at input of the liquefying compartment
    cXA0_4 = 2; % (g/l) Value of biomass at starting of the iterative procedure
    share2 = .6; % sharing ratio of liquid at output of compart 2 (Rhodo) towards Nitri
elseif typloop == 3
    nRat = 8.5; % number of rats in the consumer compartment
    nMan = .2; % ratio of 1 man_waste at input of the liquefying compartment
    cXA0_4 = 2; % (g/l) Value of biomass at starting of the iterative procedure
    cover_p=.20; % possible choice of 'cover'

```

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meeting)
    % Recall:HPC has to furnish 20 % of the need of 1 man (Toulouse and Guelph
share2 = .8; % sharing ratio of liquid at output of compart 2 (Rhodo) towards Nitri
elseif typloop == 4
    nRat = 8.5; % number of rats in the consumer compartment
    nMan = .23; % ratio of 1 man_waste at input of the liquefying compartment
    cXA0_4 = 1.4; % (g/l) Value of biomass at starting of the iterative procedure
    cover_p=.20; % possible choice of 'cover'
    % Recall:HPC has to furnish 20 % of the need of 1 man (Toulouse and Guelph
meeting)
    share2 = .7 ;% sharing ratio of liquid at output of compart 2 (Rhodo) towards Nitri
end
% The G flow rate of the Spirulina compart is set to the other compartments.
Gin_4 = 180; % incoming gas flow rate (l/h) (from TN 43.110 p.26, UAB)
% The recirculating L flow is set to 0.77 l/h (previous value of flow through Spiru).
% Then the residence time in Spiru is now > 100 h
% The volume of the Nitri compart is modified to keep its residence time unchanged
% The volume of Rhodo is set to 9 l : minimum for Fr=400 W/m2 and a biomass production of
.118 g/h
Fcirc = .77; % Recirculating L flow rate (arbitrary value) (l/h)
Fin_1 = Fcirc; % liquid flow rate through Lique (l/h)
Fin_2 = Fcirc; % liquid flow rate through Rhodo (l/h)
Fin_5 = Fcirc; % liquid flow rate through HPC (l/h)
Fin_3 = Fcirc*share2;% liquid flow rate through Nitri(l/h)
Fin_4 = Fin_3; % liquid flow rate through Spiru(l/h)
% Initializing parameters of compart.
% =====
Matom = [12; 1; 16; 14; 32; 31]; % C H O N S P atomik mass
i_sim_0
i_sim_1
i_sim_2
i_sim_3
i_sim_4
i_sim_5
% Initializing indices used in the links between compart.
% =====
% 1. Link from Rhodo to Nitri
ind_2u = [1, 2, NG_2+2, NG_2+1]; % index of CO2_L NH3_L PO4 SO4 at Rhodo L output
ind_2v = [2, 3, NG_3+3, NG_3+4]; % index of CO2_L NH3_L PO4 SO4 at Nitri L input
% 2. Link from Nitri to Spiru
i1 = (NB_3+1)*NG_3+1; % index of O2_G in part C of nitri column
i2 = (NB_3+2)*NG_3+(NB_3+1)*(NG_3+NL_3)+1; % index of O2_L in part C of Nitri
i3 = i2+NG_3+1; % index of NO3 in part C of nitri column
% i3+1 and i3+2 : indices of PO4 and SO4, respectively in part C
ind_3u = [i1, i1+1, i2, i2+1, i3, i3+2, i3+1]; % O2_G CO2_G O2_L CO2_L NO3 SO4 PO4
% 3. Link from Rhodo and Spiru to HPC
ind_3u5 = i2+2; % index of NH3_L at Nitri output vector

% Conversion due to dissociation in the links between compartments
% =====
% CO2_L NH3_L AcOH_L SO4 PO4
rKdis_1 = [(1+Kdis_1)/(1+Kdis_2); 1; 1]; % from Lique to Rhodo
% CO2_L NH3_L PO4 SO4
rKdis_2 = [(1+Kdis_2(1:2))/(1+Kdis_3(2:3)); 1; 1]; % from Rhodo to Nitri
% O2_G CO2_G O2_L CO2_L NO3 SO4 PO4
rKdis_3 = [1; 1; 1; (1+Kdis_3(2))/(1+Kdis_4(2)); 1; 1; 1];% from Nitri to Spiru

% Initializing yield of acetate consumption in Rhodo
% =====
Yx_AcOH = .995; % value supposed low enough to avoid C limitation
% Set point of conc. of the main compounds at output of HPC
% =====
fm_O2_0 = .21; % O2 G (molar fraction of O2 at output of HPC)
fm_CO2_0 = 3e-3; % CO2 G (molar fraction of CO2 at output of HPC)
spNH3_5 = 3.0e-4; % (mol/l) NH3 L total at output of HPC
spNO3_5 = 1.0e-2; % (mol/l) NO3 at output of HPC
spNO3_5 = 2.0e-3; % (mol/l) NO3 at output of HPC
spSO4_5 = 1.0e-3; % (mol/l) SO4 at output of HPC
spPO4_5 = 1.0e-3; % (mol/l) PO4 at output of HPC
% Initializing parameters
% =====
% Production rate of CO2 : 4e-2 mol/h/rat

```

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```

rCO2_0 = rCO2r_0*nRat; % mol/h for n rats
% Consumption rate of O2 : 4.45e-2 mol/h/rat
rO2_0 = rO2r_0*nRat; % mol/h for n rats
% Conc. of N2 and H2O in gas phase (perfect gases at T='Temp' Kelvin and P=1 atm)
% (molar conc. same for all the compart because gas flow rate not depending on T)
% =====
fm_H2O_0 = 5.796e-2; % H2O (molar fraction)
fm_N2_0 = 1 - fm_O2_0 - fm_H2O_0; % N2 (molar fraction); CO2 neglected
cN2_0 = fm_N2_0 / VM_0; % mol/l
cH2O_0 = fm_H2O_0 / VM_0; % mol/l
cN2_2 = cN2_0; cH2O_2 = cH2O_0;
cN2_3 = cN2_0; cH2O_3 = cH2O_0;
cN2_4 = cN2_0; cH2O_4 = cH2O_0;
% Yield of the non-constrained compartments (Lique, Rhodo, HPC)
% =====
% Yield of products of the Liquefying compartment
Faec = 9.5e-2/3; % mol/h (faeces of 1 man; according to TN35.1, ADERSA)
Urea = 1.036e-1/3; % mol/h (urea of 1 man; according to TN35.1, ADERSA)
Yp_lp = (Faec*Yxf_1 + Urea*Yxu_1); % Yield of products (H2 CO2 NH3 AcOH BuOH) for 1
man_waste (faeces + urea)
Yp_1(1,1) = -Yp_lp(1,1)/2-Yp_lp(5,1); % Lique consumption yield of O2
Yp_1(2:3,1) = Yp_lp(2:3,1); % Lique production yield of CO2 and NH3
Yp_1(4,1) = Yp_lp(4,1)+2*Yp_lp(5,1); % Lique production yield of AcOH
% Yield of substrates of the Rhodobacter : Yp(1) NH3 + Yp(2) AcOH --> CO2
Yp_2 = Yx1_2(2:3) / Yx1_2(1); % conversion yield of NH3 AcOH into CO2
% Variation rate of substrates and product of HPC (O2 CO2 NH3 NO3 SO4 PO4)
ri_5 = Yx1e_5 * Diete_5' + Yx1w_5 * Dietw_5'; % mol/h (food need of 1 man per day)
% Computation of the max production of active biomass of Spiru
% =====
for ii=1:10
%>1.Input of Spiru
% 1.1.Estimation of gas input of Spiru
CG0_4 = [fm_O2_0/VM_0+rO2_0/Gin_4; (rCO2_0+nMan*Yp_1(2))/Gin_4]; % O2 CO2 (mol/l)
% 2.2.Estimation of liquid input of Spiru
cNO3 = -1.2*Yx1_4(3,1)*cXA0_4; % Excess of NO3 needs to avoid mineral limitation
CL0_4 = [0; % O2 (mol/l)
fm_CO2_0*55.56/kpartN_4(2); % CO2 (mol/l) : G/L equilibrium
cNO3; % NO3 (mol/l)
sum(Yx1_4(4,:))/Yx1_4(3,1)*cNO3; % SO4 (mol/l)
Yx1_4(5,1)/Yx1_4(3,1)*cNO3]; % PO4 (mol/l)
% 1.3.Steady state of Spiru
[FR0_4, X0_4, Y0_4] = stesta_4( ...
NG_4, NL_4, NO_4, vNB_4, vNM_4, Fin_4, VL_4, Yx1_4, ...
A2_4, B2_4, GG1_4, GG2_4, CG0_4, CL0_4, cXA0_4, ...
FRmin_4, FRmaxc_4, fI_4, zPC_4, zCH_4, ...
RT_4, Ea_4, Es_4, muM_4, muEPS_4, Kj_4, KjEPS_4, Fmin_4, zmin_I_4, ...
KSNO3_4, KSSO4_4, KSPO4_4, KSPC_4);
if (isempty(FR0_4) | isempty(X0_4))
disp(' FR0_4 or X0_4 empty')
break
end
%>2. End of iterative computation
delta = (FRmax_4-FR0_4)/(FRmax_4);
if (abs(delta) < 1e-2), break, end
cXA0_4 = cXA0_4*(1+5*delta); % with relaxation coefficient
end
if (isempty(FR0_4) | isempty(X0_4)), break, end
%>3. Max production of active biomass of Spiru
rs=[0, cXA0_4*Fin_4]; % min and max of production (g/h) of XA in Spiru
cover_v = [0, .05, .1, .15, .2, .25]; % vector of values of 'cover'
% Local yield of Spiru
% =====
Yp_4 = zeros(3,1);
DO2 = (Y0_4(1) - CG0_4(1)) * Gin_4 + (X0_4(1) - CL0_4(1)) * Fin_4;
Yp_4(1) = ((Y0_4(NG_4)-CG0_4(NG_4))*Gin_4 + (X0_4(NG_4)-
CL0_4(NG_4))*(1+Kdis_4(NG_4))*Fin_4)/DO2;
Yp_4(2) = (X0_4(NG_4+1)-CL0_4(NG_4+1))*Fin_4/DO2;
Yp_4(3) = X0_4(NG_4+4)*Fin_4/DO2;
% Local yield of Nitri
% =====
% 1.1.Gas phase (mol/l of O2 CO2 NH3 (NH3:null) from Consu only) :
cO2 = fm_O2_0/VM_0+rO2_0/Gin_3; % O2 consumed in Consu

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cCO2 = fm_CO2_0/VM_0+rCO2_0/Gin_3; % CO2 produced by Consu
CG0_3 = [cCO2; cCO2; 0]; % mol/l
% 1.2.Liquid phase :
%CL0_3 = [C_O2; C_CO2; C_NH3; C_NO2; C_NO3; C_PO4; C_SO4];
cCO2 = nMan*(Yp_1(2)-Yp_1(4)*Yx_AcOH/Yp_2(2))/Fin_3; % CO2 produced by Lique and Rhodo
cNH3 = (-Yx1_4(3,1))*cXA0_4; % NH3 necessary for NO3 needed by Spiru
CL0_3 = [0; cCO2; cNH3]./(1+Kdis_3); % mol/l ; molecular form
cSO4 = sum(Yx1_3(7,:)) / sum(Yx1_3(3,:))*cNH3; % mol/l (SO4 stoichiometric to NH3)
cPO4 = sum(Yx1_3(6,:)) / sum(Yx1_3(3,:))*cNH3; % mol/l (PO4 stoichiometric to NH3)
CL0_3 = [CL0_3; 0; spNO3_5; cPO4; cSO4];
%1.3.Steady state of Nitri
[X0_3, Y0_3, dX0_3] = stesta_3( ...
NL_3, NG_3, NS_3, NB_3, NX_3, NO_3, NI_3, NV_3, ...
Ae_3, Be_3, Ce_3, De_3, E_3, WX_3, WYG_3, WYL_3, ...
iO2_3, iCO2_3, iNH3_3, iNO2_3, iSub_3, iXNs_3, iXNb_3, iXag_3, ...
KlNs_3, KlNb_3, KmNs_3, KmNb_3, mumax_3, maint_3, Yx_3, Yx1_3, Ym1_3, ...
CG0_3, CL0_3, RL_3, indG_3, indL_3);
if isempty(X0_3)
disp(' X0_3 empty')
break
end
%1.4.Yield of substrates O2 CO2 and NH3 : Yp(1) O2 + Yp(2) CO2 + Yp(3) NH3 --> NO3
indG = (NB_3+1)*NG_3+[1:NG_3]; % indices of O2 CO2 NH3 G in output vector Y0
indL = (NB_3+1)*(NG_3+NL_3)+[1:NG_3];% indices of O2 CO2 NH3 L in state vector X0
indN = (NB_3+1)*(NG_3+NL_3)+NG_3+1;% indices of NO2 in state vector X0
Dp = (Y0_3(indG)-CG0_3)*Gin_3 + (X0_3(indL)-CL0_3(1:NG_3)).*(1+Kdis_3)*Fin_3;
Dc = ((X0_3(indN+1)-CL0_3(NG_3+2))-(X0_3(indN)-CL0_3(NG_3+1)))*Fin_3; % NO3-NO2
Yp_3 = Dp / Dc; % conversion yield of O2 CO2 NH3 into NO3
% Computation of ksi for the following matrices AA
% =====
ksi = Yp_1(3,1)-Yp_2(1,1)/Yp_2(2,1)*Yp_1(4,1);
% Closed loop for O2 and CO2
% =====
if typloop == 1
% Computation of active biomass Spiru 'cXA0_4' and of incoming waste ratio 'nMan'
AA = [ 1/Yp_4(3,1)*Fin_4, Yp_1(1,1)-ksi*Yp_3(1,1)/Yp_3(3,1);
Yp_4(1,1)/Yp_4(3,1)*Fin_4, Yp_1(2,1)-Yp_1(4,1)/Yp_2(2,1)-ksi*Yp_3(2,1)/Yp_3(3,1)];
A1 = inv(AA);
X = -A1*[rO2_0+cover_p*(ri_5(1)-Yp_3(1,1)/Yp_3(3,1)*ri_5(3));
rCO2_0+cover_p*(ri_5(2)-Yp_3(2,1)/Yp_3(3,1)*ri_5(3))];
cXA0_4 = X(1);
nMan = X(2);
plotting=0; display=1; t_sim_m % results display
if istudy == 1
% 1. Min and max values of 'nRat' and 'nMan'
for kk = 1:max(size(cover_v))
cover = cover_v(kk);
for jj=1:2
AA = [rO2r_0, Yp_1(1,1)-ksi*Yp_3(1,1)/Yp_3(3,1);
rCO2r_0, Yp_1(2,1)-Yp_1(4,1)/Yp_2(2,1)-ksi*Yp_3(2,1)/Yp_3(3,1)];
A1 = inv(AA);
X = -A1*[1/Yp_4(3,1)*rs(jj)+cover*(ri_5(1)-Yp_3(1,1)/Yp_3(3,1)*ri_5(3));
Yp_4(1,1)/Yp_4(3,1)*rs(jj)+cover*(ri_5(2)-Yp_3(2,1)/Yp_3(3,1)*ri_5(3))];
minmaxRat(kk,jj) = X(1);
minmaxNu(kk,jj) = X(2);
end
end
%if idisp, minmaxRat, minmaxNu, end
% 2. Plotting
plotting=1; display=0; t_sim_m
end
% Closed loop for O2 , CO2 and NH3
% =====
elseif typloop == 2
% Computation of active biomass Spiru 'cXA0_4', incoming waste ratio 'nMan' and 'cover'
AA = [ 1/Yp_4(3,1)*Fin_4, Yp_1(1,1)-ksi*Yp_3(1,1)/Yp_3(3,1),
ri_5(1)-Yp_3(1,1)/Yp_3(3,1)*ri_5(3);
Yp_4(1,1)/Yp_4(3,1)*Fin_4, Yp_1(2,1)-Yp_1(4,1)/Yp_2(2,1)-
ksi*Yp_3(2,1)/Yp_3(3,1), ri_5(2)-Yp_3(2,1)/Yp_3(3,1)*ri_5(3);
-Yp_3(3,1)*Yp_4(2,1)/Yp_4(3,1)*Fin_4, ksi,
ri_5(3)-Yp_3(3,1)*ri_5(4)];
A1 = inv(AA);

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X = -A1*[rO2_0; rCO2_0; 0];
cXA0_4 = X(1);
nMan = X(2);
cover_p = X(3);
plotting=0; display=1;      t_sim_m % results display
if istudy == 1
% Min and max values of 'nRat' , 'nMan' and 'cover'
for jj=1:2
AA = [rO2r_0,      Yp_1(1,1)-ksi*Yp_3(1,1)/Yp_3(3,1),      ri_5(1)-
Yp_3(1,1)/Yp_3(3,1)*ri_5(3);
      rCO2r_0,      Yp_1(2,1)-Yp_1(4,1)/Yp_2(2,1)-ksi*Yp_3(2,1)/Yp_3(3,1), ri_5(2)-
Yp_3(2,1)/Yp_3(3,1)*ri_5(3);
      0,      ksi,      ri_5(3)-
Yp_3(3,1)*ri_5(4)];
A1 = inv(AA);
X = -A1*rs(jj)*[1/Yp_4(3,1);
                Yp_4(1,1)/Yp_4(3,1);
                -Yp_3(3,1)*Yp_4(2,1)/Yp_4(3,1)];
minmaxRat(jj) = X(1);
minmaxNu(jj) = X(2);
minmaxCov(jj) = X(3);
end
if idisp, minmaxRat, minmaxNu      , minmaxCov, end
end
end
if (typloop == 1 | typloop == 2) , break, end % Useless to pursue simulation

% Variation rates of HPC ('cover_p' food needs of 1 man/h) :
ry_5 = ri_5*cover_p;
% Closed loop for O2 and NH3/NO3
% =====
if typloop == 3 % closing O2 and NH3/NO3
% Computation of active biomass Spiru 'cXA0_4', incoming waste ratio 'nMan'
AA = [      1/Yp_4(3,1)*Fin_4,      Yp_1(1,1)-ksi*Yp_3(1,1)/Yp_3(3,1);
      -Yp_3(3,1)*Yp_4(2,1)/Yp_4(3,1)*Fin_4, ksi      ];
A1 = inv(AA);
BB = [rO2_0 + ry_5(1)-Yp_3(1,1)/Yp_3(3,1)*ry_5(3);
      ry_5(3)-Yp_3(3,1)*ry_5(4)      ];
X = -A1*BB;
cXA0_4 = X(1);
nMan = X(2);
plotting=0; display=1;      t_sim_m % results display
if istudy == 1
for kk = 1:max(size(cover_v))
cover = cover_v(kk);
for jj=1:2
AA = [rO2r_0,      Yp_1(1,1)-ksi*Yp_3(1,1)/Yp_3(3,1);
      0,      ksi      ];
A1 = inv(AA);
X = -A1*[1/Yp_4(3,1)*rs(jj)+cover*(ri_5(1)-Yp_3(1,1)/Yp_3(3,1)*ri_5(3));
        -Yp_3(3,1)*Yp_4(2,1)/Yp_4(3,1)*rs(jj)+cover*(ri_5(3)-Yp_3(3,1)*ri_5(4))];
minmaxRat(kk, jj) = X(1);
minmaxNu(kk, jj) = X(2);
end
end
%if idisp, minmaxRat, minmaxNu, end
% 2. Plotting
plotting=1; display=0;      t_sim_m
end
% Closed loop for CO2 and NH3/NO3
% =====
elseif typloop == 4 % closing CO2 and NH3/NO3
% Computation of active biomass Spiru 'cXA0_4', incoming waste ratio 'nMan'
AA = [      Yp_4(1,1)/Yp_4(3,1)*Fin_4,      Yp_1(2,1)-Yp_1(4,1)/Yp_2(2,1)-
ksi*Yp_3(2,1)/Yp_3(3,1);
      -Yp_3(3,1)*Yp_4(2,1)/Yp_4(3,1)*Fin_4, ksi
];
A1 = inv(AA);
BB = [rCO2_0+ry_5(2)-Yp_3(2,1)/Yp_3(3,1)*ry_5(3);
      ry_5(3)-Yp_3(3,1)*ry_5(4)      ];
X = -A1*BB;
cXA0_4 = X(1);

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nMan = X(2);
plotting=0; display=1;      t_sim_m % results display
if istudy == 1
for kk = 1:max(size(cover_v))
cover = cover_v(kk);
for jj=1:2
AA = [rCO2r_0,  Yp_1(2,1)-Yp_1(4,1)/Yp_2(2,1)-ksi*Yp_3(2,1)/Yp_3(3,1);
      0,        ksi
      ];
A1 = inv(AA);
X = -A1*[Yp_4(1,1)/Yp_4(3,1)*rs(jj)+cover*(ri_5(2)-Yp_3(2,1)/Yp_3(3,1)*ri_5(3));
        -Yp_3(3,1)*Yp_4(2,1)/Yp_4(3,1)*rs(jj)+cover*(ri_5(3)-Yp_3(3,1)*ri_5(4))];
minmaxRat(kk,jj) = X(1);
minmaxNu(kk,jj) = X(2);
end
end
%if idisp, minmaxRat, minmaxNu, end
% 2. Plotting
plotting=1; display=0;      t_sim_m
end
end

%=====
%      SIMULATION OF THE MELISSA LOOP      |
%=====
%> 1. INITIALIZATION
% Init of input of the process for the first iteration
% 1. O2_L CO2_L at input of the open loop (concentration in mol/l)
YO2_5 = 0; % approximate O2_L outgoing from HPC (mol/l)
YCO2_5 = fm_CO2_0*55.56/kpartN_4(2); % expected set point of CO2_L outgoing from HPC (mol/l)
: G/L equilibrium
% 2. L phase going into Rhodo (considered as non computable iteratively):
YAc_2= nMan*(1-Yx_AcOH)*Yp_1(4,1)/Fin_2; % AcOH_GL outgoing from Rhodo at previous step
initAcOH = YAc_2/(1+Kdis_2(NG_2));
% 3. L phase going into Rhodo input :
initNH3 = spNH3_5/(1+Kdis_2(2)); %(mol/l) NH3 GL coming from HPC output and going into L
phase of Rhodo input
% 4. L phase going into Nitri :
initNO2 = 1.3e-4; %(mol/l) NO2 outgoing from Nitri (value deduced from previous simulations)
% 5. SO4 P04 at input of the open loop (concentration in mol/l)
qS_2=-Yx1_2(4)/Yx1_2(3)*Yp_1(4,1)*nMan; % consumption of Rhodo
qS_3=-Yx1_3(7,1)/Yx1_3(2,1)*Yp_3(2,1)/Yp_3(3,1)*ksi*nMan*share2; % consumption of Nitri
qS_4=sum(Yx1_4(4,:))/Yx1_4(2,1)*Yp_4(1,1)/Yp_4(3,1)*cXA0_4*Fin_4;% consumption of Spiru and
HPC
qS_5=ry_5(5); % consumption of HPC
qP_2=-Yx1_2(5)/Yx1_2(3)*Yp_1(4,1)*nMan; % consumption of Rhodo
qP_3=-Yx1_3(6,1)/Yx1_3(2,1)*Yp_3(2,1)/Yp_3(3,1)*ksi*nMan*share2; % consumption of Nitri
qP_4=Yx1_4(5,1)/Yx1_4(2,1)*Yp_4(1,1)/Yp_4(3,1)*cXA0_4*Fin_4; % consumption of Spiru and
HPC
qP_5=ry_5(6); % consumption of HPC
D_S = qS_2+qS_3+qS_4+qS_5; % (mol/h) total SO4 consumed in the open loop
D_P = qP_2+qP_3+qP_4+qP_5; % (mol/h) total P04 consumed in the open loop
initLiqueL = [spSO4_5;spPO4_5]-[D_S;D_P]/Fin_1; % (mol/l) SO4 P04 at input of Lique
% 6. Addition rate of CO2 G (mol/h) at HPC input if necessary
if typloop == 3 % closing O2 and NH3/NO3
addO2=0;
crit = rCO2_0 + (Yp_1(2,1)-Yp_1(4,1)/Yp_2(2,1))*nMan -
Yp_3(2,1)/Yp_3(3,1)*(ksi*nMan+ry_5(3)) ...
+ Yp_4(1,1)/Yp_4(3,1)*cXA0_4*Fin_4 + ry_5(2); % global variation in the open loop
if crit < 0
addCO2 = -1.5*crit; % addition of CO2 in excess in first iterations to prevent C
limitation
else
addCO2 = -.5*crit; % removing CO2 partly
end
% 7. Supply rate of O2 G (mol/h) at HPC input if necessary
elseif typloop == 4 % closing CO2 and NH3/NO3
addCO2=0;
crit = rO2_0 + Yp_1(1,1)*nMan - Yp_3(1,1)/Yp_3(3,1)*(ksi*nMan+ry_5(3)) ...
+ 1/Yp_4(3,1)*cXA0_4*Fin_4 + ry_5(1); % global variation in the open loop
addO2 = -crit; % addition of O2 exactly as needed
end
% Computation of 'share2', 'Fin_3' and 'Fin_4'

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ksi = Yp_1(3,1)-Yp_2(1,1)/Yp_2(2,1)*Yp_1(4,1);
qNH3 = nMan*ksi; % estimated NH3 flow rate outgoing from Rhodo
share2 = 1 + ry_5(3)/qNH3; % sharing ratio of liquid at output of compart 2 (Rhodo) towards
Nitri
Fin_3 = Fcirc*share2;% liquid flow rate through Nitri(l/h)
Fin_4 = Fin_3; % liquid flow rate through Spiru(l/h)
% Init of spy variables
Yp_2p=Yp_2;Yp_3p=Yp_3;Yp_4p=Yp_4;Yp_5p=ri_5(2:NG_5+1)/ri_5(1);
% Initializing the input of the system to solve
EE = [cXA0_4; nMan];

%> 2. ITERATIVE COMPUTATION
for iter = 1:niter
% 1. Simulation of the process : open loop of Melissa
% =====
[CG0_0, Y0_0, Y0_1, CG0_2, CL0_2, FR0_2, X0_2, Y0_2, ...
CG0_3, CL0_3, X0_3, Y0_3, CG0_4, CL0_4, FR0_4, X0_4, Y0_4, CG0_5, CL0_5, Y0_5, ry_5]
= ...
simpro(EE, fm_O2_0, fm_CO2_0, rO2_0, rCO2_0, initNH3, initNO2, initAcOH, initLiqueL, ...
addCO2, addO2, Yx_AcOH, YO2_5, YCO2_5, spNO3_5, share2, cover_p);

if idisp
CG0_5p=[CG0_5p,CG0_5]
CL0_5p=[CL0_5p,CL0_5]
Y0_5p=[Y0_5p,Y0_5]
end
if (isempty(FR0_2) | isempty(FR0_4) | isempty(Y0_5)), break, end

% 2. Identification : yields of Rhodo, Nitri and Spiru
% =====
% 2.1. Rhodo: Yield of CO2 and NH3 : Yp(1) NH3 + Yp(2) AcOH --> Yp(3) CO2
ind=1:NG_2;
DC = (Y0_2(ind)-CG0_2)*Gin_2 + (X0_2(ind)-CL0_2(ind)).*(1+Kdis_2)*Fin_2; % CO2 NH3 AcOH
Yp_2(1:2,1) = DC(2:3)/DC(1);
% 2.2. Nitri: Yield of O2 CO2 and NH3 : Yp(1) O2 + Yp(2) CO2 + Yp(3) NH3 --> NO3
indG = (NB_3+1)*NG_3+[1:NG_3]; % indices of O2 CO2 NH3 G in output vector Y0
indL = (NB_3+1)*(NG_3+NL_3)+[1:NG_3];% indices of O2 CO2 NH3 L in state vector X0
indN = (NB_3+1)*(NG_3+NL_3)+NG_3+1;% indices of NO2 in state vector X0
Dp = (Y0_3(indG)-CG0_3)*Gin_3 + (X0_3(indL)-CL0_3(1:NG_3)).*(1+Kdis_3)*Fin_3;
Dc = ((X0_3(indN+1)-CL0_3(NG_3+2))-(X0_3(indN)-CL0_3(NG_3+1)))*Fin_3; % NO3-NO2
Yp_3 = Dp / Dc; % conversion yield of O2 CO2 NH3 into NO3
% 2.3. Spiru: Yield of CO2 and NO3 : Yp(1) CO2 + Yp(2) NO3 --> O2 + Yp(3) XA
DO2 = (Y0_4(1) - CG0_4(1)) * Gin_4 + (X0_4(1) - CL0_4(1)) * Fin_4;
Yp_4(1) = ((Y0_4(NG_4)-CG0_4(NG_4))*Gin_4 + (X0_4(NG_4)-
CL0_4(NG_4))*(1+Kdis_4(NG_4))*Fin_4)/DO2; % CO2
Yp_4(2) = (X0_4(NG_4+1)-CL0_4(NG_4+1))*Fin_4/DO2; % conversion yield of NO3
Yp_4(3) = X0_4(NG_4+4)*Fin_4/DO2; % production yield of XA
% 2.4. HPC: Yield of CO2 NH3 and NO3 : Yp(1) CO2 + Yp(2) NH3 + Yp(3) NO3 --> O2
% (iterative identification not necessary because yields of HPC are constant)
if idisp
DO2 = (Y0_5(1) - CG0_5(1)) * Gin_5 + (Y0_5(NG_5+1) - CL0_5(1)) * Fin_5;
Yp_5(1:2,1) = ((Y0_5(2:NG_5)-CG0_5(2:NG_5))*Gin_5 + (Y0_5(NG_5+[2:NG_5]) -
CL0_5(2:NG_5)).*(1+Kdis_5(2:NG_5))*Fin_5)/DO2; % CO2 NH3
Yp_5(3,1) = (Y0_5(2*NG_5+1)-CL0_5(NG_5+1))*Fin_5/DO2; % NO3
end

if idisp
Yp_2p=[Yp_2p,Yp_2]
Yp_3p=[Yp_3p,Yp_3]
Yp_4p=[Yp_4p,Yp_4]
Yp_5p=[Yp_5p,Yp_5]
end
% 3. Computation of the output of the identified model (for checking or debugging)
% =====
% 3.1. Screen display
if idisp
disp(['iter=',num2str(iter)])
ri_5 = ry_5/cover_p;
plotting=0; display=1; t_sim_m % results display
p6O2=lambda*(Y0_5(1)-fm_O2_0/VM_0)*Gin_5 % correction of O2 variation
p6NO3=lambda*(Y0_5(2*NG_5+1)-spNO3_5)*Fin_5 % correction of NO3 variation
pause

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```

end
% 3.2. Saving estimations on file
ksi = Yp_1(3,1)-Yp_2(1,1)/Yp_2(2,1)*Yp_1(4,1);
Tvar(iter)=iter;
initNH3t(iter,:) = initNH3;
initNO2t(iter,:) = initNO2;
initAcOHt(iter,:) = initAcOH;
addCO2t(iter,:) = addCO2;
addO2t(iter,:) = addO2;
evarO2_1(iter,:) = nMan*Yp_1(1,1);
%evarO2_3(iter,:) = - Yp_3(1,1)/Yp_3(3,1)*(ksi*nMan+ry_5(3));
evarO2_3(iter,:) = - Yp_3(1,1)/Yp_3(3,1)*ksi*nMan*share2;
evarO2_4(iter,:) = cXA0_4/Yp_4(3,1)*Fin_4;
evarO2_5(iter,:) = ry_5(1);
evarCO2_1(iter,:) = nMan*Yp_1(2,1);
evarCO2_2(iter,:) = -nMan*Yp_1(4,1)/Yp_2(2,1);
%evarCO2_3(iter,:) = -Yp_3(2,1)/Yp_3(3,1)*(ksi*nMan+ry_5(3));
evarCO2_3(iter,:) = -Yp_3(2,1)/Yp_3(3,1)*ksi*nMan*share2;
evarCO2_4(iter,:) = cXA0_4*Yp_4(1,1)/Yp_4(3,1)*Fin_4;
evarNH_1(iter,:) = nMan*Yp_1(3,1);
evarNH_2(iter,:) = -nMan*Yp_1(4,1)*Yp_2(1,1)/Yp_2(2,1);
evarNH_3(iter,:) = -Yp_3(3,1)*(cXA0_4*Yp_4(2,1)/Yp_4(3,1)*Fin_4 + ry_5(4));
evarNO_3(iter,:) = evarNH_3(iter,)/Yp_3(3,1);
evarNO_4(iter,:) = cXA0_4*Yp_4(2,1)/Yp_4(3,1)*Fin_4;
evarNH_5(iter,:) = ry_5(3);
evarNO_5(iter,:) = ry_5(4);
evarS_2(iter,:)= -Yx1_2(4)/Yx1_2(3)*Yp_1(4,1)*nMan; % consumption of
Rhodo
evarS_3(iter,:)= -Yx1_3(7,1)/Yx1_3(2,1)*Yp_3(2,1)/Yp_3(3,1)*ksi*nMan*share2; % consumption of
Nitri
evarS_4(iter,:)=sum(Yx1_4(4,:))/Yx1_4(2,1)*Yp_4(1,1)/Yp_4(3,1)*cXA0_4*Fin_4;% consumption of
Spiru and HPC
evarS_5(iter,:)=ry_5(5); % consumption of
HPC
evarP_2(iter,:)= -Yx1_2(5)/Yx1_2(3)*Yp_1(4,1)*nMan; % consumption of
Rhodo
evarP_3(iter,:)= -Yx1_3(6,1)/Yx1_3(2,1)*Yp_3(2,1)/Yp_3(3,1)*ksi*nMan*share2; % consumption of
Nitri
evarP_4(iter,:)=Yx1_4(5,1)/Yx1_4(2,1)*Yp_4(1,1)/Yp_4(3,1)*cXA0_4*Fin_4; % consumption of
Spiru and HPC
evarP_5(iter,:)=ry_5(6); % consumption of
HPC
% Global variation of O2 and CO2 from Consu input to HPC output
svareO2t(iter,:) = rO2_0 + evarO2_1(iter,:) + evarO2_3(iter,:) ...
+ evarO2_4(iter,:) + ry_5(1); % global variation of O2
svareCO2t(iter,:) = rCO2_0 + evarCO2_1(iter,:) + evarCO2_2(iter,:) + evarCO2_3(iter,:) ...
+ evarCO2_4(iter,:) + ry_5(2); % global variation of CO2

% Saving variables
addSO4t(iter,:) = -D_S;
addPO4t(iter,:) = -D_P;
share2t(iter,:) = share2;
Fin_3t(iter,:) = Fin_3;
Fin_4t(iter,:) = Fin_4;
YO2_5t(iter,:) = YO2_5;
YCO2_5t(iter,:) = YCO2_5;
FR0_2t(iter,:) = FR0_2;
FR0_4t(iter,:) = FR0_4;
nMant(iter,:) = nMan;
dG_0t(iter,:) = CG0_0';
cs_0(iter,:) = Y0_0';
cs_1(iter,:) = Y0_1';
dG_2t(iter,:) = CG0_2';
dL_2t(iter,:) = CL0_2';
cs_2(iter,:) = Y0_2';
dG_3t(iter,:) = CG0_3';
dL_3t(iter,:) = CL0_3';
cs_3(iter,:) = Y0_3';
dG_4t(iter,:) = CG0_4';
dL_4t(iter,:) = CL0_4';
cs_4(iter,:) = Y0_4';
dG_5t(iter,:) = CG0_5';
dL_5t(iter,:) = CL0_5';

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```

cs_5(iter,:) = Y0_5';

% 4. Inputs of the process for the next iteration
% =====
% 4.1. Active biomass Spiru and ratio of incoming waste
% Computation of ksi for the following matrices AA
ksi = Yp_1(3,1)-Yp_2(1,1)/Yp_2(2,1)*Yp_1(4,1);
if typloop == 3 % closing O2 and NH3/NO3
if 0 % algorithm where 'share2' is implicit
AA = [ 1/Yp_4(3,1)*Fin_4, Yp_1(1,1)-ksi*Yp_3(1,1)/Yp_3(3,1);
      -Yp_3(3,1)*Yp_4(2,1)/Yp_4(3,1)*Fin_4, ksi ];
A1 = inv(AA);
BB = [rO2_0 + ry_5(1)-Yp_3(1,1)/Yp_3(3,1)*ry_5(3);
      ry_5(3)-Yp_3(3,1)*ry_5(4) ];
else % algorithm where 'share2' is explicit (more rigorous)
AA = [ 1/Yp_4(3,1)*Fin_4, Yp_1(1,1)-ksi*share2*Yp_3(1,1)/Yp_3(3,1);
      -Yp_3(3,1)*Yp_4(2,1)/Yp_4(3,1)*Fin_4, ksi ];
A1 = inv(AA);
BB = [rO2_0 + ry_5(1);
      ry_5(3)-Yp_3(3,1)*ry_5(4)] + ...
      lambda * [(Y0_5(1)-fm_O2_0/VM_0)*Gin_5; % correction of O2 variation
                (Y0_5(2*NG_5+1)-spNO3_5)*Fin_5]; % correction of NO3 variation
end
elseif typloop == 4 % closing CO2 and NH3/NO3
AA = [ Yp_4(1,1)/Yp_4(3,1)*Fin_4, Yp_1(2,1)-Yp_1(4,1)/Yp_2(2,1)-
ksi*Yp_3(2,1)/Yp_3(3,1);
      -Yp_3(3,1)*Yp_4(2,1)/Yp_4(3,1)*Fin_4, ksi ];
A1 = inv(AA);
BB = [rCO2_0+ry_5(2)-Yp_3(2,1)/Yp_3(3,1)*ry_5(3);
      ry_5(3)-Yp_3(3,1)*ry_5(4) ] + ...
      lambda * [(Y0_5(2)-fm_CO2_0/VM_0)*Gin_5; % correction of CO2 variation
                (Y0_5(2*NG_5+1)-spNO3_5)*Fin_5]; % correction of NO3 variation
end
EE = -A1*BB;
cXA0_4 = EE(1);
nMan = EE(2);
% Computation of 'share2', 'Fin_3' and 'Fin_4'
share2 = 1 + ry_5(3)/nMan/ksi; % sharing ratio of liquid at output of compart 2 (Rhodo)
towards Nitri
Fin_3 = Fcirc*share2;% liquid flow rate through Nitri(l/h)
Fin_4 = Fin_3; % liquid flow rate through Spiru(l/h)
i_sim_3
i_sim_4
% 4.2. L phase going into Lique : SO4 PO4 at input of the open loop (concentration in mol/l)
indL = (NB_3+2)*NG_3+(NB_3+2)*(NG_3+NL_3);% index of SO4 in output vector Y0_3
D_S=Fin_2*(Y0_2(2*NG_2+1) - CL0_2(NG_2+1)) + ... % variation of SO4 in Rhodo
Fin_3*(Y0_3(indL) - CL0_3(NG_3+NL_3)) + ... % variation of SO4 in Nitri
Fin_4*(Y0_4(2*NG_4+2) - CL0_4(NG_4+2)) + ... % variation of SO4 in Spiru
Fin_5*(Y0_5(2*NG_5+2) - CL0_5(NG_5+2)); % variation of SO4 in HPC
D_P=Fin_2*(Y0_2(2*NG_2+NL_2) - CL0_2(NG_2+NL_2)) + ... % variation of PO4 in Rhodo
Fin_3*(Y0_3(indL-1) - CL0_3(NG_3+NL_3-1)) + ... % variation of PO4 in Nitri
Fin_4*(Y0_4(2*NG_4+NL_4) - CL0_4(NG_4+NL_4)) + ... % variation of PO4 in Spiru
Fin_5*(Y0_5(2*NG_5+NL_5) - CL0_5(NG_5+NL_5)); % variation of PO4 in HPC
initLiqueL = [spSO4_5; spPO4_5] - [D_S; D_P]/Fin_1;
% 4.3. L phase going into Rhodo :
if 1 % computing 'initAcOH' from estimation (stable convergency)
YAc_2= EE(2)*(1-Yx_AcOH)*Yp_1(4,1)/Fin_2; % AcOH_GL outgoing from Rhodo at previous step
initAcOH = YAc_2/(1+Kdis_2(NG_2)); % (mol/l)
else % computing 'initAcOH' from value at previous step ==> small oscillations
initAcOH = Y0_2(NG_2)*Gin_2/Fin_2/(1+Kdis_2(NG_2)) + Y0_2(2*NG_2);
end
% 4.4. L phase going into Rhodo input :
% computing 'initNH3' from value at previous step
initNH3 = (Y0_5(NG_5)*Gin_5 + spNH3_5*Fin_5) / ...
((1+Kdis_2(2))*Fin_2); % (mol/l) NH3 GL coming from HPC output and going into L
phase of Rhodo input
% 4.5. L phase going into Nitri input :
indN2 = (NB_3+2)*NG_3+(NB_3+1)*(NG_3+NL_3)+NG_3+1;% index of NO2 in output vector
initNO2 = Y0_3(indN2); % (mol/l) NO2 outgoing from Nitri at previous step
% 4.6. O2_L CO2_L at input of the open loop (concentration in mol/l)
Y02_5 = fm_O2_0/VM_0/Y0_5(1)*Y0_5(NG_5+1); % expected set point of O2_L outgoing from HPC

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YCO2_5 = fm_CO2_0/VM_0/Y0_5(2)*Y0_5(NG_5+2)*(1+Kdis_5(2))/(1+Kdis_2(1)); % expected set
point of CO2_L outgoing from HPC
% 4.7. Supply rate of CO2 G (mol/h) at HPC input if necessary
if typloop == 3 % closing O2 and NH3/NO3
addO2=0;
crit = rCO2_0 + (Yp_1(2,1)-Yp_1(4,1)/Yp_2(2,1))*nMan -
Yp_3(2,1)/Yp_3(3,1)*(ksi*nMan+ry_5(3)) ...
+ Yp_4(1,1)/Yp_4(3,1)*cXA0_4*Fin_4 + ry_5(2); % global variation in the open loop
if crit < 0
if iter < 5
addCO2 = -1.5*crit; % addition of CO2 in excess in first iterations to prevent C
limitation
else
addCO2 = -crit; % addition of CO2 exactly as needed
end
else
addCO2 = -.5*crit; % removing CO2 partly
end
% 4.8. Supply rate of O2 G (mol/h) at HPC input if necessary
elseif typloop == 4 % closing CO2 and NH3/NO3
addCO2=0;
crit = rO2_0 + Yp_1(1,1)*nMan - Yp_3(1,1)/Yp_3(3,1)*(ksi*nMan+ry_5(3)) ...
+ 1/Yp_4(3,1)*cXA0_4*Fin_4 + ry_5(1); % global variation in the open loop
addO2 = -crit; % addition of O2 exactly as needed
end

disp(['Iteration ',num2str(iter),' finished'])

end
if (isempty(FR0_2) | isempty(FR0_4) | isempty(Y0_5)),FR0_2, FR0_4, Y0_5, break, end
disp(' === End of iteration ===')
% Lique (1) :
% CG0 = []
% CL0 = [Faeces Urea]
% Y0 = [H2 CO2 NH3 AcOH BuOH SO4 PO4]
% Rhodo (2) :
% CG0 = [CO2 NH3 AcOH]
% CL0 = [CO2 NH3 AcOH SO4 PO4]
% X0 = [CO2 NH3 AcOH SO4 PO4 XA]
% Nitri (3) :
% CG0 = [O2 CO2 NH3]
% CL0 = [O2 CO2 NH3 NO2 NO3 PO4 SO4]
% X0 = [O2 CO2 NH3 NO2 NO3 PO4 SO4 XA_Ns XA_Nb XG_Ns XG_Nb] for each tank
% Spiru (4) :
% CG0 = [O2 CO2]
% CL0 = [O2 CO2 NO3 SO4 PO4]
% X0 = [O2 CO2 NO3 SO4 PO4 XA XV EPS PC CH]
% HPC (5) :
% CG0 = [O2_G CO2_G NH3_G]
% CL0 = [O2_L CO2_L NH3_L NO3 SO4 PO4]
% X0 = [O2_G CO2_G NH3_G O2_L CO2_L NH3_L NO3 SO4 PO4 Tomato Rice ...]
% Nitri:
% Indice in state vector Compound
% (i-1)*NE + 1 O2 in Liquid phase
% (i-1)*NE + 2 CO2 in Liquid phase
% (i-1)*NE + NG NH3 in Liquid phase
% (i-1)*NE + NG + 1 NO2
% (i-1)*NE + NG + 2 NO3
% Outputs
% The output vector is composed of the concentrations of the compounds
% of the column in gas and liquid phases.
% Indices of the compounds in the state vector :
% For a tank i (i between 1 and NB+2)
% Indice Compound
% (i-1)*NG + 1 O2 in Gas phase
% (i-1)*NG + 2 CO2 in Gas phase
% (i-1)*NG + 3 NH3 in Gas phase

```

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## 6.2. Simulation of the open extended MELISSA loop

```

%*****
%      Connected compartments 0,1,2,3,4A and 4B      *
%      Version 3.0      October 2001                  *
%                                                    *
%      simpro.m      Simulation of the extended MELISSA loop      *
%                  (HPC included)                              *
%                  Open loop and Steady state                  *
%                                                    *
%*****
function [CG0_0, Y0_0, Y0_1, CG0_2, CL0_2, FR0_2, X0_2, Y0_2, ...
         CG0_3, CL0_3, X0_3, Y0_3, CG0_4, CL0_4, FR0_4, X0_4, Y0_4, CG0_5, CL0_5, Y0_5, ri_5]
= ...
simpro(EE, fm_O2_0, fm_CO2_0, rO2_0, rCO2_0, initNH3, initNO2, initAcOH, initLiqueL, ...
      addCO2, addO2, Yx_AcOH, YO2_5, YCO2_5, spNO3_5, share2, cover)

global VM_0  Gin_0
global Gin_1  Fin_1  NG1_1  NG_1  NL_1  Kdis_1  rKdis_1  Yp_1p
global Gin_2  Fin_2  NG_2  NL_2  NO_2  vNB_2  vNM_2  VL_2  Yx1_2  Kdis_2  KSSO4_2  ...
      A2_2  B2_2  GG1_2  GG2_2  ...
      FRmin_2  FRmax_2  fI_2  RT_2  Ea_2  Es_2  muM_2  KJ_2  EpsJ_2  q_rhod_2  zmin_I_2
global Gin_3  Fin_3  NL_3  NG_3  NS_3  NB_3  NX_3  NO_3  NI_3  NV_3  ...
      Ae_3  Be_3  Ce_3  De_3  E_3  WX_3  WYG_3  WYL_3  ...
      iO2_3  iCO2_3  iNH3_3  iNO2_3  iSub_3  iXNs_3  iXNb_3  iXag_3  ...
      Klns_3  Klnb_3  KmNs_3  KmNb_3  mumax_3  maint_3  Yx_3  Yx1_3  Yml_3  ...
      RL_3  indG_3  indL_3  Kdis_3
global Fin_4  NG_4  NL_4  NO_4  vNB_4  vNM_4  VL_4  Yx1_4  Kdis_4  ...
      A2_4  B2_4  GG1_4  GG2_4  ...
      FRmin_4  FRmax_4  FRmaxc_4  fI_4  zPC_4  zCH_4  ...
      RT_4  Ea_4  Es_4  muM_4  muEPS_4  Kj_4  KjEPS_4  Fmin_4  zmin_I_4  ...
      KSNO3_4  KSSO4_4  KSPO4_4  KSPC_4
global Gin_5  Fin_5  NG_5  NL_5  NS_5  VG_5  VL_5  Yx1e_5  Yx1w_5  Kdis_5  ...
      Diete_5  Dietw_5  A2_5  B2_5  ind_3u5
global idisp

%>>> CONSU
% Concentrations in the incoming Gas of Consu
% =====
CG0_0 = [fm_O2_0; fm_CO2_0]/VM_0; % mol/l of O2 CO2 going into Consu
% Initial output vector of Consu (static state)
% =====
Y0_0 = CG0_0 + [rO2_0; rCO2_0]/Gin_0;

%>>> LIQUE
% Concentrations in the incoming Gas and Liquid flows of Lique
% =====
%1. Gas phase : inert gas
%2. Liquid phase :
%cFaec_0 = qFaec_0/Fin_1; % mol/l
%cUrea_0 = qUrea_0/Fin_1; % mol/l
%cSO4_0 = qSO4_0/Fin_1; % mol/l
%cPO4_0 = qPO4_0/Fin_1; % mol/l
% Output vector of Lique (static state)
% =====
Y_1 = EE(2)*Yp_1p; % (mol/h): production rate of H2 CO2 NH3 AcOH BuOH
NY = NG1_1+2*NG_1+NL_1;
NY1= NG1_1+2*NG_1;
% Gas concentration in mol/l (H2 and CO2 are totally under Gas phase)
Y0_1 = zeros(NY,1);
Y0_1(1:NG1_1) = Y_1(1:NG1_1)/Gin_1; % output conc. of H2 in Gas (mol/l)
% Liquid concentration in mol/l (NH3 and AcOH are totally under Liquid phase)
% Butyric acid is transformed into acetic acid (with fictitious consumption of O2 for mass
balance)
Y0_1(NY1+[1:2]) = Y_1(NY1+[1:2])/Fin_1./(1+Kdis_1(1:2)); % conc. in mol/l of CO2 NH3 molec.
form
Y0_1(NY1+3) = (Y_1(NY1+3)+2*Y_1(NY1+4))/Fin_1/(1+Kdis_1(3)); % conc. in mol/l of AcOH molec.
form
Y0_1(NY1+5:NY) = initLiqueL; % conc. SO4 PO4 in mol/l
Y0_1(NY1+4) = 0; % conc. in mol/l of BuOH total (transformed into AcOH)

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```

%>>> RHODO
% Initial concentrations in the incoming Gas and Liquid flows of Rhodo
% =====
%1. Gas phase (loop of inert gas) :
fm_CO2_2 = 0; % no CO2 (molar fraction)
fm_NH3_2 = 0; % no NH3 (molar fraction)
fm_Ac_2 = 0; % no AcOH (molar fraction)
CG0_2 = [fm_CO2_2; fm_NH3_2; fm_Ac_2] / VM_0; % mol/l
%2. Liquid phase :
%CL0_2 = [cCO2_0; cNH3_0; cAc_0; cSO4_0; cPO4_0] % mol/l
ind = [NY1+1:NY1+3,NY1+5:NY];
CL0_2 = Y0_1(ind).*rKdis_1; % mol/l of the molecular form CO2 NH3 AcOH
CL0_2(1) = CL0_2(1) + YCO2_5; % addition of CO2 coming from HPC output
CL0_2(2) = CL0_2(2) + initNH3; % NH3 GL coming from HPC output and going into L phase of
Rhodo input
CL0_2(NG_2) = CL0_2(NG_2) + initAcOH; % AcOH at L Rhodo input
% Initial concentration of biomass in Rhodo (to consume 'Yx_AcOH' part of AcOH load)
% =====
cX0_2 = -CL0_2(NG_2)*(1+Kdis_2(NG_2))/Yx1_2(NG_2)*Yx_AcOH; % g/l
% Initial light flux and state vector of Rhodo (steady state)
% =====
[FR0_2, X0_2, Y0_2] = stesta_2(...
NG_2, NL_2, NO_2, vNB_2, vNM_2, VL_2, Fin_2, Yx1_2, KSSO4_2, ...
A2_2, B2_2, GGL_2, GG2_2, CG0_2, CL0_2, cX0_2, ...
FRmin_2, FRmax_2, fI_2, RT_2, Ea_2, Es_2, muM_2, KJ_2, EpsJ_2, q_rhod_2, zmin_I_2);
%1. CO2 NH3 in G phase of Rhodo going into L phase of Rhodo :
X0_2(1:2) = X0_2(1:2) + (Y0_2(1:2)*Gin_2/Fin_2)./(1+Kdis_2(1:2)); % modif of state vector
%2. Modification of output vector
Y0_2(1:2) = zeros(2,1);
Y0_2(NG_2+[1:2]) = X0_2(1:2); % modif of output vector

%>>> NITRI
% Concentrations in the incoming Gas and Liquid flows of Nitri
% =====
%1. Gas phase (O2 CO2 from Consu, O2 used for H2 and butyric acid transformation) :
CG0_3 = [Y0_0; 0]; % mol/l of O2 CO2 NH3 (NH3:null) from Consu
CG0_3(1) = CG0_3(1) - (Y_1(1)/2 + Y_1(NY1+4))/Gin_3; %O2 used for H2 and butyric acid
transformation
%2. Liquid phase (from Rhodo):
%CL0_3 = [C_O2_0; C_CO2_0; C_NH3_0; C_NO2_0; C_NO3_0; C_PO4_0; C_SO4_0];
CL0_3 = link2_3(X0_2)';
CL0_3(1) = Y02_5; % function of expected set point of O2_L at Spiru output
CL0_3(NG_3+2) = spNO3_5*Fin_5/Fin_3; % set point of NO3 at HPC output
CL0_3(NG_3+1) = CL0_3(NG_3+1) + initNO2; % NO2 from previous step
% Initial state and output vectors of Nitri (steady state)
% =====
if idisp, CG0_3,CL0_3,end
[X0_3, Y0_3, dX0_3] = stesta_3( ...
NL_3, NG_3, NS_3, NB_3, NX_3, NO_3, NI_3, NV_3, ...
Ae_3, Be_3, Ce_3, De_3, E_3, WX_3, WYG_3, WYL_3, ...
iO2_3, iCO2_3, iNH3_3, iNO2_3, iSub_3, iXNs_3, iXNb_3, iXag_3, ...
KlNs_3, KlNb_3, KmNs_3, KmNb_3, mumax_3, maint_3, Yx_3, Yx1_3, Yml_3, ...
CG0_3, CL0_3, RL_3, indG_3, indL_3);
if isempty(X0_3), break, end
if idisp,X0_3p = [X0_3(indL_3);X0_3(indL_3(3)+1);X0_3(indL_3(3)+2)],end

%>>> SPIRU
% Initial concentrations in the incoming Gas and Liquid flows of Spiru
% =====
CGL0 = link3_4(Y0_3); % G and L from Nitri
%1. Gas phase :
CG0_4 = CGL0(1:NG_4); % mol/l
%2. Liquid phase [O2 CO2 NO3 SO4 PO4]
CL0_4 = CGL0(NG_4+1:2*NG_4+NL_4); % mol/l
% Initial light flux and state vector of Spiru (steady state)
% =====
if idisp, CG0_4,CL0_4,end
[FR0_4, X0_4, Y0_4] = stesta_4( ...
NG_4, NL_4, NO_4, vNB_4, vNM_4, Fin_4, VL_4, Yx1_4, ...
A2_4, B2_4, GGL_4, GG2_4, CG0_4, CL0_4, EE(1), ...
FRmin_4, FRmaxc_4, fI_4, zPC_4, zCH_4, ...

```

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```

RT_4, Ea_4, Es_4, muM_4, muEPS_4, Kj_4, KjEPS_4, Fmin_4, zmin_I_4, ...
KSN03_4, KSS04_4, KSPO4_4, KSPC_4);
if (isempty(FR0_4) | isempty(X0_4)), break, end
if idisp, X0_4, FR0_4, end

%>>> HPC
% Concentrations in the incoming Gas and Liquid flows of HPC
% =====
%1. Gas phase [O2 CO2 NH3]:
indN1 = (NB_3+2)*NG_3; % index of NH3 G in output vector of Nitri
%CG0_5 = [Y0_4(1)+addO2/Gin_5;Y0_4(NG_4)+addCO2/Gin_5;Y0_3(indN1)]; % O2 CO2 NH3
CG0_5 = [Y0_4(1:NG_4)+[addO2;addCO2]/Gin_5;Y0_3(indN1)]; % O2 CO2 NH3
%2. Liquid phase [O2 CO2 NH3 NO3 SO4 PO4]
CL0_5 = link245(X0_2,Y0_3,X0_4,share2,NG_2,Kdis_2,...
               NG_3,ind_3u5,Kdis_3,NG_4,NL_4,Kdis_4,NG_5,Kdis_5);
% Initial state and variation rates vectors of HPC (steady state)
% =====
if idisp, CG0_5,CL0_5,end
[X0_5, ri_5] = stesta_5(...
    NG_5, NL_5, NS_5, VG_5, VL_5, Fin_5, Yx1e_5, Yx1w_5, ...
    Diete_5, Dietw_5, cover, A2_5, B2_5, CG0_5, CL0_5);
Y0_5=X0_5;
if idisp, Y0_5, end

```

### 6.3. Parameters of the compartments

```

%*****
%      Consumer compartment (static behaviour)      *
%      Version 2      October 2001                  *
%                                                    *
%      Data according to TN 54.3                    *
%                                                    *
%      i_sim_0.m : Initialization of the simulation *
%                                                    *
%*****

arret = 0;

% General parameters of the simulated process
% -----
NG1= 2; % number of mono-phase substrates in the Gas phase : O2, CO2
% Parameters of the consumer compartment
% -----
Gin = Gin_4; % incoming gas volumetric rate (l/h)
rCO2r = .04; % (mol/h) CO2 production rate for 1 rat (according to TN47.3 p.8 by UAB)
rO2r = -.0445; % (mol/h) O2 consumption rate for 1 rat (according to TN47.3 p.8 by UAB)
Temp = 293; % K
VM = 22.4 * Temp / 273; % molar volume of perfect gas (l/mol)
% Saving the specific variables of the Consumer compartment
% =====
NG1_0 = NG1; VM_0 = VM;
Gin_0 = Gin;
rCO2r_0 = rCO2r; rO2r_0 = rO2r;

if arret
    break
end
disp(' *** Consumer - End of initialization ***')

```

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```

%*****
%      Liquefying compartment (static behaviour)      *
%      Version 2      October 2001                    *
%                                                     *
%      Data according to TN 54.3                      *
%                                                     *
%      i_sim_1.m : Initialization of the simulation   *
%                                                     *
%*****

arret = 0;

% General parameters of the simulated process
% -----
NG1= 1;    % number of mono-phase substrates in the Gas phase : H2
NG = 0;    % number of bi-phases substrates (in the L and G phases) :
NL = 6;    % number of mono-phase substrates in the Liquid phase : CO2 NH3 AcOH BuOH SO4 PO4
NO = NG1+NL;
% Parameters of the consumer compartment
% -----
Gin = 18;    % incoming gas volumetric rate as in Rhodo (l/h): arbitrary value
Fin = Fin_1; % l/h
Temp = 330; % K (TN35.1 ADERSA)
pH = 5;     % (TN35.1 ADERSA)
% Gas/liquid transfer parameters
% -----
KLa = inf;    % CO2 NH3 CH3COOH (l/h)
% Partition coefficients
% -----
kpartN = [3181.8; 23.832; 9.9507e-2]; % CO2 NH3 CH3COOH (T=330K,non ionic form)
kpartN = [3181.8; 23.832];           % CO2 NH3 (T=330K,non ionic form)
                                         % computed from TN35.1,ADERSA

% Dissociation coefficient (for CO2)
% -----
Ka = [5.2460e-7; 7.1050e-11];          % at T=330K, from TN 35.1,ADERSA
KCO2 = Ka/(10^(-pH))*(1+Ka(2)/10^(-pH)); % [HCO3-]+[CO3--] = KCO2 * [CO2]solvated
% Dissociation coefficient (for NH3)
% -----
Kb = 1.7517e-5;          % basicity cst at T=330K, from TN 35.1,ADERSA
Ke = 7.9653e-14;        % ionic product at T=330K, from TN 35.1,ADERSA
KNH3 = Kb*10^(-pH)/Ke;  % [NH4+] = KNH3 * [NH3]solvated
% Dissociation coefficient (for AcOH)
% -----
Ka = 1.5732e-5;          % at T=330K, from TN 35.1,ADERSA
KAc = Ka/(10^(-pH));    % [AcO-] = KAc * [AcOH]
% Dissociation coefficient (for H3PO4) (unused)
% -----
Ka = 6.166e-8;          % (at T=298K, from TN 27.2,LGCB)
xx = 10^(-pH)/Ka;      KPO4 = 1+xx; % [PO4]total = f([HPO4=])
% Dissociation vector for the biphasic substrates
% -----
Kdis = [KCO2; KNH3; KAc]; % CO2 NH3 CH3COOH
% Gas/liquid thermodynamical equilibrium constants
% -----
VM = 22.4 * Temp / 273; % molar volume of perfect gas (l/mol)
alpha = kpartN / 55.56 / VM;
% Stoichiometry of the reaction of faeces decomposition
% -----
% 1. mol product / mol faeces (from TN17.1 LGCB)
Yxf = [ .89125 ; % H2
        .25 ; % CO2
        .1055 ; % NH3
        .25 ; % CH3COOH (acetic acid)
        .0625 ; % C3H7COOH (butyric acid)
        .0 ; % H2SO4
        .0 ]; % H3PO4
% change of unit of Yxf :

```

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```

Matom = [12; 1; 16; 14; 32; 31]; % C H O N S P atomik mass
% C H O N S P
Scomp = [1 1.649 .15 .1055 0 0 ]; % stoechio composition faeces
Mfaec = Scomp*Matom;
% 2. mol product/g faeces
%Yxf = Yxf ./ (ones(NG1+NG+NL,1)*Mfaec'); % (mol substrate / g faeces)
% Stoichiometry of the reaction of urea decomposition
% -----
% 1. mol product/ mol urea (from from TN17.1 LGCB)
Yxu = [ 0 ; % H2
        1 ; % CO2
        2 ; % NH3
        0 ; % CH3COOH
        0 ; % C3H7COOH
        0 ; % H2SO4
        0 ]; % H3PO4
% change of unit of Yxu :
% C H O N S P
Scomp = [1 4 1 2 0 0]; % stoechio composition urea
Murea = Scomp*Matom;
% 2. mol product/g urea
%Yxu = Yxu ./ (ones(NG1+NG+NL,1)*Murea'); % (mol substrate / g urea)
% Saving the specific variables of the Consumer compartment
% =====
NG1_1 = NG1; NG_1 = NG; NL_1 = NL; NO_1 = NO; VM_1 = VM;
Gin_1 = Gin; Fin_1 = Fin;
Yxf_1 = Yxf; Yxu_1 = Yxu;
Kdis_1 = Kdis;

if arret
    break
end
disp(' *** Lique - End of initialization ***')

%*****
% Photoheterotrophic compartment (Rhodobacter) *
% Version 2 October 2001 *
% *
% State system according to TN 54.2 *
% *
% *
% i_sim_2.m : Initialization of the simulation *
% *
% . no mineral limitation *
% . no carbon limitation *
% . no decay of biomass *
% . waste of 1 man (data computed from TN 35.1, ADERSA) *
% . carbon source : acetate (no CO2 consumed) *
% . anaerobic condition done by means of inert gas : N2 or He *
% . light limitation law according to TN 45.1; April 1999 *
% *
%*****

arret = 0;

% General parameters of the simulated process
% -----
NG = 3; % number of bi-phases subs. (in the L and G phases) : CO2 NH3 CH3COOH
NL = 2; % number of mono-phase substrates in the liquid phase : SO4, PO4
NS = 1; % number of compounds of the biomass : biomass Rhodo
NI = 2*NG+NL+1; % nb of inputs of the process (photobio reactor)
NX = NG+NL+NS; % nb of coef of state vector X
NO = NG+NX; % nb of outputs of the process (photobio reactor)
% Parameters of the PBR
% -----

```

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```

RT = .048; % radius of the reactor (m)
VL = 7 ; % volume of liquid (l)
VL = 9; % volume of liquid (l).
% Minimum volume required for FRmax=400W/m2 and a biomass production of .118 g/h
Gin = 18; % incoming gas flow rate (l/h) (same ratio as in Spirulina)
% if Gin is time variable, move 'statesys' into the S-function 'pr_rhodo'
% in order to compute the state system at each sampling period
Fin = Fin_2; % l/h
fI = .6; % illuminated surface fraction (ADERSA meeting on May 12th 1999)
Temp = 303; % K (TN35.1 ADERSA)
pH = 7; % TN35.1 ADERSA
FRmin = 1; % (W/m2)
FRmax = 400; % (W/m2)
FRmax = 1000;% (W/m2) to allow trespassing 400 W/m2 during iterative computation
% Gas/liquid transfer parameters (same as for Spirulina : TN 43.110 p.26, UAB)
% -----
KLa = 12; % CO2 NH3 CH3COOH (1/h)
% Partition coefficients
% -----
kpartN = [1853.1; 11.349; 2.6414e-2];% CO2 NH3 CH3COOH (T=303K,non ionic form)
% computed from TN35.1,ADERSA

% Dissociation coefficient (for CO2)
% -----
Ka = [4.6271e-7; 5.1173e-11]; % at T=303K, from TN 35.1,ADERSA
KCO2 = Ka(1)/10^(-pH)*(1+Ka(2)/10^(-pH)); % [HCO3-]+[CO3--] = KCO2 * [CO2]solvated
% Dissociation coefficient (for NH3)
% -----
Kb = 1.6916e-5; % basicity cst at T=303K, from TN 35.1,ADERSA
Ke = 1.4376e-14; % ionic product at T=303K, from TN 35.1,ADERSA
KNH3 = Kb*10^(-pH)/Ke; % [NH4+] = KNH3 * [NH3]solvated
% Dissociation coefficient (for AcOH)
% -----
Ka = 1.7478e-5; % at T=303K, from TN 35.1,ADERSA
KAc = Ka/(10^(-pH)); % [AcO-] = KAc * [AcOH]
% Dissociation coefficient (for H3PO4) (unused)
% -----
Ka = 6.166e-8; % (at T=298K, from TN 27.2,LGCB)
xx = 10^(-pH)/Ka; KPO4 = 1+xx; %[PO4]total = f([HPO4=])
% Dissociation vector for the biphasic substrates
% -----
Kdis = [KCO2; KNH3; KAc]; % CO2 NH3 CH3COOH
% Gas/liquid thermodynamical equilibrium constants
% -----
VM = 22.4 * Temp / 273; % molar volume of perfect gas (l/mol)
alpha = kpartN / 55.56 / VM;
% Parameters of the RHODO first principles model (LGCB TN 45.1)
% -----
Ea=270; % mean Schuster mass absorption coefficient (m2/kg) (TN 45.1 p.15)
Es=370; % mean Schuster mass scattering coefficient (m2/kg) (TN 45.1 p.15)
muM=.15; % max. specific growth rate for acetate (1/h) (TN 45.1 p.18)
KJ=15; % half saturation constant (W/m2) (TN 45.1 p.5)
EpsJ=.01; % mean efficient intensity (W/m2) (TN 45.1 p.11)
q_rhod=3.2; % max ratio of V2/V3 (no dim)(TN 45.1 p.17)
% Computation of the state system of the biphasic compounds (same for Rhodo and Spiru)
% -----
[A2,B2,GG1,GG2] = stasys_4(NG, NL, Gin, Fin, VL, alpha, Kdis, KLa);
% Stoichiometry of the reactions of production of biomass
% -----
% 1. mol substrate/1.8505 mol biomass Rhodo (from TN 39.1 p.10)
Yx1 = [ .1495 ; % CO2
- .38749 ; % NH3
-1 ; % CH3COOH
- .006292; % H2SO4
- .02813 ]; % H3PO4
Yx1 = Yx1/1.8505;
% change of unit of Yx1 :
Matom = [12; 1; 16; 14; 32; 31]; % C H O N S P atomik mass
% C H O N S P
Scomp = [1 1.5951 .3699 .2094 .0034 .0152]; % stoecho composition biomass Rhodo
Mbio = Scomp*Matom;
% 2. mol substrate/g biomass
Yx1 = Yx1 ./ (ones(NG+NL,1)*Mbio'); % (mol substrate / g biomass)

```

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```

% Limiting factors associated to mineral limitation (similar to XA of Spirulina)
% -----
KSSO4 = 2.5e-4/(Matom(5)+4*Matom(3)); % mol/l
% Mass balance checking
% =====
% Matrices of stoichiometric composition of each of compounds :
% atom :      C      N      S      P
MSG = [      1      0      0      0; % CO2 Gas
        0      1      0      0; % NH3 Gas
        2      0      0      0]; % AcOH Gas
MSL = [ 1+Kdis(1)  0      0      0; % CO2 Liquid
        0      1+Kdis(2)  0      0; % NH3 Liquid
        2*(1+Kdis(3))  0      0      0; % AcOH Liquid
        0      0      1      0; % SO4
        0      0      0      1]; % PO4
MSS = Scomp(:,[1,4,5,6]); % biomass
MSS = MSS ./ (Mbio*ones(1,4)); % atom/g biomass
% Vector of indices in state vector
% -----
vNB = 1:NG; % indices of Biphasic compounds
vNM = NG+1:NG+NL; % indices of Monophasic compounds
vNS = NG+NL+1:NG+NL+NS; % indices of Solid compounds (biomass components)
% Solution of th(z) = 1/z
% for determination of the minimum of the function Isigma in rx_rhodo or rx_spiru
% -----
[zmin_I, ii] = dichoto('tanh', '1/', 1, 2, 100, 1e-6);
% Saving the specific variables of the Rhodobacter compartment
% =====
NL_2 = NL; NG_2 = NG; NS_2 = NS;
NI_2 = NI; NX_2 = NX; NO_2 = NO;
A2_2 = A2; B2_2 = B2; GG1_2 = GG1; GG2_2 = GG2;
KSSO4_2 = KSSO4;
Kdis_2 = Kdis; kpartN_2 = kpartN;
vNB_2 = vNB; vNM_2 = vNM; vNS_2 = vNS;
Fin_2 = Fin; Gin_2 = Gin; VL_2 = VL; VM_2 = VM;
Yx1_2 = Yx1;
fI_2 = fI; FRmin_2 = FRmin; FRmax_2 = FRmax;
RT_2 = RT;
Ea_2 = Ea; Es_2 = Es; muM_2 = muM;
KJ_2 = KJ; EpsJ_2 = EpsJ; q_rhod_2 = q_rhod; zmin_I_2 = zmin_I;
MSG_2 = MSG; MSL_2 = MSL; MSS_2 = MSS;
%tau_2 = tau; Matom_2 = Matom;
Matom_2 = Matom;
if arret
    disp(' *** Rhodo : initialization aborted ***')
    break
end
disp(' *** Rhodo - End of initialization ***')

%*****
%      Nitrifying column *
%      Version 2.3      October 2001 *
% *
%      State system according to TN 44.2 *
%      . dissociation of CO2 and NH3 *
%      . column = linear combination of tanks *
% *
%      Modifications in March 2000 *
%      . vector KlNs and KlNb moved into scalar *
%      . Monod type law for maintenance in 'irate.m' *
% *
%      i_sim_3.m      Initialization of the simulation *
% *
%*****

arret = 0;

```

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```

% Column parameters
%-----
% 1.Parameters of the previous column (until TN 48.2)
NB = 1;           % number of stirred tanks in part B (fixed bed)
VA = 1.48;       % volume of part A (l)
VB = 6.17;       % volume of part B (l)
VC = 0.45;       % volume of part C (l)
epsL = .33;      % volume ratio of liquid
epsG = .04;      % volume ratio of gas
epsT = epsG + epsL;
Gin = .03*60;    % incoming gas volumetric rate (l/h)
Fin = .0028*60; % incoming liq volumetric rate (l/h)
RG = 1*99.0;    % recycling ratio of gas
RL = 1*6.42;    % recycling ratio of liquid
fG = 0;         % ratio of backward flow in a tank (gas phase)
fL = 0;         % ratio of backward flow in a tank (liquid phase)

% 2.Parameters of the column for TN 54.2
Vmin = 31.7;    % (l) volume min of the part B (fixed bed)
Vmin = 31.7/5.5;% (l) volume min of the part B for NO3 production = .012 mol/h
(october 2001)
coef_V=Vmin/epsL/VB;% multiplicative coef. of the vol of previous column
VA = VA*coef_V; % adapted volume of part A (l)
VB = VB*coef_V; % adapted volume of part B (l)
VC = VC*coef_V; % adapted volume of part C (l)
Gin = Gin*coef_V;% adapted incoming gas volumetric rate (l/h)
Fin = Fin*coef_V;% adapted incoming liq volumetric rate (l/h)
% modif. of the L and G flow rates to fit the flow of Spirulina Compart
coef_L = max(0,(1+RL)*Fin/Fin_3 - 1);
Fin = Fin_3;           % l/h
coef_G = max(0,(1+RG)*Gin/Gin_4 - 1);
Gin = Gin_4;          % l/h
% modif. of the recycling ratio RG to keep constant '(1+RG)*Gin'
RG = RG*coef_G;
% modif. of the recycling ratio RL to keep constant '(1+RL)*Fin'
RL = RL*coef_L;

VnB = VB / NB; % volume of an equivalent stirred tank

% general parameters
%-----
NG = 3;           % number of bi-phases substrates (in the L and G phases)
NL = 4;           % number of mono-phase substrates in the liquid phase
NS = 2;           % number of strains of bacteria (Ns and Nb)
NX = NG+NL+2*NS;% nb of coef of state vector Xi for any tank
NO = NX+NG;       % nb of outputs for any tank
NI = 2*NG + NL;
NV = NI * (NB + 2);

% kinetic parameters
%-----
Nls = 4;           % nb of limiting substrates
Nis = 2;           % nb of inhibitory substrates

%           Ns           Nb
mumax = [5.7e-2 ; 3.6e-2]; % max specific growth rate (1/h)
maint = [3.38e-3; 7.92e-3]; % maintenance coefficient (1/h*(mol/gbio))

KlNs = [5.05e-6           ; % limiting substrate for growth : O2 (mol/l)
        6.625e-5          ; % limiting substrate for growth : NH3 (mol/l)
        1e-10             ]; % no limitation with HCO3- for growth (mol/l)

KlNb = [           1.7e-5 ; % limiting substrate for growth : O2 (mol/l)
        3.6e-4      ; % limiting substrate for growth : NO2- (mol/l)
        1e-10     ]; % no limitation with HCO3- for growth (mol/l)

In = [1e30 1e30 ; % inhibitory substrate : NO2- (mol/l)
      1e30 1e30]; % inhibitory substrate : NO3- (mol/l)

KmNs = KlNs(1:2,1); % limiting substrate for maintenance : O2; NH3 (mol/l)
KmNb = KlNb(1:2,1); % limiting substrate for maintenance : O2; NO2- (mol/l)

```

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```

% stoichiometric parameters
% -----
% inverse of yield of biosynthesis :
% (mol substr./mol biomass)
Yx1 = [-5.4269  -6.5106 ;
       -1        -1      ;
       -4.5341  -0.1994 ;
       4.3347   -15.1714;
       0        15.1714;
       -0.0089  -0.0089 ;
       -0.0035  -0.0035];
% 4.3099  -0.0248 ;
% 1        1      ];
% O2
% HCO3-
% NH3
% NO2-
% NO3-
% HPO4--
% SO4--
% H+ (unused for simplification)
% HO- (unused for simplification)

% inverse of yield of maintenance :
% (mol substr./mol maintenance substr.)
Ym1 = [-1.5  -0.5  ;
       0      0    ;
       -1     0    ;
       1     -1   ;
       0      1   ;
       0      0   ;
       0      0   ];
% O2
% HCO3-
% NH3
% NO2-
% NO3-
% HPO4--
% SO4--

% change of unit of Yx1 :
Matom = [12; 1; 16; 14; 32; 31]; %C H O N S P atomik mass
Scomp = [1 1.6147 .3906 .1994 .0035 .0089]; % stoechio composition
M_nitri = Scomp*Matom;
Yx1 = Yx1 / M_nitri; % (mol substrate / g biomass)

Yx(1,1) = 1/Yx1(3,1); % yield for (global) growth of Ns (g X/mol NH3)
Yx(2,1) = 1/Yx1(4,2); % yield for (global) growth of Nb (g X/mol NO2-)

% gas/liquid transfer parameters
% -----
KLa = 1*[51; 51; 500]; % O2 CO2 NH3 (1/h)

% partition coefficients
% -----
kpartN = [4.599e4; 1853.1; 11.349 ]; % O2 CO2 NH3 (T=303K,non ionic form)
% computed from TN35.1,ADERSA

% dissociation coefficient (for CO2)
% -----
Ka = 4.627e-7; % at T=303K, from TN 35.1,ADERSA
KCO2 = Ka / 1e-8; % [HCO3-] = KCO2 * [CO2]solvated

% dissociation coefficient (for NH3)
% -----
Kb = 1.6916e-5; % basicity cst at T=303K, from TN 35.1,ADERSA
Ke = 1.4376e-14; % ionic product at T=303K, from TN 35.1,ADERSA
KNH3 = Kb * 1e-8 / Ke; % [NH4+] = KNH3 * [NH3]solvated

% dissociation coefficient (for H3PO4)
% -----
Ka = 6.166e-8; % (at T=298K, from TN 27.2,LGCB)
xx = 1e-8/Ka; KPO4 = 1+xx; %[PO4]total = f([HPO4=])

% dissociation vector for the biphasic substrates
% -----
Kdis = [0; KCO2; KNH3]; % O2 CO2 NH3

% liquid/gas thermodynamical equilibrium constants
% -----
VM = 22.4 * 303 / 273; % molar volume (l/mol)
alpha = kpartN / 55.56 / VM;

% Computation of the state system of the nitrifying compartment
% -----
[Ae,Be,Ce,De,E] = stasys_3(NG, NL, NB, Gin, Fin, RG, RL, fG, fL, ...
                          VA, VnB, VC, epsL, epsG, epsT, ...
                          alpha, Kdis, KLa);

% Initialization of vector of indices
% -----
iO2 = 1:NG+NL:(NB+1)*(NG+NL)+1; % indices of O2 L in the state vector
iCO2 = iO2 + 1; % indices of HCO3- in the state vector
iNH3 = iCO2 + 1; % indices of NH3 L in the state vector
iNO2 = iNH3 + 1; % indices of NO2 in the state vector

```

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```

iNO3 = iNO2 + 1; % indices of NO3 in the state vector
iPO4 = iNO3 + 1; % indices of PO4 in the state vector
iSO4 = iPO4 + 1; % indices of SO4 in the state vector
iSub = 1:(NG+NL)*(NB+2); % ind. of subs. in state vector
iXNs = 1 : 2*NS : 2*NS*(NB+1) + 1;
iXNs = iXNs + (NG+NL)*(NB+2); % ind. of act. biomass Ns in the state vector
iXNb = iXNs + 1; % ind. of act. biomass Nb in the state vector
iXag = (NG+NL)*(NB+2) + 1 :(NG+NL+2*NS)*(NB+2); % ind. of active and global
indG0 = 1:NG; indG = indG0;
indL0 = NG+1:2*NG+NL; indL = indL0;
for ii = 1:NB+1
    indG = [indG, indG0+ii*NI]; % ind. of Gas concen. in the output vector
    indL = [indL, indL0+ii*NI]; % ind. of Liq concen. in the output vector
end
% Noise
%-----
% 1. Weight vector of the noise on the derivative of the state vector
WX0 = 0*5*[0 0 1e-6 1e-6 1e-6 0 0];
WX = WX0;
for ii = 1:NB+1
    WX = [WX, WX0];
end

% 2. Weight vector of the noise on the output vector
WYG0 = 0*5*[0 0 0];
WYL0 = 0*5*[0 0 1e-5/(1+KNH3) 0 1e-5 0 0];
WYG = WYG0;
WYL = WYL0;
for ii = 1:NB+1
    WYG = [WYG, WYG0];
    WYL = [WYL, WYL0];
end

% Checking the mass balance
%-----
% 1. Matrices of stoichiometric composition of each compounds :
% atom : C N S P
MSG = [ 0 0 0 0 ; % O2 Gas
        1 0 0 0 ; % CO2 Gas
        0 1 0 0 ]; % NH3 Gas
MSL = [ 0 0 0 0 ; % O2
        1+Kdis(2) 0 0 0 ; % CO2 L and ionic forms
        0 1+Kdis(3) 0 0 ; % NH3 L and ionic forms
        0 1 0 0 ; % NO2
        0 1 0 0 ; % NO3
        0 0 0 1 ; % HPO4
        0 0 1 0 ]; % SO4
MSS = [Scomp(:, [1,4,5,6]); Scomp(:, [1,4,5,6])]; % biomass Ns and Nb
MSS = MSS ./ ([M_nitri; M_nitri]*ones(1,4)); % atom/g biomass
% 2. matrices of volume of tanks
Vg = [ VA*epsG/epsT;
        VnB*epsG*ones(NB,1);
        VC*epsG/epsT];
Vl = [ VA*epsL/epsT;
        VnB*epsL*ones(NB,1);
        VC*epsL/epsT];

% Saving the specific variables of the Nitrifying compartment
% =====
NL_3 = NL; NG_3 = NG; NS_3 = NS;
NB_3 = NB; NX_3 = NX; NO_3 = NO; NI_3 = NI; NV_3 = NV;
Kdis_3 = Kdis;
Fin_3 = Fin; Gin_3 = Gin; RL_3 = RL;
Ae_3 = Ae; Be_3 = Be; Ce_3 = Ce; De_3 = De; E_3 = E;
WX_3 = WX; WYG_3 = WYG; WYL_3 = WYL;
iO2_3 = iO2; iCO2_3 = iCO2; iNH3_3 = iNH3; iNO2_3 = iNO2;
iSub_3 = iSub; iXNs_3 = iXNs; iXNb_3 = iXNb; iXag_3 = iXag;
KlNs_3 = KlNs; KlNb_3 = KlNb; KmNs_3 = KmNs; KmNb_3 = KmNb;
mumax_3=mumax; maint_3=maint;
Yx_3 = Yx; Yx1_3 = Yx1; Ym1_3 = Ym1;
indG_3 = indG; indL_3 = indL;
MSG_3=MSG; MSL_3=MSL; MSS_3=MSS;
Vl_3 = Vl; alpha_3=alpha; KLa_3=KLa;

```

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```

if arret
    disp(' *** Nitri : initialization aborted ***')
    break
end
disp(' *** Nitri - End of initialization ***')

%*****
%      Photoautotrophic compartment (Photosynthesis)      *
%      Version 2      October 2001                          *
%                                                           *
%      State system according to TN 54.2                    *
%      . mineral limitation (NO3 SO4)                       *
%      . no carbon limitation (conclusion of TN 32.4, LGCB) *
%      . NH3 is not a substrate (not consumed by biomass)  *
%                                                           *
%                                                           *
%      i_sim_4.m : Initialization of the simulation         *
%                                                           *
%*****

arret = 0;

% General parameters of the simulated process
% -----
NG = 2;          % number of bi-phases substrates (in the L and G phases) : O2, CO2
NL = 3;          % number of mono-phase substrates in the liquid phase:NO3, SO4, PO4
NS = 5;          % number of compounds of the biomass : XA, XV, EPS, PC, CH
NI = 2*NG+NL+1; % nb of inputs of the process (photosynthetic reactor)
NX = NG+NL+NS;  % nb of coef of state vector X
NO = NG+NX;      % nb of outputs of the process (photosynthetic reactor)

% Parameters of the PBR
% -----
RT = .076;      % radius of the reactor (m)
VL = 77;        % volume of liquid (l) (from TN43.110 p.4, UAB)
Gin = Gin_4;    % incoming gas flow rate (l/h) (from TN 43.110 p.26, UAB)
                % if Gin is time variable, move 'stasys_4' into the S-function 'pr_spiru'
                % in order to compute the state system at each sampling period
Fin = Fin_4;    % incoming liquid flow rate (l/h) (if Fin variable, do as for Gin)
fI = .688;      % Illuminated surface fraction (TN43.110 p.4, UAB)
Temp = 309;     % K
pH = 9.5;
FRmin = 5;      % (W/m2)
FRmin = .001;   % (W/m2)
FRmax = 223;    % (W/m2)
FRmaxc=1000;   % (W/m2) % used in iterative computation

% gas/liquid transfer parameters (TN 43.110 p.26, UAB)
% -----
KLa = 12;       % O2 CO2 NH3 (1/h)
% partition coefficients
% -----
kpartN = [4.9856e4; 2135.7; 13.539]; % O2 CO2 NH3 (T=309K,non ionic form)
                                           % computed from TN35.1,ADERSA
                                           % (for extension to NH3 when NH3=substrate)
kpartN = [4.9856e4; 2135.7];          % O2 CO2 (T=309K,non ionic form)
% dissociation coefficient (for CO2)
% -----
Ka = [4.882e-7; 5.661e-11];          % at T=309K, from TN 35.1,ADERSA
KCO2 = Ka(1)/10^(-pH)*(1+Ka(2)/10^(-pH)); % [HCO3-]+[CO3--] = KCO2 * [CO2]solvated
% dissociation coefficient (for NH3)
% -----
Kb = 1.7241e-5;                       % basicity cst at T=309K, from TN 35.1,ADERSA
Ke = 2.1900e-14;                       % ionic product at T=309K, from TN 35.1,ADERSA
KNH3 = Kb*10^(-pH)/Ke;                 % [NH4+] = KNH3 * [NH3]solvated
% dissociation coefficient (for H3PO4)
% -----
Ka = 6.166e-8;                         % (at T=298K, from TN 27.2,LGCB)

```

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```

xx = 10^(-pH)/Ka;   KPO4 = 1+xx;   %[PO4]total = f([HPO4=])
% dissociation vector for the biphasic substrates
% -----
Kdis = [0; KCO2; KNH3]; % O2 CO2 NH3 (for extension to NH3 when NH3=substrate)
Kdis = [0; KCO2];      % O2 CO2
% liquid/gas thermodynamical equilibrium constants
% -----
VM = 22.4 * Temp / 273; % molar volume of perfect gas (l/mol)
alpha = kpartN / 55.56 / VM;
% parameters of the Spirulina growth (TN19.2, LGCB)
% -----
zCH = .01; % mass biotic fraction of CH
zPC = .162; % mass biotic fraction of PC
Ea=872; % global absorption mass coef. (m2/kg)
Es=200; % global scattering mass coef. (m2/kg)
muM=.45; % max growth rate for biomass in relation to phycocyanins (1/h)
muEPS=1.852; % max growth rate for EPS in relation to phycocyanins (1/h)
Kj=20; % half satur. cste for energy to active biomass (W/m2)
KjEPS=750; % half satur. cste for energy to EPS synthesis (W/m2)
Fmin=1; % min incident light energy flux (W/m2)

% Computation of the state system of the biphasic compounds
% -----
[A2,B2,GG1,GG2] = stasys_4(NG, NL, Gin, Fin, VL, alpha, Kdis, KLa);
% Stoichiometry of the reactions of production of biomass
% -----
% 1. mol substrate/mol biomass
%
%      XA      EPS      Glycogen
Yx1 = [ 1.437    0.96    1.0745; % O2
       -1        -1        -1 ; % CO2
       -0.1921   0         0 ; % NO3-
       -0.0052  -0.015   -0.008 ; % H2SO4
       -0.0063   0         0 ]; % H3PO4

% change of unit of Yx1 :
Matom = [12; 1; 16; 14; 32; 31]; % C H O N S P atomik mass
%
%      C      H      O      N      S      P
Scomp = [1 1.566 .405 .1921 .0052 .0063; % stoechio composition XA
         1 1.65 .95 0 .015 0 ; % stoechio composition EPS
         1 1.67 .71 0 .008 0 ]; % stoechio composition G
Mbio = Scomp*Matom;
% 2. mol substrate/g biomass
Yx1 = Yx1 ./ (ones(NG+NL,1)*Mbio'); % (mol substrate / g biomass)
% Limiting factors associated to mineral limitation
% -----
KSNO3 = 5e-4/(Matom(4)+3*Matom(3)); % mol/l
KSSO4 = 2.5e-4/(Matom(5)+4*Matom(3)); % mol/l
KSPO4 = KSSO4; % mol/l (according to JFC)
KSPC = .06; % g/l
% Vector of indices in state vector
% -----
vNB = 1:NG; % indices of Biphasic compounds
vNM = NG+1:NG+NL; % indices of Monophasic compounds
vNS = NG+NL+1:NG+NL+NS; % indices of Solid compounds (biomass components)
% Solution of th(z) = 1/z
% for determination of the minimum of the function Isigma in rx_rhodo or rx_spiru
% -----
[zmin_I, ii] = dichoto('tanh', '1/', 1, 2, 100, 1e-6);

% Mass balance checking
% =====
% Matrices of stoichiometric composition of each of compounds :
% atom : C N S P
MSG = [ 0 0 0 0; % O2 Gas
        1 0 0 0]; % CO2 Gas
MSL = [ 0 0 0 0; % O2 Liquid
        1+Kdis(2) 0 0 0; % CO2 Liquid and ionic forms
        0 1 0 0; % NO3
        0 0 1 0; % SO4
        0 0 0 1]; % PO4
MSS = Scomp(:, [1,4,5,6]); % XA, EPS, G
MSS = MSS ./ (Mbio*ones(1,4)); % atom/g biomass

```

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```

% Saving the specific variables of the Spirulina compartment
% =====
NL_4 = NL;      NG_4 = NG;      NS_4 = NS;
NI_4 = NI;      NX_4 = NX;      NO_4 = NO;
A2_4 = A2;      B2_4 = B2;      GG1_4 = GG1;  GG2_4 = GG2;
KSPC_4 = KSPC;  KSN03_4 = KSN03;
KSSO4_4 = KSSO4;      KSPO4_4 = KSPO4;
Kdis_4 = Kdis;  kpartN_4 = kpartN;
vNB_4 = vNB;   vNM_4 = vNM;   vNS_4 = vNS;
Fin_4 = Fin;   Gin_4 = Gin;   VL_4 = VL;
Yx1_4 = Yx1;
fI_4 = fI;     FRmin_4 = FRmin;          FRmax_4 = FRmax;      FRmaxc_4 = FRmaxc;
zPC_4 = zPC;  zCH_4 = zCH;
RT_4 = RT;
Ea_4 = Ea;    Es_4 = Es;      muM_4 = muM;      muEPS_4 = muEPS;
Kj_4 = Kj;    KjEPS_4 = KjEPS;          Fmin_4 = Fmin;
MSG_4 = MSG;  MSL_4 = MSL;  MSS_4 = MSS;
zmin_I_4 = zmin_I;

if arret
    disp(' **=* Spiru : initialization aborted **=*')
    break
end
disp(' *** Spiru - End of initialization ***')

%*****
%           Higher Plants Chamber (HPC)                               *
%           Version 1.0      October 2001                             *
%                                                                 *
%           State system according to TN 54.4                         *
%           HPC simulated according to TN 32.3 by LGCB                *
%                                                                 *
%           i_sim_5.m  Initialization of the simulation                *
%                                                                 *
%*****

arret = 0;

% General parameters of the simulated process (HPC)
% -----
NG = 3;          % number of bi-phases substrates (in the L and G phases): O2, CO2, NH3
NL = 3;          % number of mono-phase substrates in the liquid phase: NO3, SO4, PO4
NS = 8;          % number of plants : Tomato, Rice, Lettuce, Potato, Soybean, Spinach, Onion,
Wheat
NI = 2*NG+NL;    % nb of inputs of the process
NX = 2*NG+NL+NS;% nb of coef of state vector X
NO = NX;         % nb of outputs of the process

% Parameters of the HPC
% -----
VG = 4e4;        % volume of Gas (l) (from Toulouse and Guelph meetings)
VL = 100;        % volume of liquid (l)(arbitrary value)
Gin = Gin_4;    % incoming gas flow rate (l/h) (from TN 43.110 p.26, UAB)
                % if Gin is time variable, move 'stasys_5' into the S-function 'pr_hpc'
                % in order to compute the state system at each sampling period
Fin = Fin_5;    % incoming liquid flow rate (l/h) (if Fin variable, do as for Gin)
Temp = 293;     % K
pH = 5.8;

% Gas/liquid transfer parameters (arbitrary value)
% -----
KLa = 10*ones(NG,1); % O2 CO2 NH3 (1/h)
% Partition coefficients
% -----
kpartN = [3.9034e4; 1.4168e3; 8.3186]; % O2 CO2 NH3 (T=293K,non ionic form)
% Dissociation coefficient (for CO2)
% -----
Ka = [4.0726e-7; 4.1500e-11]; % at T=293K, from TN 35.1,ADERSA

```

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KCO2 = Ka(1)/10^(-pH)*(1+Ka(2)/10^(-pH)); % [HCO3-]+[CO3--] = KCO2 * [CO2]solvated
% computed from TN35.1,ADERSA

% Dissociation coefficient (for NH3)
% -----
Kb = 1.6041e-5; % basicity cst at T=293K, from TN 35.1,ADERSA
Ke = 6.7220e-15; % ionic product at T=293K, from TN 35.1,ADERSA
KNH3 = Kb*10^(-pH)/Ke; % [NH4+] = KNH3 * [NH3]solvated
% Dissociation coefficient (for H3PO4)
% -----
Ka = 6.166e-8; % (at T=298K, from TN 27.2,LGCB)
xx = 10^(-pH)/Ka; KPO4 = 1+xx; %[PO4]total = f([HPO4=])
% Dissociation vector for the biphasic substrates
% -----
Kdis = [0; KCO2; KNH3]; % O2 CO2 NH3
% Liquid/gas thermodynamical equilibrium constants
% -----
VM = 22.4 * Temp / 273; % molar volume of perfect gas (l/mol)
alpha = kpartN / 55.56 / VM;
% Computation of the state system of the biphasic compounds (both G and L; not L alone)
% -----
A2 = [-diag((Gin + KLa./alpha*VL)/VG), diag(KLa*VL/VG);
diag(KLa./alpha./(1+Kdis)), -diag(Fin/VL + KLa./(1+Kdis))];
B2 = [diag(Gin/VG*ones(NG,1)), zeros(NG,NG), diag(ones(NG,1)), zeros(NG,NG);
zeros(NG,NG), diag(Fin/VL*ones(NG,1)), zeros(NG,NG),
diag(1./(1+Kdis))];
% Stoichiometric composition for 1 mol of dry plant
% -----
% 1. edible
% 1.1. digestible
%
% Coeff C H O N S P
Scomp1= [1 1 1.7928 0.8004 0.0546 0.0005 0; % Tomato
1 1 1.6650 0.7546 0.0257 0.0006 0; % Rice
1 1 1.7107 0.4464 0.1348 0.0019 0; % Lettuce
1 1 1.6492 0.7750 0.0335 0.0006 0; % Potato
1 1 1.6878 0.2952 0.1321 0.0035 0; % Soybean
1 1 1.6406 0.2835 0.1870 0.0088 0; % Spinach
1 1 1.8113 0.7510 0.0742 0.0010 0; % Onion
1 1 1.6548 0.7215 0.0430 0.0012 0]; % Wheat

% 1.2. fibre
%
% Coeff C H O N S P
Scomp2= [0.4040 1 1.6560 0.8280 0 0 0; % Tomato
0.0335 1 1.6667 0.8333 0 0 0; % Rice
0.5016 1 1.6537 0.8268 0 0 0; % Lettuce
0.1413 1 1.6513 0.8257 0 0 0; % Potato
0.2022 1 1.6000 0.8000 0 0 0; % Soybean
0.4215 1 1.6467 0.8233 0 0 0; % Spinach
0.4183 1 1.6560 0.8280 0 0 0; % Onion
0.1320 1 1.6667 0.8333 0 0 0]; % Wheat

% 1.3. edible = disgestible + fibre (for 1 mol of dry edible part of plant)
inde = 2:7; % indices of atoms CHONSP in 'Scomp1' and 'Scomp2'
Scomp= (Scomp1(:,1)*ones(size(inde))).*Scomp1(:,inde) +
(Scomp2(:,1)*ones(size(inde))).*Scomp2(:,inde);
% 2. waste
%
% Coeff C H O N S P
Scomp1= [1 1 1.43 0.62 0.017 0.007 0; % Tomato
1 1 1.43 0.62 0.017 0.007 0; % Rice
1 1 1.43 0.62 0.017 0.007 0; % Lettuce
1 1 1.43 0.62 0.017 0.007 0; % Potato
1 1 1.43 0.62 0.017 0.007 0; % Soybean
1 1 1.43 0.62 0.017 0.007 0; % Spinach
1 1 1.43 0.62 0.017 0.007 0; % Onion
1 1 1.43 0.62 0.017 0.007 0]; % Wheat
Scompw=(Scomp1(:,1)*ones(size(inde))).*Scomp1(:,inde); % for 1 mol of dry waste part of
plant
% Stoichiometry of the reactions of production of biomass
% -----
% 1. mol substrate/mol dry edible plant (edible = digestible + fiber)
%
% Tomato Rice Lettuce Potato Soybean Spinach Onion Wheat
Yx1e= [ 1.4744 1.0836 1.7627 1.1803 1.5344 1.7777 1.5266 1.2039; %
O2 -1.4040 -1.0335 -1.5016 -1.1413 -1.2022 -1.4215 -1.4183 -1.1320; %
CO2

```

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```

NH3      -0.0232  -0.0109  -0.057371 -0.0142  -0.0562  -0.0796  -0.0316  -0.0183;  %
NO3-     -0.0313  -0.0147  -0.0774   -0.0192  -0.0758  -0.1074  -0.0426  -0.0247;  %
H2SO4    -0.0005  -0.0006  -0.0019  -0.0006  -0.0035  -0.0088  -0.0010  -0.0012;  %
H3PO4     0         0         0         0         0         0         0         0 ];  %
Yxle1=[-1.1799  -0.8360  -1.1435  -0.9097  -0.8799  -0.9855  -1.1823  -0.8963];  %
H2O
% 2. mol substrate/mol dry waste plant
%   Tomato   Rice   Lettuce   Potato   Soybean   Spinach   Onion   Wheat
Yxlw= [ 1.0648  1.0648  1.0648  1.0648  1.0648  1.0648  1.0648  1.0648;  %
O2      -1.0000  -1.0000  -1.0000  -1.0000  -1.0000  -1.0000  -1.0000  -1.0000;  %
CO2     -0.0072  -0.0072  -0.0072  -0.0072  -0.0072  -0.0072  -0.0072  -0.0072;  %
NH3     -0.0098  -0.0098  -0.0098  -0.0098  -0.0098  -0.0098  -0.0098  -0.0098;  %
NO3-    -0.0070  -0.0070  -0.0070  -0.0070  -0.0070  -0.0070  -0.0070  -0.0070;  %
H2SO4    0         0         0         0         0         0         0         0 ];  %
H3PO4    Yxlw1=[-0.6923  -0.6923  -0.6923  -0.6923  -0.6923  -0.6923  -0.6923  -0.6923];  %
H2O
%% 3. checking the mass balance of the global chemical equations (atoms C H O N S P):
% % atom : C      H      O      N      S      P
% MSC = [ 0      0      2      0      0      0      ; % O2
%         1      0      2      0      0      0      ; % CO2
%         0      3      0      1      0      0      ; % NH3
%         0      1      3      1      0      0      ; % HNO3
%         0      2      4      0      1      0      ; % H2SO4
%         0      3      4      0      0      1      ; % H3PO4
%         0      2      1      0      0      0      ]; % H2O
% mass_balance_e=[Yxle;Yxle1]*MSC + Scmpe;
% mass_balance_w=[Yxlw;Yxlw1]*MSC + Scmpw;
% if ~all(all(abs(mass_balance_e) <= 1e-3 & abs(mass_balance_w) <= 1e-3))
%   disp('Mass is unbalanced in stoichiometry of reactions')
%   arret = 1;
% end
% 4. change of unit of Yx1 :
Matom = [12; 1; 16; 14; 32; 31]; % C H O N S P atomik mass
Mbioe = Scmpe*Matom; % edible
Mbiow = Scmpw*Matom; % waste
% 5. mol substrate/g dry plant
Yxle = Yxle ./ (ones(NG+NL,1)*Mbioe'); % (mol substrate / g dry edible plant)
Yxlw = Yxlw ./ (ones(NG+NL,1)*Mbiow'); % (mol substrate / g dry waste plant)
% Diet composition (1 man.hour). From TN32.3 Table 17.c p.24
% -----
%   Tomato   Rice   Lettuce   Potato   Soybean   Spinach   Onion   Wheat
Diete= [3.45  69.06  2.07  126.79  6.91  6.91  6.91  207.17]/24;% g
dry edible plant
Dietw= [32.97  82.71  1.77  63.34  3.85  10.88  10.9  315.93]/24;% g
dry waste plant
% Checking the mass balance of the process
% -----
% Matrices of stoichiometric composition of each compounds :
% atom : C      N      S      P
MSG = [ 0      0      0      0      ; % O2 Gas
%       1      0      0      0      ; % CO2 Gas
%       0      1      0      0      ]; % NH3 Gas
MSL = [ 0      0      0      0      ; % O2
%       1+Kdis(2)  0      0      0      ; % CO2 L and ionic forms
%       0      1+Kdis(3)  0      0      ; % NH3 L and ionic forms
%       0      1      0      0      ; % NO3
%       0      0      1      0      ; % SO4
%       0      0      0      1      ]; % PO4
inde = [1,4,5,6]; % indices of atoms CNSP in 'Scmpe' and 'Scmpw'
MSe= Scmpe(:,inde); % Tomato, Rice ...
MSSe= MSe ./ (Mbioe*ones(size(inde))); % CNSP atom/g dry edible plant
MSSw= Scmpw(:,inde); % Tomato, Rice ...

```

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MSSw= MSSw ./ (Mbiow*ones(size(inde)));           % CNSP atom/g dry waste plant
% Saving the specific variables of the HPC compartment
% =====
NL_5 = NL;      NG_5 = NG;      NS_5 = NS;
NI_5 = NI;      NX_5 = NX;      NO_5 = NO;
A2_5 = A2;      B2_5 = B2;
Kdis_5 = Kdis;  kpartN_5 = kpartN;
Fin_5 = Fin;   Gin_5 = Gin;   VL_5 = VL;  VG_5 = VG;
Yxle_5 = Yxle; Yxlw_5 = Yxlw; Diete_5 = Diete; Dietw_5 = Dietw;
MSG_5 = MSG;   MSL_5 = MSL;   MSSE_5 = MSSE; MSSw_5 = MSSw;

if arret
    disp(' *** HPC : initialization aborted ***'), break
else
    disp(' *** HPC - End of initialization ***')
end
% HPC (5) :
% CG0 = [O2_G CO2_G NH3_G]
% CL0 = [O2_L CO2_L NH3_L NO3 SO4 PO4]
% X0  = [O2_G CO2_G NH3_G O2_L CO2_L NH3_L NO3 SO4 PO4 Tomato Rice ...]

```

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