MELISSA

Memorandum of Understanding
ECT/FG/MMM/97.012

ESTEC/Contract N° 12924/98/NL/MV
Contract change notice No 03 of August 2001

TECHNICAL NOTE : 64.2

Mass balance of the global simulator

Version : 1
Issue : 0

J.-J. LECLERCQ

October 2002

10, rue de la Croix Martre
91873 PALAISEAU Cedex
Téléphone : (33) 1 60 13 53 53
Télécopie : (33) 1 69 20 05 63
Courriel : adersa@adersa.com

Document Change Log

Version	Issue	Date	Observation
0	0	September 2002	Draft
1	0	October 2002	Original version

TABLE OF CONTENTS

1. INTRODUCTION

The matter conservation principle is used to establish the model of any matter transformation process. As this rule is included in the simulation programme, the results are bound by it and it should be checked within the tolerance error due to modelling approximations and, in a lesser degree, numerical computations. So checking that the results are actually bound by this rule is a way of checking the simulation programme itself. The condition is not sufficient to establish the reliability of the software but it is necessary.

So far, any simulation software of a MELISSA compartment has passed the test for each of the atoms C, N, S and P implied in the chemical reactions. The atoms H and O have not been taken into consideration because the transformation of H_2O has not been modelled as the variations of this compound is low (about 10^{-3} in relative proportion) compared to the flow rate of the reactional medium.

In this study, the variations of H_2O are included in the modelling and the checking of the matter conservation principle is extended to the atoms H and O in the following programmes :

- global simulator;
- dynamical behaviour of the 3 connected compartments 2,3 and 4a (Rhodobacter, Nitrifying and Spirulina).

Status of the models :

The status of achievement of the simulated compartments is unchanged compared to TN 54.4 and is recalled hereafter:

1_ The Consumer compartment, which is considered from the gaseous aspect only, is simply represented by a consumption rate of O_2 and a production rate of CO_2. In the examples given hereafter, these data are (according to TN 47.3 by UAB) :

- O_2 consumption = 4.45 10^{-2} mol/h/rat;
- CO_2 production = 4 10^{-2} 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 :

$$1\,[\text{faeces}] + 0.975\,H_2O \rightarrow \qquad \text{(R1)}$$
$$0.25\,CO_2 + 0.89125\,H_2 + 0.25\,C_2H_4O_2 + 0.0625\,C_4H_8O_2 + 0.1055\,NH_3$$

$$CH_4ON_2 + H_2O \rightarrow CO_2 + 2\,NH_3 \qquad \text{(R2)}$$

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 :

$$C_3H_7COOH + O_2 \rightarrow 2\,CH_3COOH \qquad \text{(R3)}$$

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 :

$$CO_2 + 0.827\ H_2O + 0.008\ H_2SO_4 \rightarrow C\ H_{1.67}\ O_{0.71}\ S_{0.008} + 1.0745\ O_2 \qquad (R4)$$

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 :

$$CO_2 + NH_3 + HNO_3 + H_2SO_4 + H_2O \rightarrow O_2 + [CHONS]_{digestible} + [CHONS]_{fibre} \qquad (R5)$$

and

$$CO_2 + NH_3 + HNO_3 + H_2SO_4 + H_2O \rightarrow O_2 + [CHONS]_{waste} \qquad (R6)$$

whose stoechiometric coefficients are given in TN 32.3 table 15.

2. METHOD

2.1. Mass balance

Given a reactor with a constant volume V. Given q the volumetric flow rate passing through the reactor. Given x and y the concentrations of an atom j in the input flow and in the reactor, respectively.

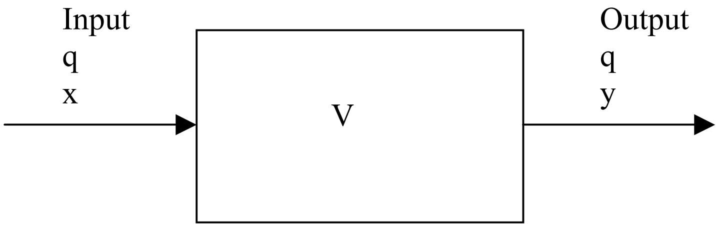

Figure 1 : General flow sheet of a reactor

The matter conservation principle can be expressed as follows :
the input flow rate $q \cdot x$ is equal to the output flow rate $q \cdot y$ increased with the variation inside the reactor $V \cdot \frac{dy}{dt}$.

$$q \cdot x = q \cdot y + V \cdot \frac{dy}{dt} \tag{1}$$

Given for each atom C, H, O, N, S and P :

c_{Gi} : molar concentration in the incoming gas phase
c_{Li} : molar concentration in the incoming liquid phase
c_G : molar concentration in the reactor or outgoing gas phase
c_L : molar concentration in the reactor or outgoing liquid phase
c_S : molar concentration in the reactor or outgoing solid phase

The total input molar flow rate, i.e. the molar flow rate of an atom j before the transformation, is expressed by :

$$r_{Ti} = q_G \cdot c_{Gi} + q_L \cdot c_{Li} \tag{2}$$

The variable r_{Ti} represents the left-hand side term of the expression (1).
The right-hand side term of (1) is expressed by :

$$r_T = V_G \cdot \frac{dc_G}{dt} + q_G \cdot c_G + V_L \cdot \frac{dc_L}{dt} + q_L \cdot c_L + V_L \cdot \frac{dc_S}{dt} + q_L \cdot c_S \tag{3}$$

Given c_m the concentration in the liquid and solid phases of the reactor :

$$c_m = c_L + c_S \tag{4}$$

the relation (3) becomes :

$$r_T = V_G \cdot \frac{dc_G}{dt} + q_G \cdot c_G + V_L \cdot \frac{dc_m}{dt} + q_L \cdot c_m \tag{5}$$

Given the matrices M_{Gj}, M_{Lj} and M_{Sj} whose coefficients are the stoechiometric composition in atom j (C, H, O, N, S or P) of the Gas, Liquid and Solid phases (theses matrices are detailed for each compartment in annex).
The molar concentrations defined above are expressed by :

$$
\begin{aligned}
c_{Gij} &= d_G \cdot M_{Gj} \\
c_{Lij} &= d_L \cdot M_{Lj} \\
c_{Gj} &= a \cdot M_{Gj} \\
c_{Lj} &= b \cdot M_{Lj} \\
c_{Sj} &= b_S \cdot M_{Sj}
\end{aligned}
\qquad (6)
$$

where :

- d_G and d_L are general notation of the molar concentrations of the different phases Gas and Liquid of the incoming flow;
- a, b and b_S are the molar concentrations of the different phases Gas, Liquid and Solid of the output flow.

In this system (6), d_G, d_L, a, b and b_S are row vectors (depending on time) and M_j are column vectors for atom j.

Checking the mass balance consists in checking the relation (1), equivalent to :

$$r_{Ti} = r_T \qquad (7)$$

And, if the incoming flow rate is not zero, the relative distance is expressed by :

$$\delta = \frac{r_T - r_{Ti}}{r_{Ti}} \qquad (8)$$

These 3 variables (r_{Ti} , r_T and δ) are traced in every simulation in order to reveal the existence of a bug in the software.

2.2. Modelling the production or consumption of water

As the variations of water as product or substrate of the chemical reactions are small compared to the water of the reactional medium, there is no risk that water may interfere in the reactions. So there is no need to take the water concentration in the equations describing the process.

The variations of water implied by the chemical reactions are simply computed in stoechiometric proportion of the variations of biomass (for compartments Rhodo, Nitri, Spiru and HPC) and of urea and faeces (for the Liquefying compartment).

3. EXAMPLES

3.1. Dynamic behaviour of the 3 connected compartments 2, 3 and 4a

The simulator of these 3 compartments has already been described in TN54.2 and is recalled in the figure 2.

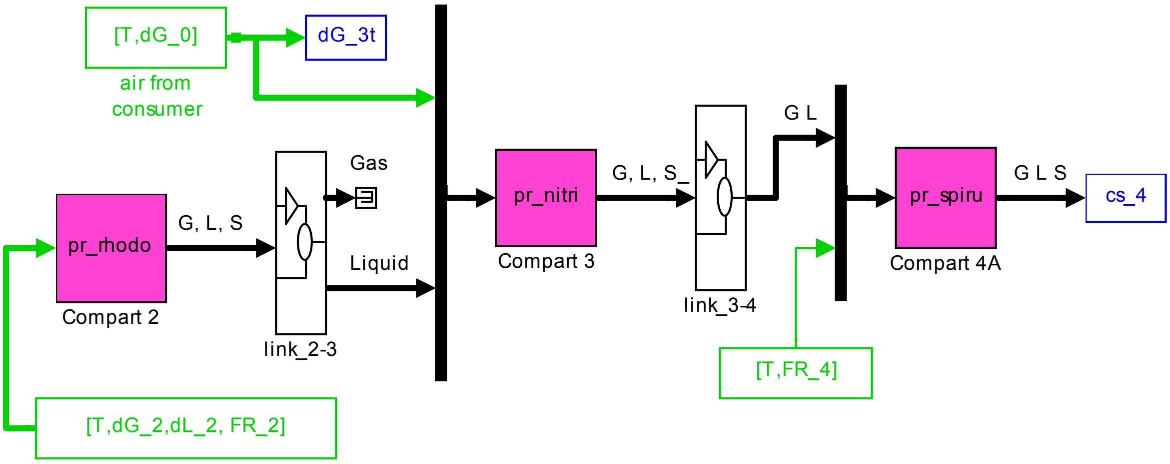

Figure 2 : Simulator of the 3 connected compartments

The conditions of the simulation are the same as in TN54.2 . The test consisted of a light flux step at Rhodo compartment at time 20 h. Only the 100 first hours are plotted in order to zoom in the transient behaviour. In TN 54.2, the mass balance was checked for the atoms C, N, S and P only. The present aim is to show the extension of the mass balance checking to the atoms H and O for each of the compartments (figures 3 to 5).

The following figures 3 to 5, related to the compartments Rhodo, Nitri and Spiru respectively, show that the mass balance is checked for all these 6 atoms within a relative error tolerance of less than 10^{-4}, even during the transient where approximations on time constants could have imbalanced matter transformation.

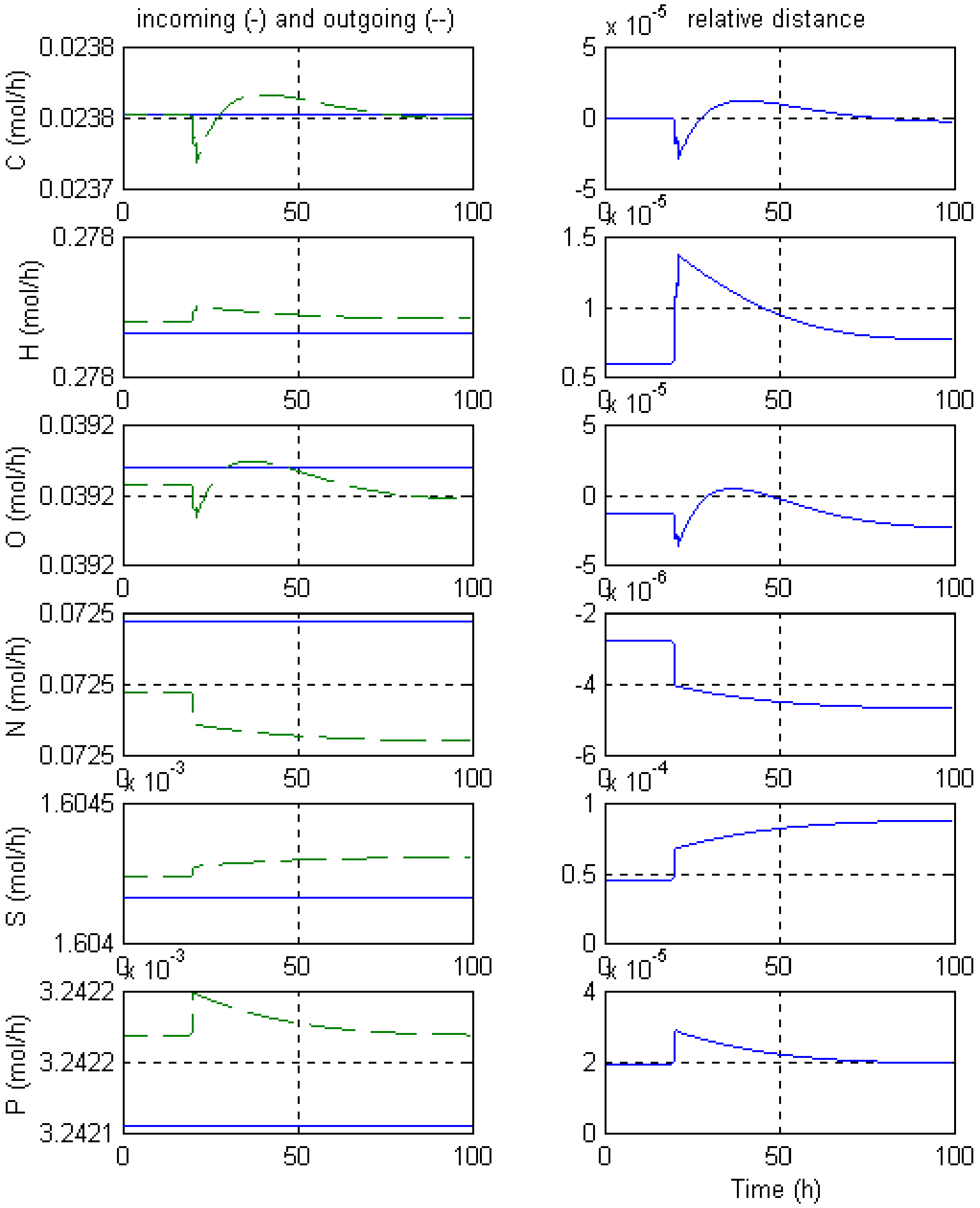

Figure 3 : Mass Balance (atoms C H O N S P) in Rhodo
The variables r_{Ti} and r_T of relation (7) are shown in the left-hand side column of figure (blue and green lines respectively).
The relative distance δ of relation (8) is lower than 10^{-4} for each atom C H O N S and P (right hand side column of figure).

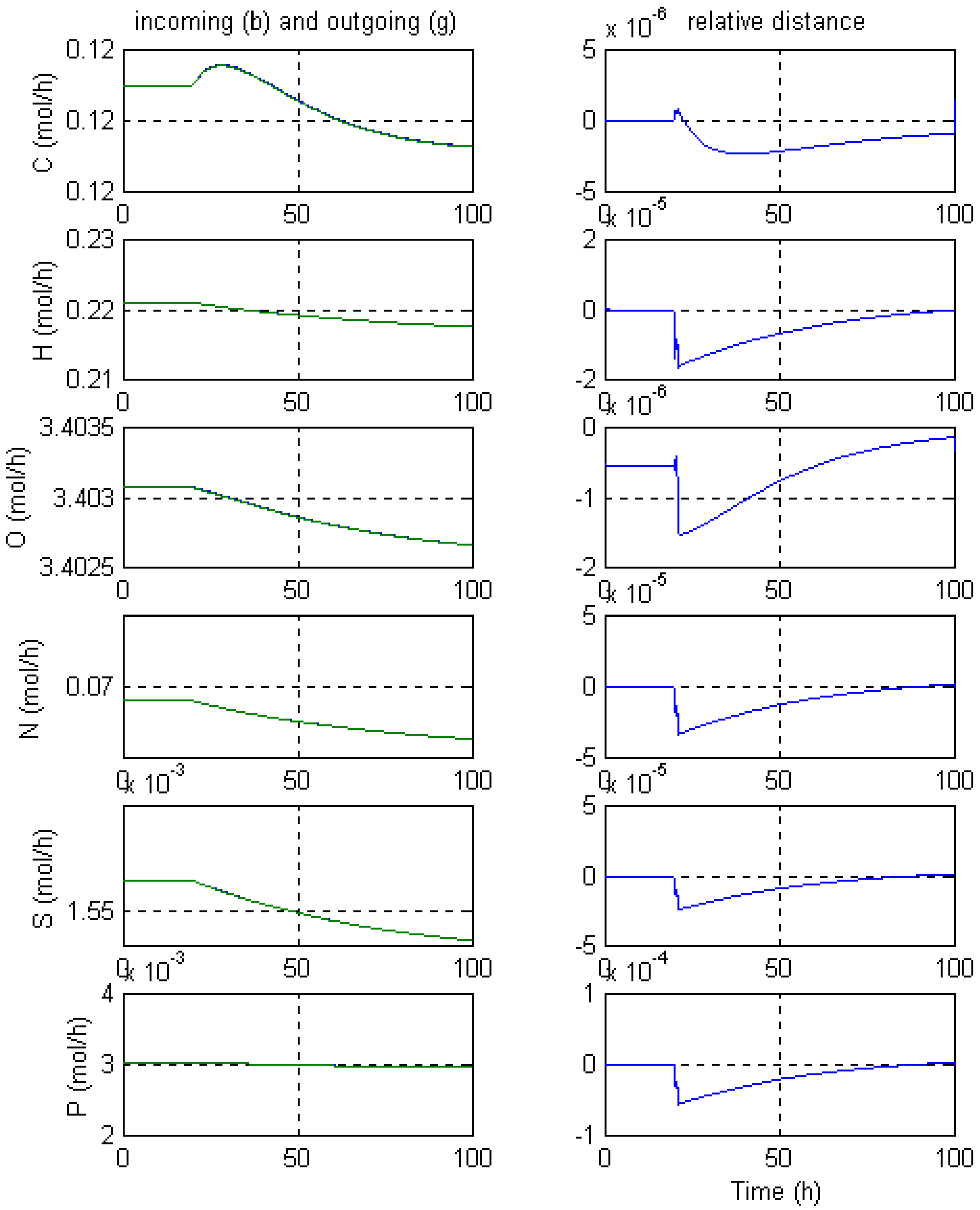

Figure 4 : Mass Balance (atoms C H O N S P) in Nitri
The variables r_{Ti} and r_T of relation (7) are shown in the left-hand side column of figure (blue and green lines respectively).
The relative distance δ of relation (8) is lower than 10^{-4} for each atom C H O N S and P (right hand side column of figure).

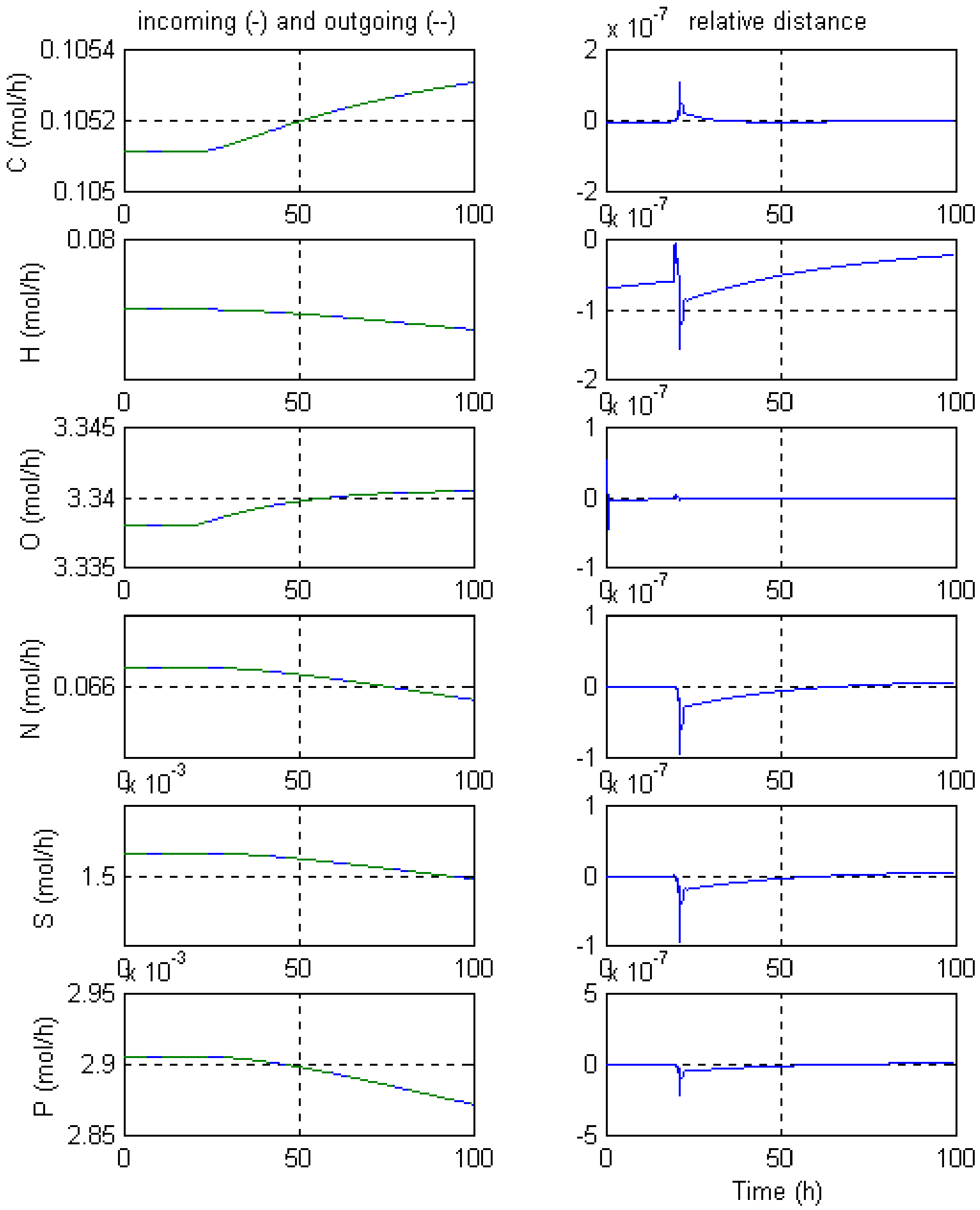

Figure 5 : Mass Balance (atoms C H O N S P) in Spiru
The variables r_{Ti} and r_T of relation (7) are shown in the left-hand side column of figure (blue and green lines respectively).
The relative distance δ of relation (8) is lower than 10^{-6} for each atom C H O N S and P (right hand side column of figure).

3.2. Global simulator

The global simulator, in its steady state behaviour, has already been described in TN54.4 and is recalled in figure 6. It has been modified here in order to take into account the production of butyric acid in the Liquefying compartment.

In TN 54.4, butyric acid was supposed to be transformed into acetic acid (R1) before entering Rhodo, because the transformation of butyric acid inside Rhodo was not modelled yet by LGCB. That fictitious reaction :

$$C_4H_8O_2 + O_2 \rightarrow 2\ C_2H_4O_2 \qquad \text{(R1)}$$

was criticizable because, even if the mass balance was respected, it was too far from physical phenomenon.

So, in the present study, the model of Rhodo is modified in order to degrade butyric acid according to the stoechiometry of TN 39.1 by LGCB (R2) and assuming that the light law is the same as for acetic acid (assumption by ADERSA which will be cancelled as soon as the modelling of transformation of butyric acid is done by LGCB) :

$$C_4H_8O_2 + 0.9689\ NH_3 + 0.0704\ H_3PO_4 + 0.0156\ H_2SO_4 + 0.6261\ CO_2 \qquad \text{(R2)}$$
$$\rightarrow 4.6261\ CH_{1.5951}O_{0.3699}N_{0.2094}S_{0.0034}P_{0.0152} + 1.8850\ H_2SO_4$$

This second approach, if not completely satisfactory, is more rigorous.

The results of 2 examples of closing the MELISSA loop, previously described in TN 54.4, are presented in the following tables 1 and 2. They show that the mass transformation is balanced within a relative error tolerance lower than 4 10^{-4}.

Example 1 : closing O_2 and NH_3/NO_3 :

	C	**H**	**O**	**N**	**S**	**P**
input rate (mol/h)	3.7425e-001	5.7502E-001	9.9841e-001	1.6825e-002	1.7711e-003	3.3555e-004
output rate (mol/h)	3.7425e-001	5.7500e-001	9.9838e-001	1.6830e-002	1.7712e-003	3.3557e-004
relative distance	1.1192e-005	3.3059e-005	2.8329e-005	2.9704e-004	2.4809e-005	3.7238e-005

Table 1 : mass balance of atoms C H O N S and P

Example 2 : closing CO_2 and NH_3/NO_3 :

	C	**H**	**O**	**N**	**S**	**P**
input rate (mol/h)	3.5259e-001	5.4054E-001	9.8650e-001	1.3768e-002	1.6043e-003	2.2547e-004
output rate (mol/h)	3.5258e-001	5.4053e-001	9.8647e-001	1.3773e-002	1.6043e-003	2.2548e-004
relative distance	1.1600e-005	2.8526e-005	2.6505e-005	3.6678e-004	2.2389e-005	4.4922e-005

Table 2 : mass balance of atoms C H O N S and P

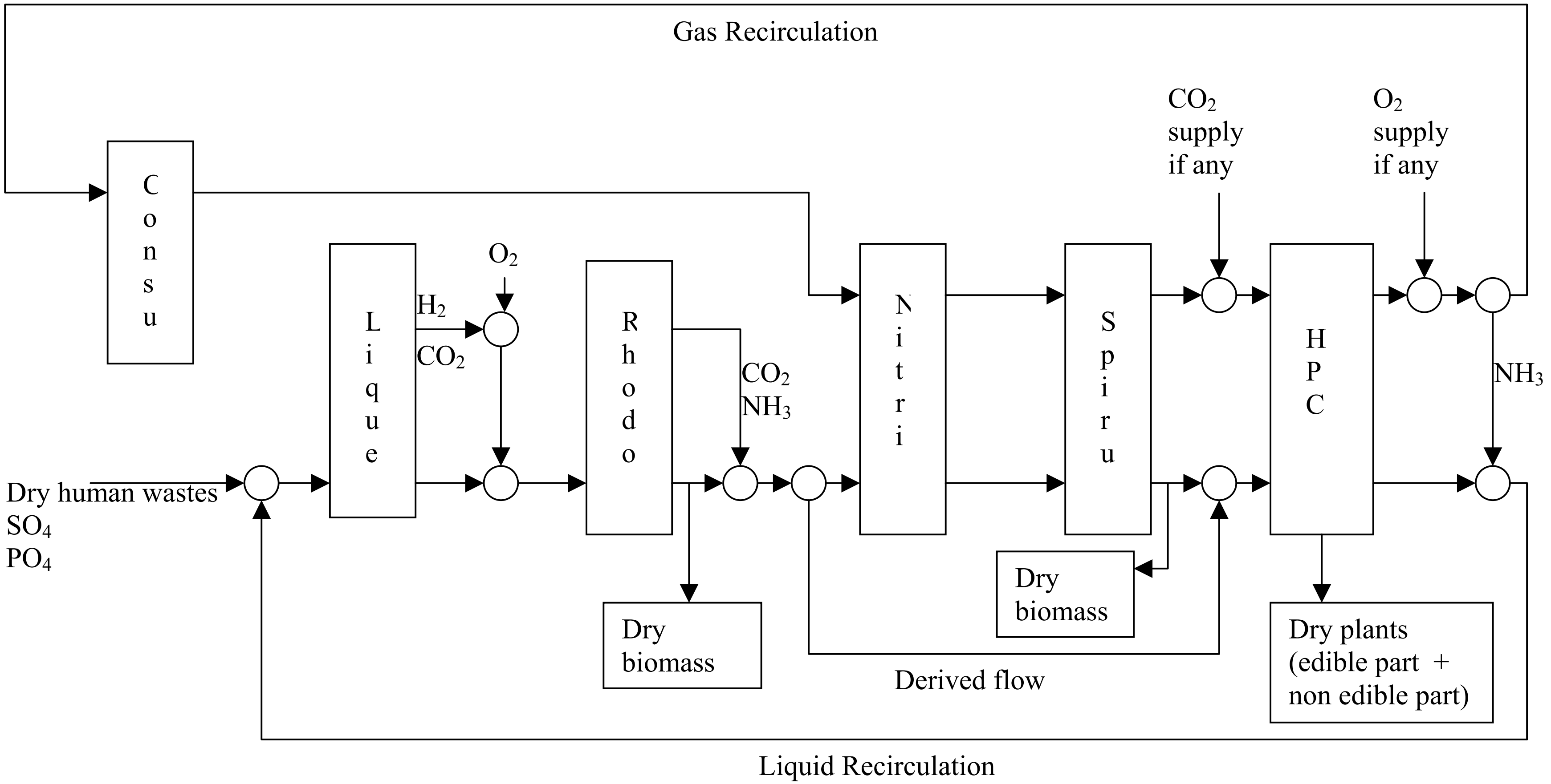

Figure 6 : Gas and Liquid connections between compartments

One remembers that the consumption of gaseous O_2 *at output of the Liquefying compartment is not physically possible; but, in the simulator, it is needed for the transformation of* H_2 *, produced by Lique, into* H_2O*.*

4. CONCLUSION

Before this technical note, the simulator of each compartment was equipped with a programme in charge of checking the mass balance of each atom C, N, S and P at any moment in order to reveal the trace of a mistake that be could introduced when the software is modified.

The checking is now extended to atoms H and O, which improves the reliability of simulator.

5. REFERENCES

LECLERCQ J.-J. : "Steady state of the compartments : Rhodobacter, Nitrifying and Spirulina". Contract ESTEC n° 12924/98/NL/MV, Contract change notice n° 1 of May 1999. March 2001. TN 54.1.

LECLERCQ J.-J. : "Overall strategy for the interfacing of the HPC to the MELISSA loop". Contract ESTEC n° 12924/98/NL/MV, Contract change notice n° 2 of May 2000. November 2001. TN 54.4.

POUGHON L. "Towards a dynamic model of the MELISSA loop". ESTEC contract PO 161031, November 1998, TN 39.1.

6. ANNEX

6.1. Stoechiometry matrices of compounds for each compartment

The matrices M_G, M_L and M_S (composed of the column vectors M_{Gj}, M_{Lj} and M_{Sj} of relation (6)) are designed MSG, MSL and MSS respectively in the following statements of the software.

6.1.1. Liquefying

```
% Stoechiometry matrix of the chemical compounds (atoms C H O N S P):
% atom : C         H         O         N         S         P
MSC = [  0         2         0         0         0         0       ;  % H2
         1         0         2         0         0         0       ;  % CO2
         0         3         0         1         0         0       ;  % NH3
         2         4         2         0         0         0       ;  % CH3COOH
         4         8         2         0         0         0       ;  % C3H7COOH
         0         2         4         0         1         0       ;  % SO4H2
         0         3         4         0         0         1       ]; % PO4H3
Scompf =[1         1.649      .15       .1055    0         0   ]; % stoechio
composition faeces
Scompu =[1         4         1         2         0         0]; % stoechio
composition urea
```

6.1.2. Rhodobacter

```
% Stoechiometry matrix of the chemical compounds (atoms C H O N S P):
% atom : C         H         O         N         S         P
MSC = [  1         0         2         0         0         0       ;  % CO2
         0         3         0         1         0         0       ;  % NH3
         2         4         2         0         0         0       ;  % CH3COOH
         4         8         2         0         0         0       ;  % C3H7COOH
         0         2         4         0         1         0       ;  % H2SO4
         0         3         4         0         0         1       ]; % H3PO4
Scompr= [1     1.5951  0.3699  0.2094  0.0034 0.0152]; % stoechio composition
biomass Rhodo
```

```
% Stoechiometry matrices of compounds in Gas Liquid and Solid phases :
MSG = MSC(1:NG,:);                        % CO2 NH3 AcOH BuOH : Gas
MSL = MSC;
MSL(1:NG,:) = diag(1+Kdis)*MSL(1:NG,:);   % CO2 NH3 AcOH BuOH : solvated and ionic
forms
MSS = Scompr ./ (Mbio*ones(size(Matom')));% CHONSP atom/g biomass Rhodo
```

6.1.3. Nitrifying

```
% Stoechiometry matrix of the chemical compounds (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         2         1         0         0       ;  % NO2H
         0         1         3         1         0         0       ;  % NO3H
         0         3         4         0         0         1       ;  % PO4H3
         0         2         4         0         1         0       ]; % SO4H2
Scompn = [1     1.6147 .3906 .1994 .0035 .0089]; % stoechio composition biomass
nitri
% Stoechiometry matrices of compounds in Gas Liquid and Solid phases :
MSG = MSC(1:NG,:);  % O2 CO2 NH3 : Gas
MSL = MSC;
MSL(1:NG,:) = diag(1+Kdis)*MSL(1:NG,:); % O2 CO2 NH3 : solvated and ionic forms
MSS = Scompn ./ (M_nitri*ones(size(Matom')));  % CHONSP atom/g biomass Ns or  Nb
MSS = [MSS; MSS];                              % CHONSP atom/g biomass Ns and Nb
```

6.1.4. Spirulina

```
% Stoechiometry matrix of the chemical compounds (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         1         3         1         0         0       ;  % NO3H
         0         2         4         0         1         0       ;  % SO4H2
         0         3         4         0         0         1       ]; % PO4H3
%        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
% Stoechiometry matrices of compounds in Gas Liquid and Solid phases :
MSG = MSC(1:NG,:);                        % O2 CO2 : Gas
MSL = MSC;
MSL(1:NG,:) = diag(1+Kdis)*MSL(1:NG,:);   % O2 CO2 : solvated and ionic forms
MSS = Scomp ./ (Mbio*ones(size(Matom'))); % CHONSP atom/g biomass XA, EPS, G
```

6.1.5. HPC

```
% Stoechiometry matrix of the chemical compounds (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       ;  % NO3H
         0         2         4         0         1         0       ;  % SO4H2
         0         3         4         0         0         1       ]; % PO4H3
% Stoechiometry matrix of 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'
Scompe=(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
% Stoechiometry matrices of compounds in Gas Liquid and Solid phases :
MSG = MSC(1:NG,:);                        % O2 CO2 NH3 : Gas
MSL = MSC;
MSL(1:NG,:) = diag(1+Kdis)*MSL(1:NG,:);   % O2 CO2 NH3 : solvated and ionic forms
MSSe=Scompe ./ (Mbioe*ones(size(Matom')));% CHONSP atom/g dry edible part of plant
MSSw=Scompw ./ (Mbiow*ones(size(Matom')));% CHONSP atom/g dry waste  part of plant
```

6.2. Programme of the mass balance checking of the MELISSA loop

```
%***********************************************************************
%       Global simulator                                               *
%       Version 1.0     September 2002                                 *
%                                                                      *
%       Models of the MELISSA loop described in TN 64.2                *
%                                                                      *
%       loop_bal.m   Checking the mass balance of the MELISSA loop     *
%                                                                      *
%***********************************************************************
% If the Workspace is empty,
% data have to be loaded into the Workspace from the file 'simloop3' or 'simloop4'

i_sauv = 0; % 1 for saving
if i_sauv, diary results, end

% Flux of H2O as substrate or product of the chemical reaction in each compart
% Flux > 0 when H2O is production or consumption?  by the chemical reaction
% (= flux inside the reactor)
dH2O = zeros(1,6); % Compartments 0 to 4B
% 1. Flux of H2O in Consu (compartment 0)
dH2O(1,1) = 0; % no flux of H2O in Consu (not yet)
% 2. Flux of H2O in Lique (compartment 1)
```

```
% 2.1. Init of variables
Yxf = Yxf_1;  Yxf1 = Yxf1_1;  Yxu1 = Yxu1_1;
% 2.2. Computation of H2O flux based on consumption rate of faeces and urea
%      Recall : 'Yxf(1)' H2O is produced by combustion of 'Yxf(1)' H2
dH2O(1,2) = nMan*(Faec/abs(Yxf1(2))*(Yxf1(1)+Yxf(1)) + Urea/abs(Yxu1(2))*Yxu1(1));
% 3. Flux of H2O in Rhodo (compartment 2)
% 3.1. Init of variables
[m,n] = size(cs_3);
cX_2 = cs_2(m,2*NG_2+NL_2+1); % conc. of biomass Rhodo at reactor output
% 3.2. Flux of H2O as substrate or product of the chemical reaction
rAcBu = cs_2(m,NG_2+3) ./ (sum(cs_2(m,NG_2+[3,4])')'); % ratio of AcOH versus
(AcOH+BuOH)
dH2O(1,3) = Fin_2*cX_2*([rAcBu,(1-rAcBu)]* Yx11_2(1,:)');    % mol/h of H2O
% 4. Flux of H2O in Nitri (compartment 3)
% 4.1. Init of variables
[m,n] = size(cs_3);
iXNs = iXNs_3;  iXNb = iXNb_3;  Vg = Vg_3;  Vl = Vl_3;
iO2 = iO2_3;  iCO2 = iCO2_3;  iNH3 = iNH3_3;  iNO2 = iNO2_3;
KlNs = KlNs_3;  KlNb = KlNb_3;  KmNs = KmNs_3;  KmNb = KmNb_3;
mumax=mumax_3;  maint=maint_3;
Yx11 = Yx11_3;  Ym11 = Ym11_3;
MSC1=MSC1_3;
NG=NG_3; NB=NB_3; NS=NS_3;
% 4.2. Computation of H2O flux based on production rates of active biomass Ns and
Nb
x = cs_3(m,NG*(NB+2)+1:n)'; % State vector at point m
% Computation of the matrix J (as done in 'pr_nitri' and adapted to H2O)
[mui,mai,rmu] = irate(x,iO2,iCO2,iNH3,iNO2,KlNs,KlNb,KmNs,KmNb,mumax,maint);
dim = 1; % only one compound : H2O
J = zeros(dim*(NB+2),NS*(NB+2));
ind1 = 1:dim;
ind2 = 1:NS;
for ii = 1:NB+2
  Ji = Yx11(1,:)*diag(mui(:,ii)) + Ym11*diag(mai(:,ii)); % stoechio of H2O
  J(ind1,ind2) = Ji;
  ind1 = ind1 + dim;
  ind2 = ind2 + NS;
end
Cx = [x(iXNs)'; x(iXNb)'];  % (g/l) conc. of active biomass Ns and Nb
Cx = reshape(Cx,NS*(NB+2),1);
dH2O(1,4) = Vl'*J*Cx; % (mol/h) flux of H2O due to the chemical reaction in Nitri
% 5. Flux of H2O in Spiru (compartment 4a)
% 5.1. Init of variables
ind = 2*NG_4+NL_4;
cX_4 = [cs_4(m,ind+[1,3]), cs_4(m,ind+2)-cs_4(m,ind+1)]; % biomass XA EPS G
% 5.2. Flux of H2O as substrate or product of the chemical reaction
dH2O(1,5) = Fin_4*cX_4*Yx11_4(1,:)'; % (mol/h of H2O)
% 6. Flux of H2O in HPC (compartment 4b)
dH2O(1,6) = cover_p*(Diete_5*Yx1e1_5(1,:)' + Dietw_5*Yx1w1_5(1,:)');

% Input flow rate (mol/h) of atoms CHONSP
inmol = zeros(8,6);
inmol(1,:) = nMan*Faec*Scompf;                 % faeces
inmol(2,:) = nMan*Urea*Scompu;                 % urea
inmol(3,:) = nRat*rCO2r*[1 0 2 0 0 0];         % CO2 rejected by rats
inmol(4,:) = addO2* [0 0 2 0 0 0];             % addition of O2 at HPC output
inmol(5,:) = addCO2*[1 0 2 0 0 0];             % addition of CO2 at HPC input
inmol(6,:) = (-D_S)*[0 2 4 0 1 0];             % addition of SO4H2
inmol(7,:) = (-D_P)*[0 3 4 0 0 1];             % addition of PO4H3
inmol(8,:) = (-sum(dH2O))*[0 2 1 0 0 0];       % consumption of H2O by the chemical
reactions

% Computation of production of decayed biomass of Nitri (g/h)
% Recall : at steady state, decay rate = global rate
```

```
nx = zeros(1, NS_3);% decay rate (g/h) of biomass k of the whole column
for k = 1:NS_3      % for biomass Ns Nb
  ind = NS_3+k : 2*NS_3 : (NB_3+1)*(2*NS_3)+NS_3+k;
  ind = ind+(NG_3+NL_3)*(NB_3+2); % indices of global biomass in state vector
  nx(1,k) = dX0_3(ind,1)' * Vl_3; % production rate (g/h) of global biomass
end
dx_3 = nx*MSS_3; % (g/h) production of decayed biomass of Nitri

% Molar output flow rate (mol/h) of atoms CHONSP
outmol = zeros(6,6);
outmol(1,:) = Fin_2*cX_2*MSS_2;             % production of biomass Rhodo
outmol(2,:) = dx_3;                         % production of biomass Nitri
outmol(3,:) = Fin_4*cX_4*MSS_4;             % production of biomass Spiru
outmol(4,:) = cover_p*Diete*MSSe;           % production of edible part of plants
outmol(5,:) = cover_p*Dietw*MSSw;           % production of waste  part of plants
outmol(6,:) = nRat*(-rO2r)*[0 0 2 0 0 0];   % sink of O2 due to rats

format short e
disp(' ')
disp('Balance of atoms CHONSP :')
disp('=========================')
disp('  rows 1 to 3 : input rate (mol/h); output rate (mol/h); relative distance')
disp('     C            H            O            N            S            P')
disp([sum(inmol);sum(outmol);abs((sum(inmol)-sum(outmol))./sum(inmol))])
```