MELISSA

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TECHNICAL NOTE : 54.3

Overall strategy for the interfacing of the HPC to the MELISSA loop

Phase I : closing the loop (without HPC)

Version : 1
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Abbreviations or notations:
AcOH : Acetic acid
CH : chlorophyll
CO_2 : carbon dioxide (gaseous or solvated)
EPS : exopolysaccharide
HPC : Higher Plant Chamber
NH_3 : ammonia (gaseous or solvated)
NO_2 : nitrite ion
NO_3 : nitrate ion
N_s : Nitrosomonas
N_b : 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.

1. INTRODUCTION

During 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 that will be added to the fundamental loop composed of the Liquefying, Rhodobacter, Liquefying and Spirulina compartments (compartments 1 to 4A).

The closing of the extended loop (fundamental + HPC) at the same time is probably not feasible and the easiest way is to proceed in two steps : first the fundamental loop alone will work and then, when the expected performances are reached, the HPC will be added to it. Moreover the fundamental part has to be able to work alone in case of a dys-functioning of the HPC. So the present study deals with the fundamental loop only and the study of the extended MELISSA loop will be pursued in a next Technical Note.

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 on condition that assumed operations are physically feasible. 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.

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.

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

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

$$CH_4ON_2 + H_2O \rightarrow CO_2 + 2\ NH_3 \tag{R2}$$

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 :

$$C_3H_7COOH + O_2 \rightarrow 2\ CH_3COOH \qquad (R3)$$

The oxygen requested by this equation is produced by Spirulina.

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 :

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

2.2. Sizing of the compartments of the simulator

The Spirulina compartment, whose volume has been determined to 77 litres, is the reference to set the size of the other compartments. 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. The volume of the Rhodobacter compartment is merely increased in the ratio of the new flow rate of liquid to keep unchanged the residence time. Its volume is 42.5 l to fit the incoming liquid flow rate of 0.77 l/h.
Of course, the Consumer and the Liquefying compartments, which are reduced to mere chemical reactions, have no volume.

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 and then back to the Consumer. At Spiru output, the NH_3 Gas is supposed to be captured to 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_2 and NH_3 present in the inert gas is captured and sent into the liquid stream. The oxygen needed for oxidation of H_2 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 4 compartments : Lique, Rhodo, Nitri and Spiru. All the biomass outgoing from Rhodo and Spiru is supposed to be removed as dry matter while the biomass produced by Nitri is fixed. The human wastes (faeces and urea) are introduced continously at the input of Lique as dry matter.

The water produced or consumed by the biochemical reactions is neglected.

These circuits are represented in the figure 1.

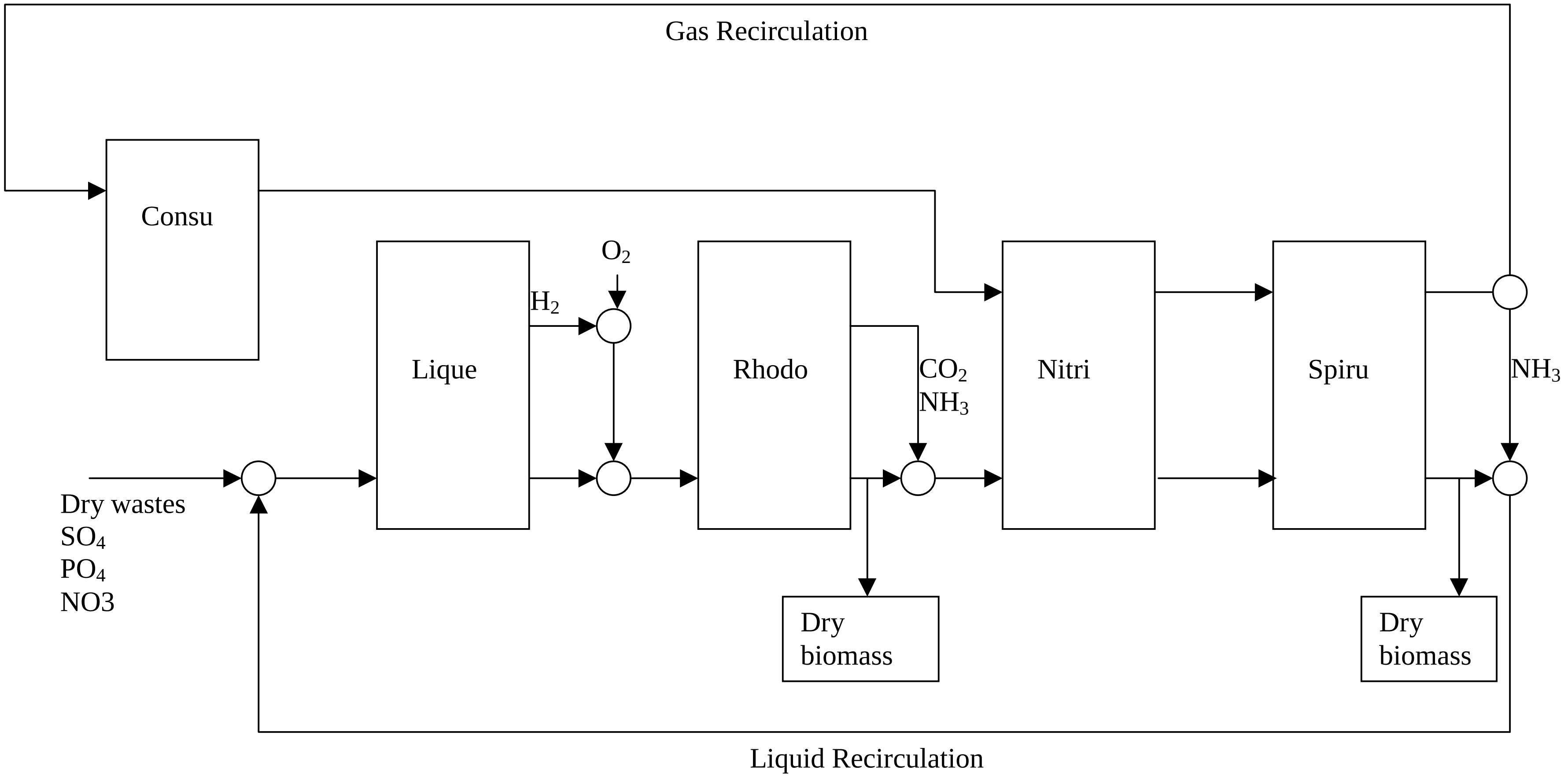

Figure 1 : Gas and Liquid connections between compartments

3. CLOSING THE GAS AND LIQUID LOOPS

Closing the gas loop is one of the main objectives of the pilot plant test.
The approach consists in setting the mathematical equations that represent the variations of O_2 and CO_2 of the whole process and in discussing the solutions.
It is obvious that the closing of the gas loop much be done permanently. So the process is considered at steady state.

3.1. Chemical equations binding the variations of O_2 and CO_2

The following chemical equations are stoechiometric 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 stoechiometric coefficients depend. For example, in the case of Spiru, the stoechiometric coefficients α_1, α_2, and α_3 cannot be explicitly given but they are computed by the simulator. The equation (R5) 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 :

$$\alpha_1\, CO_2 + \alpha_2\, NO_3 \rightarrow O_2 + \alpha_3\, XA \qquad (R5)$$

Nitri :

$$\beta_1\, O_2 + \beta_2\, CO_2 + \beta_3\, NH_3 \rightarrow NO_3 \qquad (R6)$$

Rhodo :

$$\gamma_1\, NH_3 + \gamma_2\, AcOH \rightarrow CO_2 \qquad (R7)$$

Lique :

$$\text{waste} + \varepsilon_1\, O_2 \rightarrow \varepsilon_2\, CO_2 + \varepsilon_3\, NH_3 + \varepsilon_4\, AcOH \qquad (R8)$$

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

3.2. Global balance of O_2 and CO_2

Given :

n : number of rats in the Consumer compartment
r_1 : O_2 consumption rate for 1 rat (negative value)
r_2 : CO_2 production rate for 1 rat (positive value)
x : concentration of active biomass XA in Spiru (mol/l)
ν : input rate of waste in Liquefying compartment
q : re-circulating liquid flow rate (l/h)

For each compartment, the O_2 and CO_2 variations rates (algebraic values) are as follows :

	O_2 variation rate (mol/h)	CO_2 variation rate (mol/h)
Consu	$n \cdot r_1$	$n \cdot r_2$
Lique	$\nu \cdot \varepsilon_1$ (*)	$\nu \cdot \varepsilon_2$
Rhodo	0	$-\frac{1}{\gamma_2} \cdot \varepsilon_4 \cdot \nu$

Nitri	$-\frac{\beta_1}{\beta_3}\cdot\left(\varepsilon_3-\varepsilon_4\cdot\frac{\gamma_1}{\gamma_2}\right)\cdot\nu$	$-\frac{\beta_2}{\beta_3}\cdot\left(\varepsilon_3-\varepsilon_4\cdot\frac{\gamma_1}{\gamma_2}\right)\cdot\nu$
Spiru	$\frac{1}{\alpha_3}\cdot q\cdot x$	$\frac{\alpha_1}{\alpha_3}\cdot q\cdot x$

(*) : *It is recalled 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 1 : O_2 and CO_2 variation rates of the process

The necessary condition to close the gas loop is to make nil the variation rates of O_2 and CO_2 of the whole process, which gives 2 equations.

The number of rats, n, will be fixed arbitrarily, for example, accordingly to the maximum light flux in Spiru; the liquid flow rate, q, is fixed too. So the resulting system of 2 equations has 2 unknowns : x and ν.

Then, provided that the coefficients α, β, γ, ε exist and that the NO_3 is sufficient, the closing of the gas loop has only one mathematical solution (which is physical solution if positive) : the vector X_0 that follows :

$$X_0 = A^{-1}\cdot B \tag{1}$$

with

$$X_0 = \begin{pmatrix} x_0 \\ \nu_0 \end{pmatrix} \qquad A = \begin{pmatrix} \frac{1}{\alpha_3}\cdot q & \varepsilon_1 - \frac{\beta_1}{\beta_3}\cdot\xi \\ \frac{\alpha_1}{\alpha_3}\cdot q & \varepsilon_2 - \frac{\varepsilon_4}{\gamma_2} - \frac{\beta_2}{\beta_3}\cdot\xi \end{pmatrix} \qquad B = -\begin{pmatrix} n\cdot r_1 \\ n\cdot r_2 \end{pmatrix}$$

$$\xi = \varepsilon_3 - \varepsilon_4\cdot\frac{\gamma_1}{\gamma_2}$$

The condition on NO_3 comes from the fact that the NH_3 produced by Lique has to be in sufficient amount to furnish the NO_3 necessary to the production of the active biomass of Spiru. It is expressed as follows :

$$\varepsilon_3 \geq q\cdot\beta_3\cdot\frac{\alpha_2}{\alpha_3}\cdot\frac{x}{\nu} + \varepsilon_4\cdot\frac{\gamma_1}{\gamma_2} \tag{2}$$

3.3. Method of resolution

As the coefficients α, β, γ and ε are non linear depending on the concentration of the substrates, the solution X of (1) is obtained through an iterative algorithm.

The starting point X_0 is computed from the balance of O_2 and CO_2 applied only to Nitri and Spiru where their variation rates are the biggest. The coefficients α, β, γ and ε are refreshed at each iterative step.

In order to make s_1 and s_2, the molar fractions of O_2 and CO_2 at Spiru output respectively, converge to a given value c_1 and c_2, the matrix B of (1) is replaced by :

$$B' = B - \lambda \cdot q' \cdot \begin{pmatrix} s_1 - c_1 \\ s_2 - c_2 \end{pmatrix} \quad (3)$$

where :
. λ is a relaxation coefficient to avoid instability of the algorithm that might come from the non-linearity of the pre-quoted stoechiometric coefficients;
. and q' is the re-circulating air flow rate.

It can be checked immediately that when the molar fractions of O_2 and CO_2 at Spiru output have reached their set points, then

$$s_1=c_1$$
$$s_2=c_2$$
$$B'=B$$

and the solution X of (1) is reached.

3.4. Results and discussion

The main parameters of the process are :

- $r_1 = 4.45\ 10^{-2}$ mol/h/rat : O_2 consumption for 1 rat (TN 47.3 by UAB);
- $r_2 = 4\ 10^{-2}$ mol/h/rat : CO_2 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;
- $c_1 = 0.21$: molar fraction of O_2 in the air at the Consumer input;
- $c_2 = 0.003$: molar fraction of CO_2 in the air at the Consumer input;
- input rate of 1 man wastes : $\frac{9.5\ \ 10^{-3}}{3}$ mol/h of faeces + $\frac{1.036\ \ 10^{-1}}{3}$ 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 and i_sim_4.m).

Given these data, the results are :

- number of rat in Consu : n = 1.5 ;
- input rate of man wastes : $\nu = 0.127$ rate of 1man wastes;

- O_2 production in Spiru : 0.0832 mol/h;
- O_2 consumption in Consu : 0.0668 mol/h (80.2 % of the production);
- O_2 consumption in Lique : 0.002 mol/h (2.4 % of the production);
- O_2 consumption in Nitri : 0.0144 mol/h (17.4 % of the production);

- CO_2 production in Consu : 0.0600 mol/h;
- CO_2 production in Lique : 0.0054 mol/h;
- CO_2 production in Rhodo : 0.0002 mol/h;
- CO_2 consumption in Nitri : 0.0018 mol/h;
- CO_2 consumption in Spiru : 0.0638 mol/h (97.2 % of the production);

- biomass concentration in Rhodo : 0.083 g/l production of biomass : 0.064 g/h;

- XA concentration in Spiru : 1.38 g/l production of biomass (XA+G+EPS) : 1.56 g/h;
- light flux for Rhodo : 3 W/m^2 ;
- light flux for Spiru : 200 W/m^2, which is near the upper limit 223 W/m^2 ;

- concentration of NO_3 in the liquid stream : 1 10^{-2} mol/l;
- concentration of NO_2 in the liquid stream : 1.32 10^{-4} mol/l;

- conversion yield of acetic acid in Rhodo : 0.996 ;
- conversion yield of NH_3 in Nitri : 0.974 ;
- conversion yield of CO_2 in Spiru : 0.63 ;
- conversion yield of NO_3 in Spiru : 0.56 ;

As the condition (2) is not fulfilled (the wastes do not supply a sufficient amount of NH_3) it is necessary to add some nitrate into the liquid loop. This complementary supply is 6.5 10^{-4} mol/h, which represents 1.1 molar % of the NH_3 produced by Lique.
All the SO_4 and PO_4 introduced at input of Lique are not consumed in the loop so that it is necessary to remove the part in excess. This is the only condition to actually close the liquid loop.

4. CONCLUSION

The study, done with the limited models described in section 2.1, shows that it is possible to close the gas loop of the fundamental part of the pilot plant (composed of the Consumer, Liquefying, Rhodobacter, Nitrifying and Spirulina compartments). The closing of the liquid loop is also possible under 2 conditions :

- to add some nitrate (1 molar % of NH_3 produced by Liquefying) to keep its concentration to a constant value at Spirulina output;
- to remove the excess of SO_4 and PO_4, which is more difficult to realize.

So apart from these considerations, the input matter of the MELISSA loop is the dry wastes at the rate of 0.127 unit (1 unit = wastes rate of 1 man). The output matter is all the dry biomass produced by Rhodobacter (0.064 g/h) and Spirulina (1.56 g/h). The available O_2 production rate is 0.0668 mol/h, which represents the need of 1.5 rat.
Of course these results strongly depend on the mean composition of the wastes and on the modelling of the Liquefying compartment (the other compartments (Rhodo, Nitri and Spiru) can be considered in a good state of modelling now).

5. REFERENCES

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GODIA,F.; ALBIOL,J.; CREUS,N.; PEREZ,J.; "Preliminary review of the pilot plant final loop" ESTEC/contract PRF 11549/95/NL/FG. December 2000. TN 47.3 (Issue: 0).

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LECLERCQ J.-J. : "Gas-Liquid equilibrium in global simulator". Contract ESTEC n° 12924/98/NL/MV,. January 1997. TN 35.1.

POUGHON L. "Review of models and basis of a dynamic structured model of the nitrifying compartment". ESTEC contract PRF 151739, February 1996, TN 27.1.

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6. ANNEX (Software)

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

```
%***********************************************************************
%       Connected compartments 0,1,2,3 and 4A                          *
%       Version 2.1     September 2001                                 *
%                                                                      *
%       i_sim.m   Initialization of the simulation                     *
%                 of the fundamental MELISSA loop (without 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_1p
global Gin_2  NG_2  NL_2  NO_2  vNB_2  vNM_2  VL_2  Fin_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  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  ...
   RL_3  indG_3  indL_3  Kdis_3
global NG_4  NL_4  NO_4  vNB_4  vNM_4  Fin_4  VL_4  Yx1_4  ...
   A2_4  B2_4  GG1_4  GG2_4  ...
   FRmin_4  FRmax_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 idisp

idisp=0; % flag to display intermediate variables if equal to 1
imodel=1;% choice of the computation method of cXA0_4 and nMan (1 --> explicit model approach)
if imodel==0,
  lambda = .2;   % relaxation coefficient
  niter=50; % number of iterations
else
  lambda = .05; % relaxation coefficient
  niter=20; % number of iterations
end;
% Type of test
% ============
typtst = 2;     titre = 'Team=2 rats';
typtst = 1;     titre = 'Team=1.5 rats';
% Initializing global parameters
% ==============================
  Matom = [12;    1;     16;    14;    32;   31];  % C H O N S P atomik mass
% The G and L flow rates of the Spirulina compart are set to the other compartments
% The volumes of these latest ones are modified to keep their residence time
  VL_4 = 77;        % volume of liquid (l) (from TN43.110 p.4, UAB)
  Gin_4 = 180;      % incoming gas flow rate (l/h) (from TN 43.110 p.26, UAB)
  tau_4 = .01;      % (1/h) to have residence time as in the actual reactor
  Fin_4 = tau_4*VL_4;% incoming liquid flow rate (l/h)
% Initializing parameters of compart.
% ===================================
  i_sim_0
  i_sim_1
  i_sim_2
  i_sim_3
  i_sim_4
% 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
% 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 NO3 conc. at output of Spiru
% =========================================
  spNO3_4 = 1.0e-2; % (mol/l) NO3 at output of Spiru
% Initializing the characteristics of Consu and team
% ==================================================
  fm_O2_0  = .21; % O2  (molar fraction of O2 at output of Spiru)
  fm_CO2_0 = 3e-3;   % CO2 (molar fraction)
  if typtst == 1
    nRat = 1.5;  % number of rats in the consumer compartment
  elseif typtst == 2
    nRat = 2;  % number of rats in the consumer compartment
  end
  % Initializing 'nMan' for iterative computation
  nMan = .2;   % ratio of 1 man_waste at input of the liquefying compartment
  %nMan = .15;  % ratio of 1 man_waste at input of the liquefying compartment
  % Production rate of CO2 : 4e-2 mol/h/rat
  rCO2_0 = .04*nRat;   % mol/h for n rats (according to TN47.3 p.8 by UAB)
  % Consumption rate of O2 : 4.45e-2 mol/h/rat
  rO2_0 = -.0445*nRat; % mol/h for n rats (according to TN47.3 p.8 by UAB)
% 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;
%Init of 'cXA0_4' and 'nMan'
%===========================
  % 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_1p = (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_1p(1,1)/2-Yp_1p(5,1); % Lique consumption yield of O2
  Yp_1(2:3,1) = Yp_1p(2:3,1);           % Lique production yield of CO2 and NH3
  Yp_1(4,1) = Yp_1p(4,1)+2*Yp_1p(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
  % 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)
  % Estimation of liquid input of Spiru
  cSO4_0  = nMan*.8/(Matom(5)+4*Matom(3)); % mol/l (arbitrary value)
  cPO4_0  = nMan*.4/(Matom(6)+4*Matom(3)); % mol/l (arbitrary value)
  CL0_4 = [0;                          % O2  (mol/l)
           fm_CO2_0*55.56/kpartN_4(2); % CO2 (mol/l) : G/L equilibrium
           nMan*Yp_1(3)/Fin_4;         % NO3 (mol/l)
           cSO4_0; cPO4_0];            % SO4 PO4 (mol/l)
  % Computation of the init value of the active biomass of Spiru
  cXA0_4 = 1.0; % (g/l) Value of biomass at starting of the iterative procedure
  cmul = 1.2;  % multiplicative coef applied to rO2 to estimate O2 consumed by Nitri
  for ii=1:10
    [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, FRmax_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)), break,  end
    DO2 = (Y0_4(1) - CG0_4(1)) * Gin_4 + (X0_4(1) - CL0_4(1)) * Fin_4;
    if (abs((DO2+cmul*rO2_0)/(cmul*rO2_0)) < 1e-2), break, end
    Yp_4 = zeros(3,1);
    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;
    cXA0_4 = cXA0_4 - Yp_4(3)*(DO2+cmul*rO2_0);
    CL0_4(2) = fm_CO2_0/VM_0/Y0_4(2)*X0_4(2);  % expected set point of CO2_L outgoing from
Spiru
  end
  CG0_4p=CG0_4;
  CL0_4p=CL0_4;
  if idisp
    ii
    cXA0_4
    FR0_4
    DO2
    rO2_0
    Yp_4
  end
  if (isempty(FR0_4) | isempty(X0_4)), break, end
  % Estimation of the yield of Nitri versus O2 CO2 and NH3
  %1. Gas phase (mol/l of O2 CO2 NH3 (NH3:null) from Consu and Lique) :
  cO2 = fm_O2_0/VM_0+(rO2_0-nMan*Yp_1(1))/Gin_3; % O2 consumed in Consu and Lique (H2, BuOH)
  cCO2 = (rCO2_0+nMan*Yp_1(2))/Gin_4; % CO2 produced by Consu and Lique
  CG0_3 = [cO2; cCO2; 0];  % mol/l
  %2. Liquid phase :
  %CL0_3 = [C_O2_0; C_CO2_0; C_NH3_0; C_NO2_0; C_NO3_0; C_PO4_0; C_SO4_0];
  cCO2 = -nMan*Yx_AcOH*Yp_1(4)/Yp_2(2)/Fin_3; % CO2 produced by Rhodo from AcOH
  %cNH3 = nMan*Yp_1(3)/Fin_3           % NH3 produced by Lique
  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
  CL0_3 = [CL0_3; 0; 0; cPO4_0; cSO4_0];
  %3. Initial state vector of Nitri (steady state)
  [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), break,  end
  %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
  CG0_3p = CG0_3; CL0_3p = CL0_3; X0_3p = [X0_3(indL);X0_3(indL(3)+1);X0_3(indL(3)+2)];
  % Computation of active biomass Spiru 'cXA0_4' and of incoming waste ratio 'nMan'
  ksi = Yp_1(3,1)-Yp_2(1,1)/Yp_2(2,1)*Yp_1(4,1);
  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; rCO2_0];
  cXA0_4 = X(1);
  nMan = X(2);

  if idisp
  disp(' O2           CO2')
  p0 = rO2_0;
  p1=nMan*Yp_1(1,1);
  p2=0;
  p3=nMan*(-ksi*Yp_3(1,1)/Yp_3(3,1));
  p4=cXA0_4/Yp_4(3,1)*Fin_4;
```

```
  X=[p0;p1;p2;p3;p4;p0+p1+p2+p3+p4];
  p0 = rCO2_0;
  p1=nMan*Yp_1(2,1);
  p2=nMan*(-Yp_1(4,1)/Yp_2(2,1));
  p3=nMan*(-ksi*Yp_3(2,1)/Yp_3(3,1));
  p4=cXA0_4*Yp_4(1,1)/Yp_4(3,1)*Fin_4;
  X=[X,[p0;p1;p2;p3;p4;p0+p1+p2+p3+p4]];
  disp(X)
  end
  Yp_2p=Yp_2;Yp_3p=Yp_3;Yp_4p=Yp_4;
  % Necessary condition on 'nMan'
  crit = Yp_3(3,1)*Yp_4(2,1)/Yp_4(3,1)*cXA0_4*Fin_4/nMan + ...
         Yp_2(1,1)/Yp_2(2,1)*Yp_1(4,1);
  if Yp_1(3,1)<crit
    %nMan = Yp_3(3,1)*Yp_4(2,1)/Yp_4(3,1)*cXA0_4*Fin_4 / ...
    %       (Yp_1(3,1)-Yp_2(1,1)/Yp_2(2,1)*Yp_1(4,1)
    addNO3 = -Yp_4(2,1)/Yp_4(3,1)*cXA0_4 + ...
             (Yp_1(3,1)-Yp_2(1,1)/Yp_2(2,1)*Yp_1(4,1))/Yp_3(3,1)*nMan/Fin_4;
  else
    addNO3 = 0;
  end
%------------------------------------------------
%        SIMULATION OF THE MELISSA LOOP         |
%------------------------------------------------
% Inputs of the MELISSA loop
% ==========================
% Waste of 'nMan' man (according to TN35.1, ADERSA)
% qFaec_0 = nMan*Faec;   % mol/h (faeces)
% qUrea_0 = nMan*Urea;   % mol/h (urea)
  qSO4_0  = nMan*.2/(Matom(5)+4*Matom(3))*Fin_1; % mol/l
  qSO4_0  = nMan*.6/(Matom(5)+4*Matom(3))*Fin_1; % mol/l
  qPO4_0  = nMan*.4/(Matom(6)+4*Matom(3))*Fin_1; % mol/l
  %qPO4_0  = nMan*.8/(Matom(6)+4*Matom(3))*Fin_1; % mol/l
% Init of intermediate variables (concentration in mol/l)
% ==============================
  %1. L phase going into Rhodo :
  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));
  %2. L phase going into Nitri :
  qNH3 = nMan*(Yp_1(3,1)-Yx_AcOH*Yp_2(1,1)/Yp_2(2,1)*Yp_1(4,1)); % estimated NH3 flow rate
outgoing from Rhodo
  initNH3 = 2.5e-2*qNH3/Fin_3/(1+Kdis_3(NG_3));   % estimated NH3_GL outgoing from Nitri
  initNO2 = 1.3e-4;       % NO2 outgoing from Nitri at previous step
% Init of variations of EE for the second method
% ==============================================
  deltaE = diag([1e-3,  % variation amplitude on Spiru biomasse 'cXA0_4'
                 2e-6]);% variation amplitude on 'nMan'
% Sizing variables
% ================
  AA=zeros(2);
  Tvar=[];
% Setting the objective of the output of the system to solve
% ==========================================================
  Sobj=[fm_O2_0; fm_CO2_0];
% Initializing the input of the system to solve
% =============================================
  EE = [cXA0_4; nMan];
for iter = 1:niter
  % O2_L CO2_L NO3 at input of the open loop (concentration in mol/l)
  YO2_4 = fm_O2_0/VM_0/Y0_4(1)*X0_4(1);  % expected set point of O2_L outgoing from Spiru
  YCO2_4 = fm_CO2_0/VM_0/Y0_4(2)*X0_4(2)*(1+Kdis_4(NG_4))/(1+Kdis_2(1));  % expected set point
of CO2_L outgoing from Spiru
  % SO4 PO4 at input of the open loop (concentration in mol/l)
  YSO4_4 = EE(2)*.8/(Matom(5)+4*Matom(3)); % mol/l (arbitrary value)
  YPO4_4 = EE(2)*.8/(Matom(6)+4*Matom(3)); % mol/l (arbitrary value)
  initLiqueL = [YSO4_4; YPO4_4]; % SO4 PO4
  % saving
  initNH3t(iter,:) = initNH3;
  initNO2t(iter,:) = initNO2;
  initAcOHt(iter,:) = initAcOH;

  % process (simulated pilot plant)
```

```
      [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] = ...
  simpro(EE, fm_O2_0, fm_CO2_0, rO2_0, rCO2_0, qSO4_0, qPO4_0, ...
         initNH3, initNO2, initAcOH, initLiqueL, Yx_AcOH, YO2_4, YCO2_4, spNO3_4);

  % Refreshing the yields of Nitri and Spiru
  % ========================================
  %1. Rhodo: Yield of CO2 and NO3 : 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. 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
  %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
  if idisp
    Yp_2p=[Yp_2p,Yp_2]
    Yp_3p=[Yp_3p,Yp_3]
    Yp_4p=[Yp_4p,Yp_4]
  end

  % Computation of the active biomass Spiru and the ratio of incoming waste
  % =======================================================================
  % 1. First method for computing cXA0_4 and nMan
  if imodel==1 % explicit model approach
    ksi = Yp_1(3,1)-Yp_2(1,1)/Yp_2(2,1)*Yp_1(4,1);
    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(1,1)-ksi*Yp_3(2,1)/Yp_3(3,1)];
    A1 = inv(AA);
    EE = -A1*[rO2_0  + lambda*(Y0_4(1)-fm_O2_0/VM_0 )*Gin_4; % correction of O2 variation
              rCO2_0 + lambda*(Y0_4(2)-fm_CO2_0/VM_0)*Gin_4]; % correction of CO2 variation
  % 2. Second method for computing cXA0_4 and nMan
  else
    X0_40 = X0_4;  Y0_40 = Y0_4;
    SS0 = Y0_40(1:2,1)*VM_0;  % Local output of the system to solve
    EE0=EE; % Local input of the system to solve
    for jj=1:2
      EE = EE0+deltaE(:,jj); % small variation of the local input
      % O2_L CO2_L NO3 at input of the open loop (concentration in mol/l)
      YO2_4 = fm_O2_0/VM_0/Y0_40(1)*X0_40(1);  % expected set point of O2_L outgoing from
Spiru
      YCO2_4 = fm_CO2_0/VM_0/Y0_40(2)*X0_40(2)*(1+Kdis_4(NG_4))/(1+Kdis_2(1));  % expected set
point of CO2_L outgoing from Spiru
      % SO4 PO4 at input of the open loop (concentration in mol/l)
      YSO4_4 = EE(2)*.8/(Matom(5)+4*Matom(3)); % mol/l (arbitrary value)
      YPO4_4 = EE(2)*.8/(Matom(6)+4*Matom(3)); % mol/l (arbitrary value)
      initLiqueL = [YSO4_4; YPO4_4]; % SO4 PO4

      % process output (simulated pilot plant) corresponding to the new process input
        [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] = ...
      simpro(EE, fm_O2_0, fm_CO2_0, rO2_0, rCO2_0, qSO4_0, qPO4_0, ...
             initNH3, initNO2, initAcOH, initLiqueL, Yx_AcOH, YO2_4, YCO2_4, spNO3_4);

      SS = Y0_4(1:2,1)*VM_0;  % Output of the system to solve
      AA(:,jj) = (SS-SS0)/deltaE(jj,jj); % AA = local approximate derivative of the system
    end

    AA1=inv(AA);
    EE=EE0+AA1*((Sobj-SS0)*lambda); % First method for computation of cXA0_4 and nMan
  end
  % Refreshing the intermediate variables (concentration in mol/l)
  % =====================================
```

```
  %1. 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));
 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
  %2. L phase going into Nitri :
  indN1 = (NB_3+2)*NG_3;                          % index of NH3 G in output vector
  indN2 = (NB_3+2)*NG_3+(NB_3+1)*(NG_3+NL_3)+NG_3;% index of NH3 L in output vector
 if 0  % computing 'initNH3' from estimation
  zNH3  = 1-((Y0_3(indN1)*Gin_3 + Y0_3(indN2)*Fin_3*(1+Kdis_3(NG_3))))./...
            (CG0_3(NG_3)*Gin_3 +  CL0_3(NG_3)*Fin_3*(1+Kdis_3(NG_3)))); % conversion of NH3
  qNH3 = EE(2)*(Yp_1(3,1)-Yx_AcOH*Yp_2(1,1)/Yp_2(2,1)*Yp_1(4,1));   % estimation of NH3 flow
rate outgoing from Rhodo
  initNH3 = (1-zNH3)*qNH3/Fin_3/(1+Kdis_3(NG_3));   % estimation of NH3_GL outgoing from Nitri
for next step
 else  % computing 'initNH3' from value at previous step (best method)
  initNH3 = Y0_3(indN1)*Gin_3/Fin_3/(1+Kdis_3(NG_3)) + Y0_3(indN2); % NH3_GL outgoing from
Nitri at previous step
 end
  initNO2 = Y0_3(indN2+1);       % NO2 outgoing from Nitri at previous step
  % Addition of NO3
    % variation of NH3 : output-input of the open loop
    if X0_4(NG_4+1) < spNO3_4
      addNO3 = spNO3_4 - X0_4(NG_4+1);
    else
      addNO3 = 0;
    end
  % Saving estimations (for checking or debugging)
  % ==================
  evarO2_1(iter,:) = nMan*Yp_1(1,1);
  evarO2_3(iter,:) = -nMan*(Yp_3(1,1)/Yp_3(3,1))*ksi;
  evarO2_4(iter,:) = cXA0_4/Yp_4(3,1)*Fin_4;
  evarCO2_1(iter,:) = nMan*Yp_1(2,1);
  evarCO2_2(iter,:) = -nMan*Yp_1(4,1)/Yp_2(2,1);
  evarCO2_3(iter,:) = -nMan*ksi*Yp_3(2,1)/Yp_3(3,1);
  evarCO2_4(iter,:) = cXA0_4*Yp_4(1,1)/Yp_4(3,1)*Fin_4;
  evarNO3_4(iter,:) = cXA0_4*Yp_4(2,1)/Yp_4(3,1);
  Tvar=[Tvar, iter];
  % Necessary condition on 'nMan'
  crit = Yp_3(3,1)*Yp_4(2,1)/Yp_4(3,1)*cXA0_4*Fin_4/nMan + ...
         Yp_2(1,1)/Yp_2(2,1)*Yp_1(4,1);

  cXA0_4 = EE(1);
  nMan   = EE(2);
  if idisp
  disp(['iter=',num2str(iter),'    O2           CO2'])
  p0 = rO2_0;
  p1=nMan*Yp_1(1,1);
  p2=0;
  p3=nMan*(-ksi*Yp_3(1,1)/Yp_3(3,1));
  p4=cXA0_4/Yp_4(3,1)*Fin_4;
  X=[p0;p1;p2;p3;p4;p0+p1+p2+p3+p4];
  p0 = rCO2_0;
  p1=nMan*Yp_1(2,1);
  p2=nMan*(-Yp_1(4,1)/Yp_2(2,1));
  p3=nMan*(-ksi*Yp_3(2,1)/Yp_3(3,1));
  p4=cXA0_4*Yp_4(1,1)/Yp_4(3,1)*Fin_4;
  X=[X,[p0;p1;p2;p3;p4;p0+p1+p2+p3+p4]];
  disp(X)
  pause
  end

  % Saving variables
  % ================
  YO2_4t(iter,:) = YO2_4;
  YCO2_4t(iter,:) = YCO2_4;
  addNO3t(iter,:) = addNO3;
  critt(iter,:) = crit;
  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';
  disp(['Iteration ',num2str(iter),' finished'])
  temps(iter) = iter;

end
if isempty(cs_4), break,end
titre0 = ['X_rhodo=',num2str(X0_2(NG_2+NL_2+1)),', XA_Spiru=',num2str(cXA0_4),' (g/l)'];
pou=1;
t_sim_b
disp('nouvelle fenetre graphique puis RC')
pause
pou = 2;
t_sim_b
disp('nouvelle fenetre graphique puis RC')
pause
pou = 3;
t_sim_b
disp('nouvelle fenetre graphique puis RC')
pause
pou = 4;
t_sim_b
disp('nouvelle fenetre graphique puis RC')
pause
titre = [titre0,';Conc. in Spiru'];
pou = 2;
t_sim_4

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]
% 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
```

6.2. Simulation of the open fundamental MELISSA loop

```
%***********************************************************************
%       Connected compartments 0,1,2,3 and 4A                          *
%       Version 2.1     September 2001                                 *
%                                                                      *
%       simpro.m   Simulation of the fundamental MELISSA loop          *
%                  (HPC non 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] = ...
  simpro(EE, fm_O2_0, fm_CO2_0, rO2_0, rCO2_0, qSO4_0, qPO4_0, ...
         initNH3, initNO2, initAcOH, initLiqueL, Yx_AcOH, YO2_4, YCO2_4, spNO3_4)

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  NG_2  NL_2  NO_2  vNB_2  vNM_2  VL_2  Fin_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  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  ...
   RL_3  indG_3  indL_3  Kdis_3
global NG_4  NL_4  NO_4  vNB_4  vNM_4  Fin_4  VL_4  Yx1_4  ...
   A2_4  B2_4  GG1_4  GG2_4  ...
   FRmin_4  FRmax_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 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 totaly 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 totaly 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)

%>>> 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_4;        %  addition of CO2 coming from Spiru output
  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, GG1_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);

%>>> 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) = YO2_4;        % function of expected set point of O2_L at Spiru output
  CL0_3(NG_3+2) = spNO3_4;  % set point of NO3 at Spiru output
  CL0_3(NG_3) = CL0_3(NG_3) + initNH3;      % NH3_GL from previous step
  CL0_3(NG_3+1) = CL0_3(NG_3+1) + initNO2;  % NO2 from previous step
  %3. G phase of Rhodo going into L phase of Nitri :
  YCO2_2 = Y0_2(1)*Gin_2/Fin_2;       % CO2_G outgoing from Rhodo
  YNH3_2 = Y0_2(2)*Gin_2/Fin_2;       % NH3_G outgoing from Rhodo
  CL0_3(2:NG_3) = CL0_3(2:NG_3) + [YCO2_2; YNH3_2]./(1+Kdis_3(2:NG_3));
% Initial state and output vectors of Nitri (steady state)
% ========================================================
  [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), break,  end
  if idisp
    CG0_3p = [CG0_3p, CG0_3]
    CL0_3p = [CL0_3p, CL0_3]
    X0_3p = [X0_3p, [X0_3(indL);X0_3(indL(3)+1);X0_3(indL(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_4p = [CG0_4p, CG0_4]
    CL0_4p = [CL0_4p, 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, GG1_4, GG2_4, CG0_4, CL0_4, EE(1), ...
   FRmin_4, FRmax_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)), break,    end
  if idisp, FR0_4, end
```

6.3. Parameters of the compartments

```
%******************************************************************************
%       Consumer compartment (static behaviour)                         *
%       Version 1     April 2001                                        *
%                                                                       *
%       Data according to TN 54.3                                       *
%                                                                       *
%       i_sim_0.m : Initialization of the simulation                    *
%                                                                       *
%******************************************************************************

arret = 0;

% General parameters of the simulated process
% -------------------------------------------
NG1= 3;   % number of mono-phase substrates in the Gas phase : O2, CO2 NH3
          % NG1_0 = NG_3 to fit the G inputs of Nitri
% Parameters of the consumer compartment
% --------------------------------------
Gin = Gin_4;    % incoming gas volumetric rate (l/h)
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;

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

%******************************************************************************
%       Liquefying compartment (static behaviour)                       *
%       Version 1     April 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
% Parameters of the consumer compartment
% --------------------------------------
Gin = 18;    % incoming gas volumetric rate as in Rhodo (l/h): arbitrary value
Fin = Fin_4; % l/h
```

```
Temp = 330; % K (TN35.1 ADERSA)
pH = 5;     % (TN35.1 ADERSA)
% Gas/liquid transfer parameters
% -------------------------------
KLa = inf;    % CO2 NH3 CH3COOH (1/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(1)/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 biphase 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;
% Stoechiometry 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 :
    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)
% Stoechiometry 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;            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 1     November 2000                                    *
%                                                                      *
%       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
% ---------------------
RT = .048;   % radius of the reactor (m)
VL = 7 ;     % volume of liquid (l)
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
tau = .0181; % (1/h) to have same residence time as in TN43.8, UAB
Fin = tau*VL;% incoming liquid flow rate (l/h); if Fin variable, do as for Gin
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)
% modif. of the L flow rate to fit the flow of Spirulina Compart
coef_F = Fin_4/Fin;
Fin = Fin_4; % l/h
% modif. of the volume VL to keep the residence time
VL = VL*coef_F;
% 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 biphase 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);
% Stoechiometry 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]; % stoechio composition biomass Rhodo
    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 (similar to XA of Spirulina)
% ---------------------------------------------
KSSO4 = 2.5e-4/(Matom(5)+4*Matom(3));  % mol/l
% Mass balance checking
% ====================
% Matrices of stoechiometric 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;
if arret
  disp(' *=*=* Rhodo : initialization aborted *=*=*')
  break
end
disp(' *** Rhodo - End of initialization ***')

%***********************************************************************
%       Nitrifying column                                              *
%       Version 2.2     November 2000                                  *
%       for the 3 connected compartments : 2, 3 and 4a                 *
%                                                                      *
%       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;

% 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)
        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_4 - 1);
        Fin = Fin_4;                % 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 coeffcient (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)

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

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

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


%***********************************************************************
%       Photoautotrophic compartment (Photosynthesis)                  *
%       Version 1     November 2000                                    *
%                                                                      *
%       State system according to TN 54.2                              *
%       . mineral limitation (NO3 SO4)                                 *
%       . no carbon limitation (conclusion of TN 32.4, LGCB)           *
%       . CO2 production of 4 rats (.04 mol/h)                         *
%       . waste of 1 man (data computed from TN 35.1, ADERSA)          *
%       . 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 = VL_4;   % 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
tau = tau_4; % (1/h) to have residence time as in the actual photobioreactor
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)
FRmax = 1000; % (W/m2)

% 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)
xx = 10^(-pH)/Ka;   KPO4 = 1+xx;  %[PO4]total = f([HPO4=])
% dissociation vector for the biphase 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);
% Stoechiometry 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 stoechiometric 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
% 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; KSNO3_4 = KSNO3;
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;
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 ***')
```