ADERSA

# MELISSA

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# TECHNICAL NOTE : 64.3

## Sizing of compartment from First Principles model

RHODOBACTER, NITRIFYING AND SPIRULINA COMPARTMENTS

Version : 1
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# Document Change Log

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| 0 | 0 | October 2002 | Draft |
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Abbreviations or notations:
$NH_3$ : ammonia (gaseous or solvated)
$NO_2$ : nitrite ion
$NO_3$ : nitrate ion
SO4 : sulphate ion
PO4 : phosphate ion
$N_s$ : Nitrosomonas strain
$N_b$ : Nitrobacter strain
VFA : Volatile Fatty Acid

# 1. INTRODUCTION

To justify the technical note, two previous results have to be recalled :

- In TN54.1, for each of the compartments Rhodobacter, Nitrifying and Spirulina, the study of the steady state has shown that the existence of this last one is submitted to a condition that implies the volume.
- In TN54.2 where the 3 above compartments were connected in series, it has been necessary to adapt the volumes so that the whole process could work correctly, i.e. so that each compartment could treat correctly the substances it receives at its input.

Among all the parameters of a reactor, the volume is probably the only one that can be reasonably change on a simulator, while keeping in mind that this change must not disturb the optimum operating conditions. In the case of a photobioreactor, for example, since the radial dimension is determined by optimizing the light absorption, the volume change must be obtained by reducing or extending the length of the cylindrical reactor.
So the technical note does not pretend to furnish a new design of a reactor but provides a method and a programme to determine the volumes for the Rhodobacter, Nitrifying and Spirulina compartments appropriate to a required performance. Its use is limited to the global simulator.

Due to budget considerations, the constant evolution of modelling done by LGCB cannot always be taken into account on ADERSA's simulator. So the present status of achievement of the simulated compartments for the technical note is :
1_ The Rhodobacter compartment is simulated according to the latest version of the first principles model of TN 45.1 by LGCB where the source of carbon is the acetic acid. Since TN64.2 the model of Rhodo has been modified in order to degrade butyric acid according to the stoechiometry of TN 39.1 by LGCB (R1) 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) :

$$C_4H_8O_2 + 0.9689\ NH_3 + 0.0704\ H_3PO_4 + 0.0156\ H_2SO_4 + 0.6261\ CO_2 \quad \text{(R1)}$$
$$\rightarrow 4.6261\ CH_{1.5951}O_{0.3699}N_{0.2094}S_{0.0034}P_{0.0152} + 1.8850\ H_2SO_4$$

2_ 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).

3_ 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 :

$$CO_2 + 0.827\ H_2O + 0.008\ H_2SO_4 \rightarrow C\ H_{1.67}\ O_{0.71}\ S_{0.008} + 1.0745\ O_2 \qquad (R2)$$

The rate unit of 1 man wastes is : $\frac{9.5\ \ 10^{-3}}{3}$ mol/h of faeces + $\frac{1.036\ \ 10^{-1}}{3}$ mol/h of urea (TN 35.1).

# 2. SIZING OF THE NITRIFYING COMPARTMENT

## *2.1. Aim of the sizing*

When connecting the 3 compartments Rhodobacter, Nitrifying and Spirulina (TN 54.2), it has been noted on the Nitrifying compartment particularly that the production of nitrite was very high when compared to the values obtained for the compartments taken separately. The explanation was that the volume of the column was too small compared to the increased load of ammonia implied. At that moment, the relation between the volume of liquid and the amount of by-product was not studied extensively.
Nevertheless an expression of the minimum volume of liquid was expressed (relation A4.4 in TN 54.2) :

$$V \geq \frac{1}{K_{La} \cdot \left( \frac{n_0}{k_p} \cdot y - b \right)} \cdot \varphi'$$

with $V$ : volume of liquid
$\varphi'$ : flux of O2 required by the oxidation
$b$ : $O_2$ molar concentration in liquid phase
$y$ : $O_2$ molar concentration in gas phase
$K_{La}$ : volumetric transfer coefficient in liquid phase
$n_0$ : number of mole in a litre of water
$k_p$ : partition coefficient of gas/liquid equilibrium

The purpose is now to determine the minimum volume of liquid necessary in the fixed bed (part B of column) to allow for a steady state at a given load of ammonia and producing an acceptable amount of nitrite.

## *2.2. Method*

The method consists first in computing the nitrite concentration at steady state versus the ammonia load and the parameters of the column :

- the volume of liquid of the fixed bed;

- the gas/liquid transfer parameter KLa;
- the gas recirculating ratio $R_G$;
- the liquid recirculating ratio $R_L$;

Then the minimum volume of liquid is determined versus a maximum level of acceptable concentration of nitrite, given a value of the parameters.

The relation for the computation of nitrite concentration at steady state has been established in TN 54.1 section 4 .

Remark : The ammonia load is considered as the input flow rate of ammonia and expressed in mol/h (and not mol/h/l when the load is scaled to the reactor volume). The liquid and gas flow rates are assumed fixed in the present study but they can be changed in the programme to have results at different liquid or gas flow rates. Actually as it will be seen hereafter, changing $R_G$ and $R_L$, which is nearly equivalent to change flow rate with unchanged load, has nearly no effect on the nitrite concentration.

### *2.3. Numerical application*

The general conditions of simulation are :

- the liquid and gas flow rates are not variable and set to their values in the global simulator: 180 and 0.77 l/h respectively.
- on the pilot plant at UAB, the gas and liquid recirculating ratios, $R_G$ and $R_L$, are currently set to 0 and 6, respectively (Julio Perez's e-mail on October 28$^{th}$ 2002). Although they were higher in previous ADERSA's TN's, they are now changed on the simulator to be in agreement with the parameters of the real process. So in the present study they are varying on an equivalent range : from 0 to 10.
- $CO_2$, sulfate and phosphate concentrations are not limiting;
- the input concentration of $NO_2$ is not zero : it is set to 1.4 $10^{-4}$ mol/l as it is obtained in the global simulator (TN 54.4) where the $NO_2$ produced in Nitri is assumed not removed and recirculates in the main liquid stream.

The figures 1 to 3 show the surface of $NO_2$ concentration at column output depending on the 2 parameters Volume and Load, represented in the xy plane, and depending on a third parameter, KLa, $R_G$ or $R_L$ , one per figure. In all cases, the surface has same general aspect : a flat area and a peak.
As expected, KLa has a great influence on $NO_2$ (figure 1).
The figure 2 and 3 show the surface of nitrite versus $R_G$ and $R_L$ : these 2 parameters have just a small influence on the height of the peak but no influence in the flat area, which is the area concerned in the study. So it is checked that the nitrite concentration at low level is not sensible to the recirculating ratios $R_G$ and $R_L$.

The surface is mostly nearly flat except in a small area where the $NO_2$ is increasing very quickly. The limit between the flat area and the peak could be set at 1.6 $10^{-4}$ mol/l (2.2 Nppm) for all the graphs : the surface is blue under the limit and red above.

### *2.4. Conclusion*

In the flat area, for the investigated conditions the $NO_2$ concentration never falls below 1.3 $10^{-4}$ mol/l (1.8 Nppm) as indicated in figures 1 to 3. It means that it is impossible to produce less than about 1.3 $10^{-4}$ mol/l of $NO_2$ whatever big may be the volume of liquid, KLa, $R_G$ and $R_L$.

Given a load of ammonia equal to 2 $10^{-2}$ mol/h (which is an overestimated value compared to the one computed with the global simulator in TN 54.4 : 1.5 $10^{-2}$ mol/h), the minimum volume of liquid of the fixed bed versus the main parameter KLa is given in Table1.

| **KLa (h-1)** | **25** | **50** | **100** |
|---|---|---|---|
| Minimum liquid volume (l) | 8 | 3.75 | 2 |

**Table 1 : Minimum liquid volume versus KLa**

Given a KLa greater than 50 $h^{-1}$, the volume of liquid of the fixed bed (part B of the column) should be greater than 3.75 l, which means a volume of part B greater than 11.3 l (the ratio of liquid in part B is $\varepsilon_L$=0.33).

Another interesting result is that the recycling ratios $R_G$ and $R_L$ have no influence in the domain of low level $NO_2$ concentration (flat area of figures 2 and 3). It means that, if this result could be confirmed in a dynamic behaviour, the gas and liquid recirculating pumps could be saved (which would imply less maintenance too).

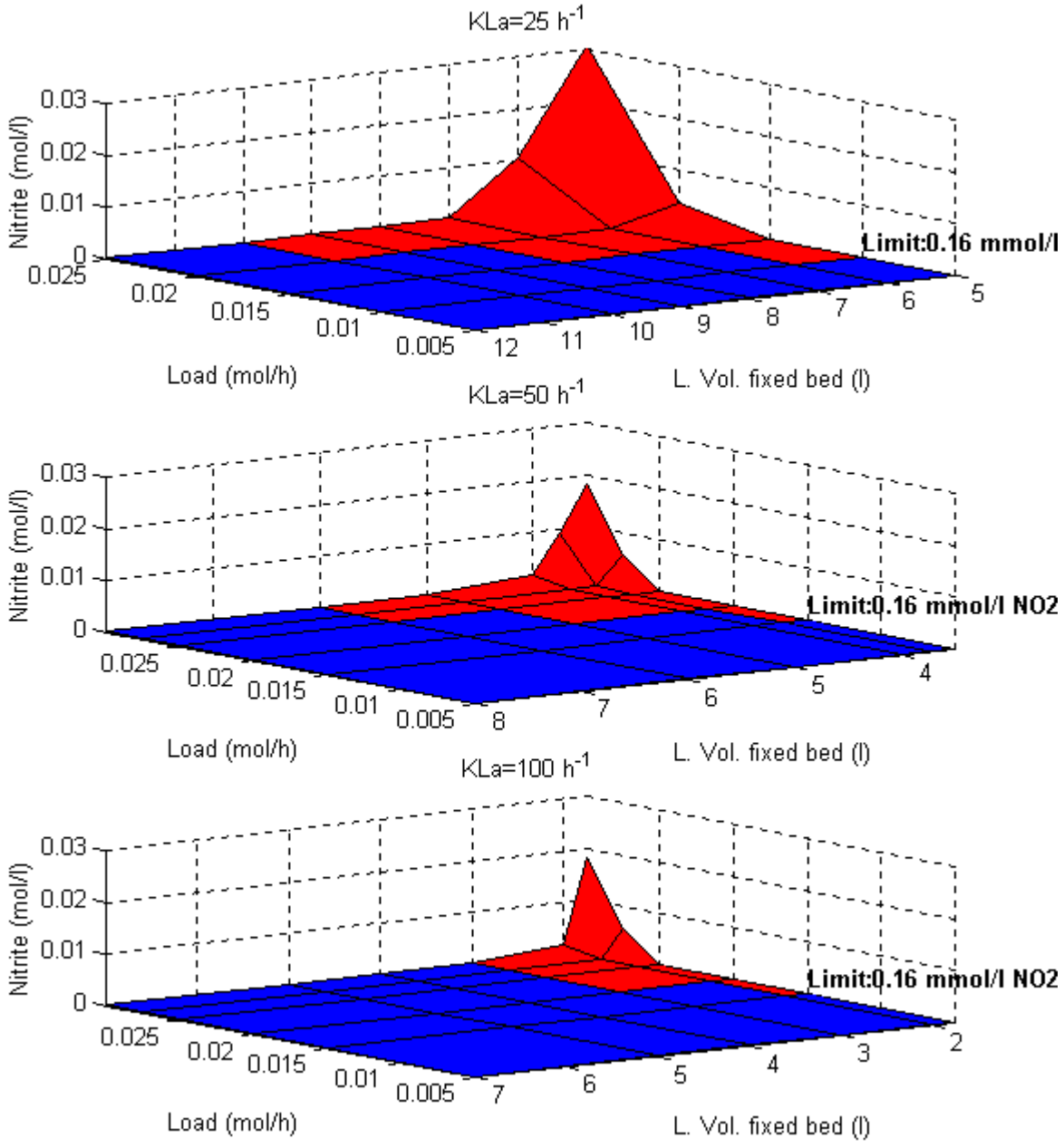


**Figure 1 : Nitrite concentration depending on Volume, Load and KLa**
**KLa = 25 , 50 and 100 $h^{-1}$ from top to bottom graphs**
**$R_G$ and $R_L$ are the same for the 3 graphs : 5 and 5, respectively**

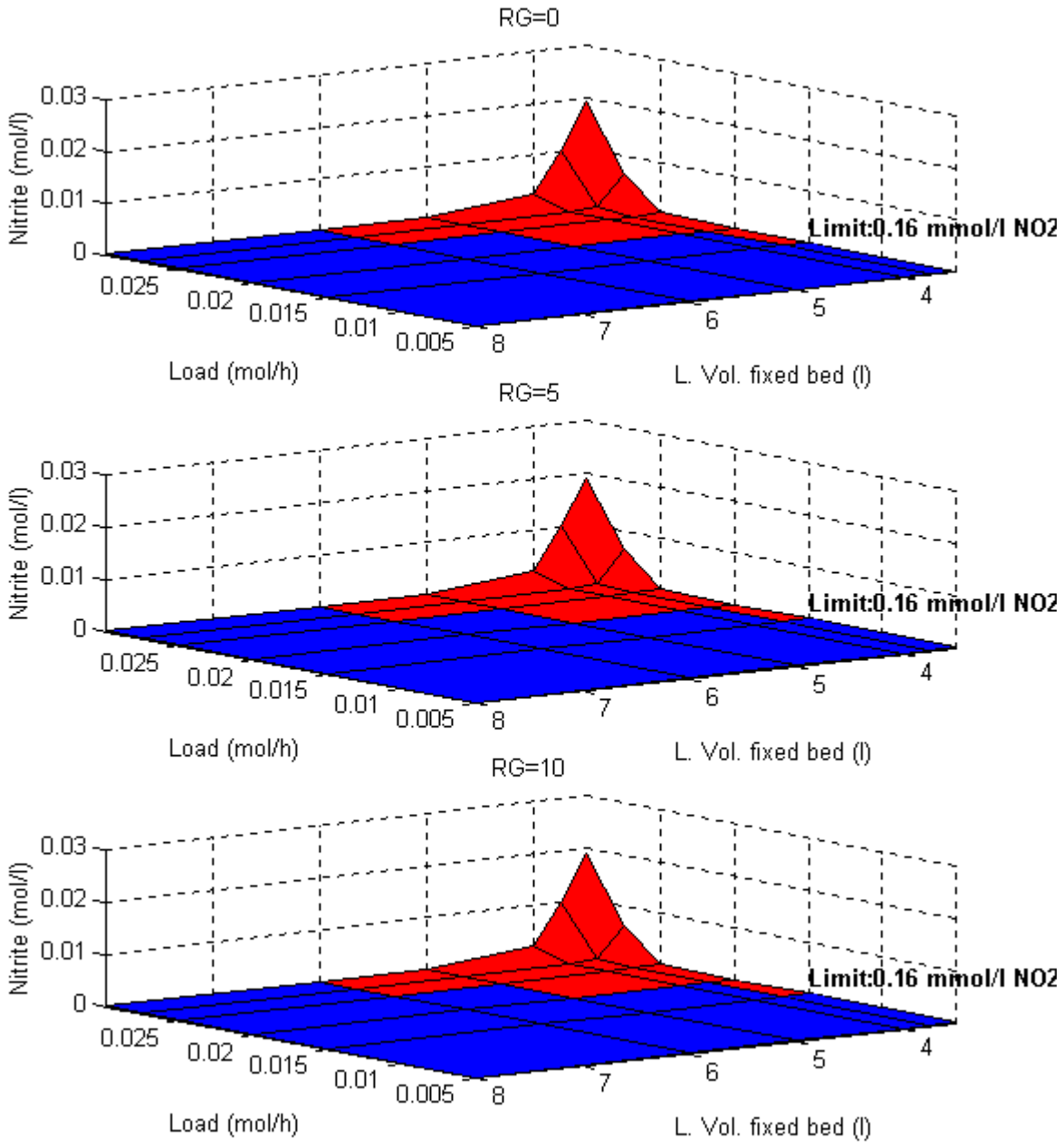


**Figure 2 : Nitrite concentration depending on Volume, Load and $R_G$**
**$R_G$ = 0, 5 and 10 from top to bottom graphs**
**Interval of parameters Load and Volume are the same for the 3 graphs**

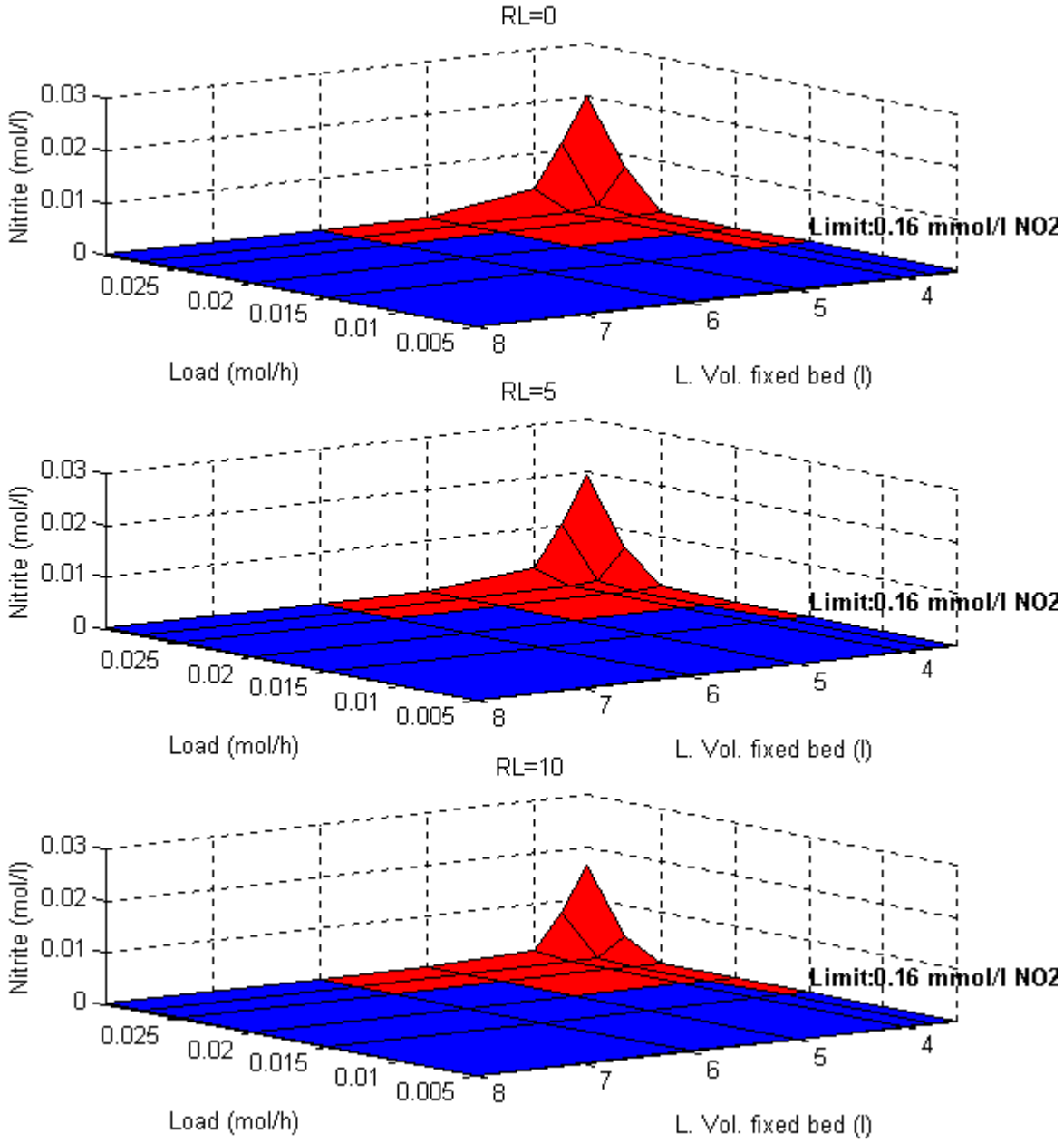


**Figure 3 : Nitrite concentration depending on Volume, Load and $R_L$**
**$R_L$ = 0, 5 and 10 from top to bottom graphs**
**Interval of parameters Load and Volume are the same for the 3 graphs**

# 3. SIZING OF THE RHODOBACTER COMPARTMENT

## *3.1. Aim of the sizing*

The aim is to determine the minimum volume of the reactor versus the load, which is the flow rate of acetate and butyrate. In order to be directly usefull for the global simulator, the load is expressed in ratio of one man wastes which is an independent variable of the global simulator.

## *3.2. Method*

First the Rhodobacter biomass production is computed to degrade a given proportion of VFA, produced by the Liquefying compartment, versus the ratio of 1 man waste. No value of the degradation proportion is known at the moment. But as the goal of this compartment is to degrade all the VFA, it seems reasonable to set the proportion at 99.5 % in the present simulations.

Then the maximum Rhodobacter biomass production (production at maximum light flux) is computed versus the volume of the photobioreactor and the residence time.

So the volume can be correlated to the ratio of 1 man wastes.

The relation for the computation of Rhodobacter production at steady state has been established in TN 54.1 section 2 .

Its relation (2.8) shows that the residence time $\tau$ belongs to an interval whose limits are depending on the range of light flux $[F_{min}, F_{max}]$ :

$$f(F_{max}) \leq \tau \leq f(F_{min}) \qquad (1)$$

## *3.3. Numerical applications*

For the computation of maximum biomass production versus volume and residence time, the substrates are non-limiting (this condition is justified by the fact that in case of limiting substrates, an increase of volume is unable to increase the production).

As no value is available for the gas/liquid transfer coefficient KLa at the moment, it is arbitrarily set at the value of the another similar photobioreactor of the project, the Spirulina compartment (12 $h^{-1}$, TN 43.110 p.26, by UAB). Of course this coefficient, that is a parameter of the programme, can be changed as soon as a real value is known.

The illuminated surface fraction $f_i$ is set to 0.6 (ESA/LGCB/ADERSA meeting on May 12$^{th}$ 1999).

The figure 4 shows the minimum volume of reactor (upper graph) and the minimum flow rate (lower graph) depending on ratio of 1 man wastes for different values of the residence time (RT=12, 15 and 25 h).

## *3.4. Conclusion*

The minimum value of the residence time is 12 hours to have 99.5 % of acetate transformed in the reactor at the maximum light flux (400 W/$m^2$).

The choice of the minimum volume has to be done considering the flow rate imposed by the Melissa loop. In the global simulator the recirculating liquid is assumed to be 0.77 l/h (arbitrarily value coming from Spirulina compartment and that can be changed). In order to optimize the volume, the minimum residence time has to be chosen (12 h).

For a ratio of 0.2 man wastes (data coming from the global simulator in TN 54.4), the minimum volume is 6.5 l and the min flow rate is 0.55 l/h (figure 4). As the flow rate of the Melissa loop is supposed to be 0.77 l/h, the volume of the reactor has to be 0.77*12 = 9.2 l.

Remark: to allow comparison with other studies, the degradation of 0.2 man wastes produces 1.58 $10^{-3}$ mol/h of acetate and 3.96 $10^{-4}$ mol/h of butyrate.

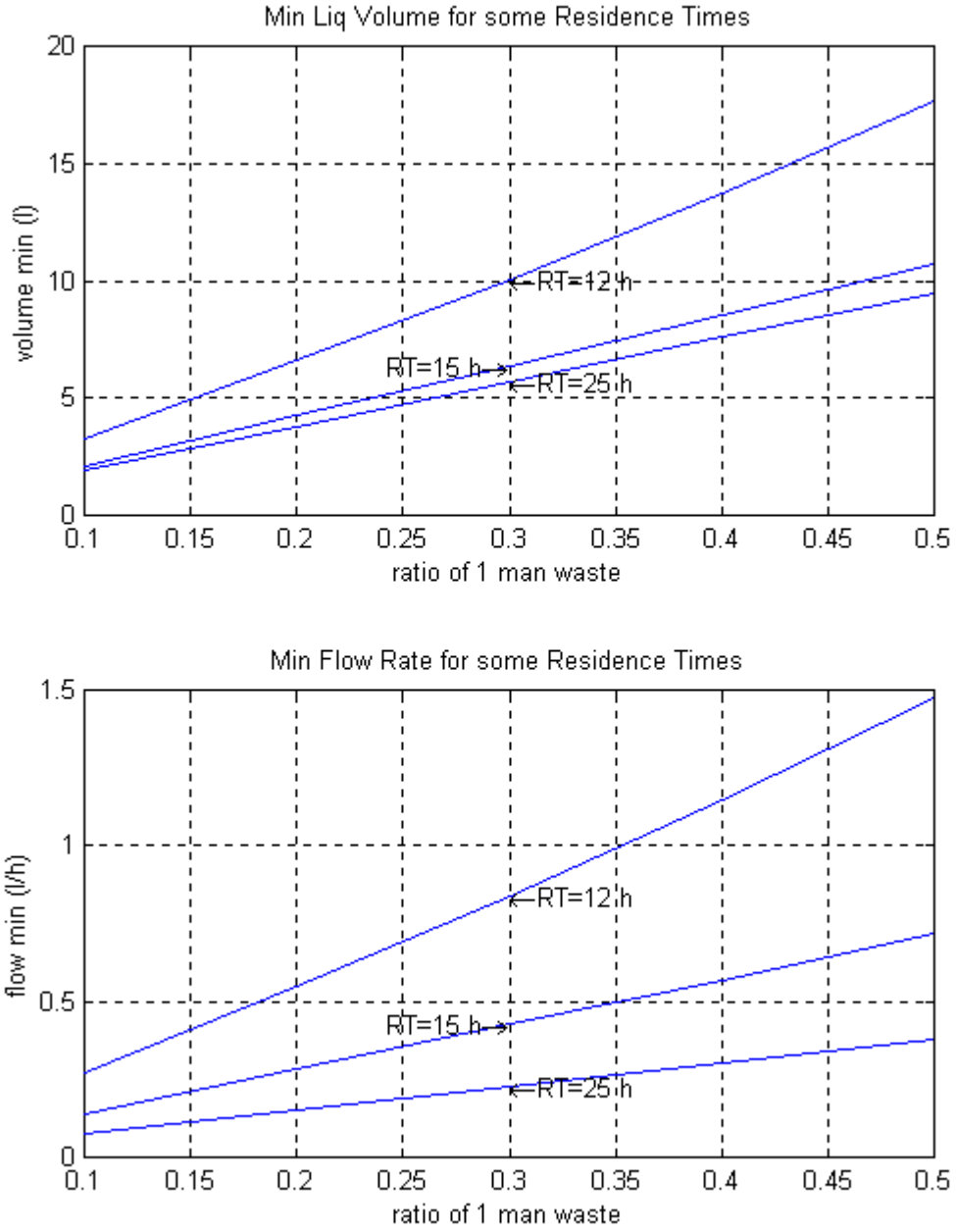


**Figure 4 : Minimum volume and flow rate of Rhodo compartment versus load (the load is the acetate and butyrate produced in Liquefying compartment by ratio of 1 man waste)**
**'Minimum' refers to 'Maximum' light flux**
**For lower light flux the curves move up**

# 4. SIZING OF THE SPIRULINA COMPARTMENT

## *4.1. Aim of the sizing*

The aim is to determine the minimum volume of the reactor so that it can produce a required amount of biomass or of oxygen at the maximum light flux (223 $W/m^2$).

## *4.2. Method*

The maximum Spirulina biomass production (production at maximum light flux) is computed versus the volume of the photobioreactor and the residence time.
The relation for the computation of Spirulina production at steady state has been established in TN 54.1 section 3 .
Its relation (3.16) shows that the residence time $\tau$ belongs to an interval whose limits are depending on the range of light flux $[F_{min}, F_{max}]$ :

$$f(F_{max}) \leq \tau \leq f(F_{min}) \qquad (2)$$

## *4.3. Numerical applications*

As in the case of the Rhodo compartment, for the computation of maximum biomass production versus volume and residence time, the substrates are non-limiting.
The gas/liquid transfer coefficient KLa is set at 12 $h^{-1}$, value obtained on the pilot plant at UAB (TN 43.110 p.26).
The illuminated surface fraction $f_i$ is set to 0.688 (TN 43.110 p.4, by UAB).

The figure 5 shows the minimum volume of reactor (upper graph) and the minimum flow rate (lower graph) depending on the required biomass production for different values of the residence time (RT=55, 100 and 150 h).

## *4.4. Conclusion*

The minimum value of the residence time is 55 hours.
The choice of the minimum volume has to be done considering the flow rate imposed by the Melissa loop. In the global simulator the recirculating liquid is assumed to be 0.77 l/h (arbitrarily value coming from Spirulina compartment and that can be changed). In order to optimize the volume, the minimum residence time has to be chosen (55 h).
The point corresponding to a biomass production rate of 1.1 g/h and a liquid flow rate of 0.77 l/h (data coming from current UAB experiments) belongs to the curve RT=100 h of the lower graph. The minimum volume on the curve RT=100 h of the upper graph is 77 l, which is exactly the volume of the reactor at UAB. It means that the reactor of the pilot plant is working at its maximum capacity for a residence time of 100 h.
The figures 5 foresees that for the same volume (77 l), the reactor could produce a maximum of 1.03 g/h for a maximum liquid flow rate of 1.4 l/h. This functioning point corresponds to a residence time of 55 h, which is its minimum value.
In addition, the figure indicates that, at a given volume (horizontal line on the upper graph), the gain of production of biomass is less than 10 % when the residence time is increased indefinitely (a multiplication factor of 3, from 55 to 150 h, on the graph).

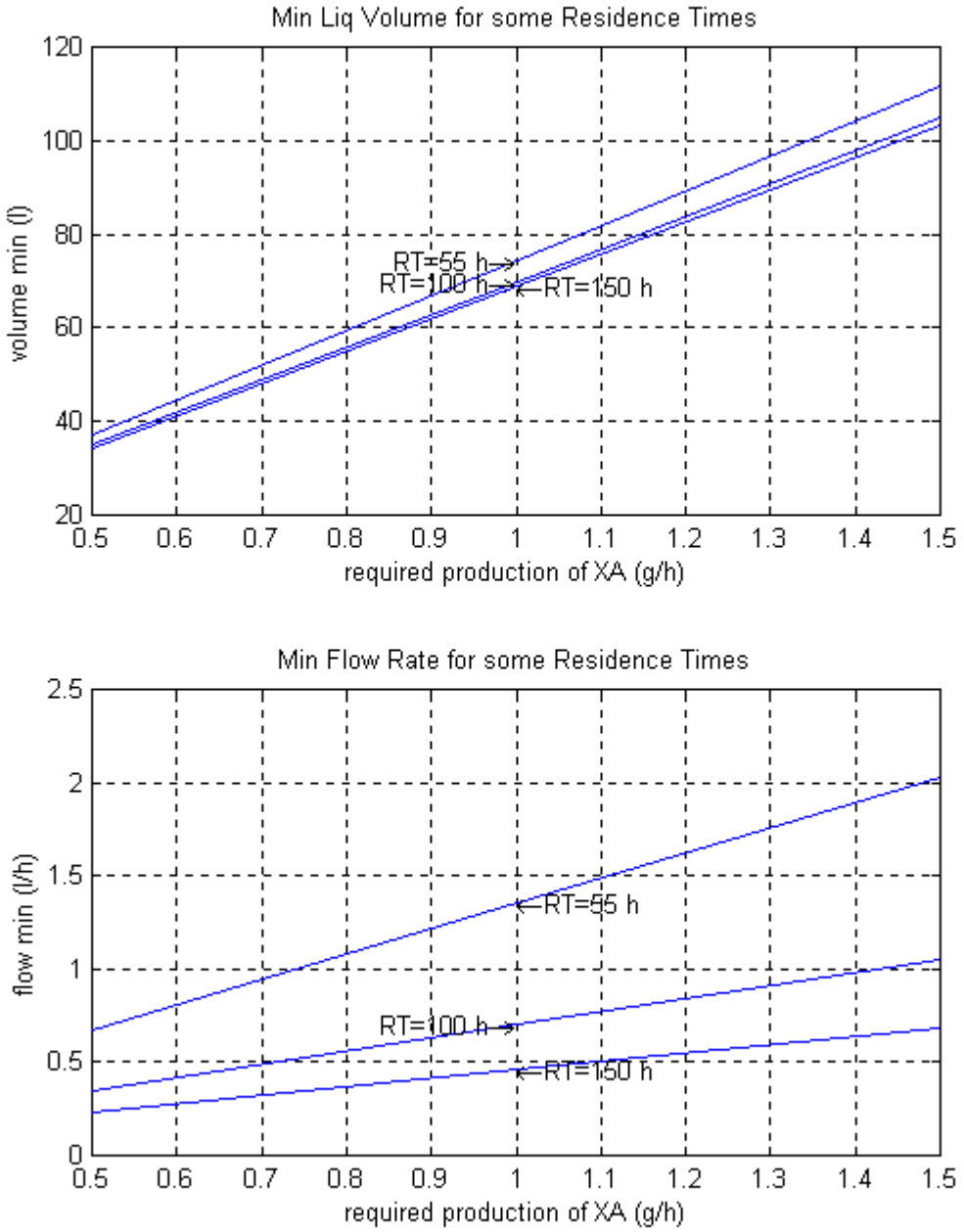


**Figure 5 : Minimum volume and flow rate of Spiru compartment versus required biomass production**
**'Minimum' refers to 'Maximum' light flux**
**For lower light flux the curves move up**

# 5. CONCLUSION

The study has contributed, by means of the First Principles models, a theoretical approach to the determination of the optimal volume of the Rhodobacter, Nitrifying and Spirulina compartments. It will very useful, when building the global simulator, to adapt the volumes according to the evolution of the project.

# 6. REFERENCES


GODIA,F.; ALBIOL, J.; CREUS, N.; PEREZ,J.; : “Preliminary review of the Pilot Plant Final Loop”. ESTEC contract 11549/95/NL/FG. December 2000, TN 47.3 .

LECLERCQ J.-J. : "Steady state of the compartments : Rhodobacter, Nitrifying and Spirulina". Contract ESTEC n° 12924/98/NL/MV, Contract change notice nº 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 nº 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.


# 7. ANNEX

## *7.1. Programme for sizing the Nitrifying compartment*

```
%**********************************************************************
%       Sizing compartment 3 (Nitri)                                   *
%       Version 1     October 2002                                     *
%                                                                      *
%       size_3.m : Main programme to help sizing Nitrifying compartment*
%                                                                      *
%**********************************************************************
clear all
global Ae_3 Be_3 Ce_3 De_3 E_3
global Fin1
global NL_3  NG_3  NS_3  NB_3  NX_3  NO_3  NI_3  NV_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  indG_3  indL_3  RG_3  RL_3  fG_3  fL_3  VA_3  VnB_3  VC_3  ...
epsL_3  epsG_3  epsT_3  alpha_3  Kdis_3  KLa_3  Gin_3  Fin_3

% The G flow rate of the Spirulina compart is set to the other compartments.
Gin_4 = 180;       % incoming gas flow rate (l/h) (from TN 43.110 p.26, UAB)
% The circulating L flow is set to 0.77 l/h (previous value of flow through Spiru).
Fcirc = .77;   % Recirculating L flow rate of the Melissa loop (arbitrary value) (l/h)
Fin_1 = Fcirc; % liquid flow rate through Lique (l/h)
Fin_3 = Fcirc; % liquid flow rate through Nitri(l/h)

% Initializing parameters of compart.
% ===================================
Matom = [12;   1;      16;    14;    32;   31];  % C H O N S P atomik mass
Fin1 = Fin_3;  % global Fin1 is used to run computation of the state matrices Ae_3,Be_3 ...
i_sim_0
i_sim_1
i_sim_3
indG = (NB_3+1)*NG_3+NG_3;          % index of outgoing NH3 G in output vector Y0
indL = (NB_3+1)*(NG_3+NL_3)+NG_3;   % index of outgoing NH3 L in state vector X0
indN = (NB_3+1)*(NG_3+NL_3)+NG_3+1; % index of outgoing NO2 in state vector X0
```

```
% Environment of the study
% ========================
nRat = 3;    % number of rats in the consumer compartment
nMan = .2;   % ratio of 1 man_waste at input 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))
spNO3_5 = 2.0e-3; % (mol/l) NO3 at HPC output (hence at Nitri input)
Yp_1p = (Faec*Yxf_1 + Urea*Yxu_1); % (mol/h/man) Production (H2 CO2 NH3 AcOH BuOH) for 1
man_waste (faeces + urea)
Yp_1(1,1) = -Yp_1p(1,1)/2;  % (mol/h/man) Lique consumption of O2
Yp_1(2:5,1) = Yp_1p(2:5,1); % (mol/h/man) Lique production of CO2 NH3 AcOH BuOH
% Production rate of CO2 : 4e-2 mol/h/rat
rCO2_0 = rCO2r_0*nRat;   % mol/h for n rats

% Concentrations at input of the column
% =====================================
% 1. Gas phase (coming from the consumer compartment) :
fm_O2_0  = .21;         % O2  (molar fraction). O2 consumed by rats is ignored
fm_CO2_0 = rCO2_0*VM_3/Gin_3;   % CO2 (molar fraction)
fm_H2O_0 = 5.796e-2;                % H2O (molar fraction)
fm_NH3_0 = 0;           % NH3 (molar fraction) : no NH3 from consumer
fm_N2_0 = 1 - fm_O2_0 - fm_CO2_0 - fm_NH3_0 - fm_H2O_0;    % N2
CG0_3 = [fm_O2_0; fm_CO2_0; fm_NH3_0] / VM_3; % mol/l
% 2.Liquid phase :
%CL0_3 = [C_O2; C_CO2; C_NH3; C_NO2; C_NO3; C_PO4; C_SO4];
cO2  = 0;                   % mol/l; No O2 L coming from Rhodo
cCO2 = nMan*Yp_1(2)/Fin_3;    % CO2 produced by Lique and Rhodo
lNH3 = nMan*Yp_1p(3,1);       % NH3 load (mol/h (NOT mol/l/h) of N total) from human waste
cNH3 = lNH3/Fin_3;            % NH3 molar conc. of N total in liquid (from human waste)
CL0_3= [cO2; cCO2; cNH3]./(1+Kdis_3); % mol/l ; molecular form
cNO2 = 1.4e-4;  % (mol/l) mean NO2 at Nitri input when MELISSA loop closed; TN 54.4 p.17
cSO4 = 10*sum(Yx1_3(7,:)) / sum(Yx1_3(3,:))*cNH3; % mol/l (SO4 excess versus stoechio to NH3)
cPO4 = 10*sum(Yx1_3(6,:)) / sum(Yx1_3(3,:))*cNH3; % mol/l (PO4 excess versus stoechio to NH3)
CL0_3= [CL0_3; cNO2; spNO3_5; cPO4; cSO4];

% Parameters to be scanned
% ========================
% 1. Vector of gas/liquid transfer parameters to be scanned
KLa_i = 1*[50; 50; 50];     % O2 CO2 NH3   (1/h)
KLa = [.5*KLa_i, KLa_i, 2*KLa_i];
% 2. Vector of recirculating ratio RG and RL to be scanned
RG=[0, 5, 10];
RL=[0, 5, 10];
% 3. Default value of parameters
idft = 2; % index of default parameter
KLa_3=KLa(:,idft);
RG_3=RG(idft); % default value of RG = its value in TN 27.2 p.13, LGCB
RL_3=RL(idft); % default value of RL = its value in TN 27.2 p.13, LGCB
% 4. Vectors of volume and load to be scanned
Vol1 = [5 6 7 8 9 10 12]; % max1 = 3.0767e-002; NB=1; KLa=.5*[50 50 50]
Vol2 = [3.5 3.75 4 5 6 8]; % max2 = 2.5939e-002; NB=1; KLa=[50 50 50]
Vol3 = [1.75 2 3 4 5 7];  % max3 = 1.7170e-002; NB=1; KLa=2*[50 50 50]
Load1 = [2.5 2 1.5 1 .5]*1e-2;      % max1 = 3.0767e-002; NB=1; KLa=.5*[50 50 50]
Load2 = [3 2.75 2.5 2 1.5 .5]*1e-2; % max2 = 2.5939e-002; NB=1; KLa=[50 50 50]
Load3 = [3 2.75 2.5 2 1.5 .5]*1e-2; % max3 = 1.7170e-002; NB=1; KLa=2*[50 50 50]

% Scanning the whole space of parameters
% ======================================
% The most influent parameters are : Volume, Load and KLa. Parameters RG and RL are minor.
% So, to shorten the computation time, the exploration of parameters space can be
% limited by setting 'nPar=1' instead of 'nPar=3' in the following statement.
nPar=3; %Three third parameters to be scanned
for iPar=1:nPar  % Iteration on the third parameter : KLa, RG or RL
  iPar
  if iPar == 1 % Third parameter = KLa
    Par=KLa;
    niter=size(KLa,2);
    eval(['ii=exist(''Vol',num2str(niter),''');'])
    if ~ii
      disp('Define more volumes to be scanned')
      break
    end
```

```
  eval(['ii=exist(''Load'',num2str(niter),''');'])
  if ~ii
    disp('Define more loads to be scanned')
    break
  end
  RG_3=RG(idft);
  RL_3=RL(idft);
elseif iPar == 2 % Third parameter = RG
  Par=RG;
  niter=length(RG);
  eval(['Vol=Vol',num2str(idft),';'])
  eval(['Load= Load',num2str(idft),';'])
  KLa_3=KLa(:,idft);
  RL_3=RL(idft);
elseif iPar == 3 % Third parameter = RL
  Par=RL;
  niter=length(RL);
  eval(['Vol=Vol',num2str(idft),';'])
  eval(['Load= Load',num2str(idft),';'])
  KLa_3=KLa(:,idft);
  RG_3=RG(idft);
end

% Computation of NO2
% ------------------
maxNO2=zeros(1,niter);
minNO2=zeros(1,niter);
for kk=1:niter % niter=dim. of the third parameter (KLa, RG or RL)
  if iPar == 1
    KLa_3 = Par(:,kk);
    eval(['Vol=Vol',num2str(kk),';'])
    eval(['Load= Load',num2str(kk),';'])
  elseif iPar == 2
    RG_3 = Par(kk);
  elseif iPar == 3
    RL_3 = Par(kk);
  end
  RG_3
  RL_3
  KLa_3
  Vol
  Load
  niterx=length(Vol);
  nitery=length(Load);
  cNO2_out=zeros(nitery,niterx);  % NO2 concentration at column output
  Yp=zeros(nitery,niterx);        % Yield NH3 --> NO3

  for itery=1:nitery
    %itery
    % Iterations on Load
    CL0_3(3) =  Load(itery)/Fin_3/(1+Kdis_3(3));
    % 1. Volume of column before variation
    VA = 1.48;      % volume of part A (l)
    VB = 6.17;      % volume of part B (l)
    VC = 0.45;      % volume of part C (l)
    % Iterations on volume
    for iterx=1:niterx
      coef_V=Vol(iterx)/epsL_3/VB;% multiplicative coef. of the vol of previous column
      VA_3 = VA*coef_V; % adapted volume of part A (l)
      VB_3 = VB*coef_V; % adapted volume of part B (l)
      VC_3 = VC*coef_V; % adapted volume of part C (l)
      VnB_3 = VB_3/NB_3;  % volume of an equivalent stirred tank

      % Computation of the state system of the nitrifying compartment
      %--------------------------------------------------------------
      [Ae_3,Be_3,Ce_3,De_3,E_3] = stasys_3(NG_3, NL_3, NB_3, Gin_3, Fin_3, ...
        RG_3, RL_3, fG_3, fL_3, VA_3, VnB_3, VC_3, epsL_3, epsG_3, epsT_3, ...
        alpha_3, Kdis_3, KLa_3);

      % Steady state of Nitri
      % ---------------------
      [X0_3, Y0_3, dX0_3] = stesta_3( ...
```

```
          NL_3, NG_3, NS_3, NB_3, NX_3, NO_3, NI_3, NV_3, 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, indG_3, indL_3, RG_3, RL_3, fG_3, fL_3, VA_3, VnB_3, VC_3, ...
          epsL_3, epsG_3, epsT_3, alpha_3, Kdis_3, KLa_3, Gin_3, Fin_3);
        if isempty(X0_3)
          disp(' X0_3 empty')
          iteration=[iterx itery]
          break
        end
        cNO2_out(itery,iterx) = X0_3((iNO2_3(NB_3+2)));  % NO2 concentration at column output
        Dp = (CG0_3(NG_3)-Y0_3(indG))*Gin_3 + (CL0_3(NG_3)-X0_3(indL))*(1+Kdis_3(NG_3))*Fin_3;
% flow of transformed NH3
        %Dp = Dp + CL0_3(NG_3+1)*Fin_3; % + ingoing NO2
        Dc = (X0_3(indN+1)-CL0_3(NG_3+2))*Fin_3; % outgoing NO3 flow rate
        Yp(itery,iterx) = Dc/Dp;  % conversion yield of  NH3+NO2 into NO3
      end
      if isempty(X0_3)
        break
      end
    end
    eval(['KLa',num2str(kk),num2str(iPar),'=KLa_3(1);'])
    eval(['RG',num2str(kk),num2str(iPar),'=RG_3;'])
    eval(['RL',num2str(kk),num2str(iPar),'=RL_3;'])
    eval(['Vol',num2str(kk),num2str(iPar),'=Vol;'])
    eval(['Load',num2str(kk),num2str(iPar),'=Load;'])
    eval(['cNO2_out',num2str(kk),num2str(iPar),'=cNO2_out;'])
    eval(['Yp',num2str(kk),num2str(iPar),'=Yp;'])
    maxNO2(kk)=max(max(cNO2_out));
    minNO2(kk)=min(min(cNO2_out));
    maxYp(kk)=max(max(Yp));
    minYp(kk)=min(min(Yp));
    end
  eval(['maxNO2',num2str(iPar),'=maxNO2'])
  eval(['minNO2',num2str(iPar),'=minNO2'])
  eval(['maxYp',num2str(iPar),'=maxYp'])
  eval(['minYp',num2str(iPar),'=minYp'])
end
%save simsiz_3

% Plotting 3D
% ===========
% 1. NO2
for iPar=1:nPar  % Iteration on the third parameter : KLa, RG or RL
  fen2tr
  for kk=1:niter
    subplot(3,1,kk)
    eval(['Vol=Vol',num2str(kk),num2str(iPar),';'])
    eval(['Load= Load',num2str(kk),num2str(iPar),';'])
    eval(['cNO2_out=cNO2_out',num2str(kk),num2str(iPar),';'])
    if 0
      Vol_lin = linspace(min(Vol), max(Vol), 11);
      Load_lin = linspace(min( Load), max( Load), 6);
      [X,Y]=meshgrid(Vol_lin, Load_lin);
      Z=griddata(Vol, Load,cNO2_out,X,Y,'cubic');
    else
      %[X,Y]=meshgrid(Vol, Load);
      Z=cNO2_out;
    end
    limitz = 1.6e-4; % max limit of acceptable NO2
    C=(Z<=limitz);
    cmap = [1 0 0 ; 0 0 1];
    colormap(cmap) % cancel by "colormap('default')"
    %h=surf(X,Y,Z,C);
    h=surf(Vol, Load,cNO2_out,C);
    set(gca,'XDir','rev')
    axis([min(Vol) max(Vol)   min(Load) max(Load)   0 .03])
    %hidden off
    xlabel('L. Vol. fixed bed (l)')
    ylabel('Load (mol/h)')
    zlabel('Nitrite (mol/l)')
    % marking the horizontal plane limit
```

```
    i1=1;
    i2 = min(find(C(:,i1)==1));
    texte = ['\bfLimit:', num2str(1e3*limitz), ' mmol/l NO2'];
    if ~(isempty(i1) | isempty(i2))
      text(Vol(i1), Load(i2),Z(i2,i1),texte,'VerticalAlignment','bottom')
    end
    if iPar == 1
      eval(['xx=KLa',num2str(kk),num2str(iPar),';'])
      title(['KLa=',num2str(xx),' h^-^1'])
    elseif iPar == 2
      eval(['xx=RG',num2str(kk),num2str(iPar),';'])
      title(['RG=',num2str(xx)])
    elseif iPar == 3
      eval(['xx=RL',num2str(kk),num2str(iPar),';'])
      title(['RL=',num2str(xx)])
    end
  end
end
% 2. Yiel NH3 --> NO3
for iPar=1:nPar  % Iteration on the third parameter : KLa, RG or RL
  fen2tr
  for kk=1:niter
    subplot(3,1,kk)
    eval(['Vol=Vol',num2str(kk),num2str(iPar),';'])
    eval(['Load= Load',num2str(kk),num2str(iPar),';'])
    eval(['Yp=Yp',num2str(kk),num2str(iPar),';'])
    if 0
      Vol_lin = linspace(min(Vol), max(Vol), 11);
      Load_lin = linspace(min( Load), max( Load), 6);
      [X,Y]=meshgrid(Vol_lin, Load_lin);
      Z=griddata(Vol, Load,Yp,X,Y,'cubic');
    else
      %[X,Y]=meshgrid(Vol, Load);
      Z=Yp;
    end
    limitz = .95; % min limit of acceptable Yield
    C=(Z<=limitz);
    cmap = [0 0 1; 1 0 0];
    colormap(cmap) % cancel by "colormap('default')"
    %h=surf(X,Y,Z,C);
    h=surf(Vol, Load,Yp,C);
    set(gca,'XDir','rev')
    set(gca,'ZDir','rev')
    axis([min(Vol) max(Vol)   min(Load) max(Load)   0 1])
    %hidden off
    xlabel('L. Vol. fixed bed (l)')
    ylabel('Load (mol/h)')
    zlabel('Yield')
    % marking the horizontal plane limit
    i1=1;
    i2 = min(find(C(:,i1)==0));
    texte = ['\bfYield Limit:', num2str(limitz)];
    if ~(isempty(i1) | isempty(i2))
      text(Vol(i1), Load(i2),Z(i2,i1),texte,'VerticalAlignment','bottom')
    end
    if iPar == 1
      eval(['xx=KLa',num2str(kk),num2str(iPar),';'])
      title(['KLa=',num2str(xx),' h^-^1'])
    elseif iPar == 2
      eval(['xx=RG',num2str(kk),num2str(iPar),';'])
      title(['RG=',num2str(xx)])
    elseif iPar == 3
      eval(['xx=RL',num2str(kk),num2str(iPar),';'])
      title(['RL=',num2str(xx)])
    end
  end
end
```

## 7.2. Programme for sizing the Rhodobacter compartment

```
%**********************************************************************
%       Sizing compartment 2 (Rhodo)                                  *
%       Version 1     October 2002                                    *
%                                                                     *
%       size_2.m : Main programme to help sizing Rhodobacter compart. *
%                                                                     *
%**********************************************************************
clear all
idisp=1; % if 1 ==> displaying details

% The G flow rate of the Spirulina compart is set to the other compart. excepted Lique and
Rhodo.
Gin_4 = 180;       % incoming gas flow rate (l/h) (from TN 43.110 p.26, UAB)
% The circulating L flow is set to 0.77 l/h (value of flow through Spiru).
Fcirc = .77;   % Recirculating L flow rate of the Melissa loop (arbitrary value) (l/h)
Fin_1 = Fcirc; % liquid flow rate through Lique (l/h)
Fin_2 = Fcirc; % liquid flow rate through Rhodo (l/h)

% Initializing parameters of compart.
% ===================================
Matom = [12;   1;      16;    14;    32;   31];  % C H O N S P atomik mass
i_sim_0
i_sim_1
i_sim_2

% Environment of the study
% ========================
nRat = 3;    % number of rats in the consumer compartment
nMan = .2;   % ratio of 1 man_waste at input 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); % (mol/h/man) Production (H2 CO2 NH3 AcOH BuOH) for 1
man_waste (faeces + urea)
Yp_1(1,1) = -Yp_1p(1,1)/2;  % (mol/h/man) Lique consumption of O2
Yp_1(2:5,1) = Yp_1p(2:5,1); % (mol/h/man) Lique production of CO2 NH3 AcOH BuOH
% Production rate of CO2 in Consu : 4e-2 mol/h/rat
rCO2_0 = rCO2r_0*nRat;   % mol/h for n rats
% Consumption rate of O2 in Consu : 4.45e-2 mol/h/rat
rO2_0 = rO2r_0*nRat;     % mol/h for n rats
% Consumption rate of O2 in Nitri
lNH3 = nMan*Yp_1p(3,1); % NH3 load (mol/h (NOT mol/l/h) of N total) from human waste
rO2_3 = -1.5*lNH3;      % approximate global stoechio in Nitri : 1.5 O2 + NH3 --> NO3
% Production rate of CO2 in Lique
rCO2_1 = nMan*Yp_1(2);
fm_O2_0  = .21;   %  O2 G (molar fraction of O2 at input of Consu)
fm_CO2_0 = 3e-4;  %  CO2 G (molar fraction of CO2 at input of Consu)

% Biomass concentration versus input rate of human waste 'nMan'
% =============================================================
Yx_AcOH = .995; % required value of yield by Rhodo
% 1.Gas phase (mol/l of CO2 NH3 AcOH BuOH from Lique assumed null) :
CG0_2 = [0; 0; 0; 0]; % mol/l
nMan_v=[.1:.1:.5]; % vector of 'nMan' values
niter=length(nMan_v);
cX=zeros(niter,1);
Yx_Bu_v=zeros(niter,1);
for iter=1:niter
  nMan=nMan_v(iter);
  % 2.Lique phase (mol/l of CO2 NH3 AcOH BuOH from Lique only) :
  CC = [Yx1_2(NG_2+[1,2],:) ./ (ones(2,1)*[Yx1_2(3,1),Yx1_2(4,2)])] * Yp_1p(4:5,1); %
(mol/h/man) SO4 PO4 consumed in Rhodo
  CL0_2 = nMan*[Yp_1p(2:5,1)./(1+Kdis_2); CC*10]/Fin_2; % mol/l of the molecular form CO2 NH3
AcOH BuOH, (SO4 & PO4) in excess
  % Concentration of biomass in Rhodo (necessary to consume 'Yx_AcOH' part of AcOH load)
  aa = 1 + Yx_AcOH*((1+Kdis_2(3))/(1+Kdis_2(NG_2))*Yx1_2(4,2)/Yx1_2(3,1) - 1);
  cX(iter) = -Yx_AcOH * (1+Kdis_2(3)) / Yx1_2(3,1)* (aa*CL0_2(3)+CL0_2(NG_2)) / aa;
  Yx_Bu_v(iter) = 1-(1-Yx_AcOH) / aa; % conversion of [BuOH]
end
prod_v=cX*Fin_2;
```

```
if idisp
  fen2tr(1);
  plot(nMan_v,prod_v),grid
  xlabel('ratio of 1 man waste')
  ylabel('biomass production (g/h)')
  title(['Biomass conc. to consume ',num2str(100*Yx_AcOH),' % of acetate'])
end
% Parameters to be scanned : Volume and Residence Time
% ========================
VL_v = [1   1  1;
        5   3  2;
        10  5  4;
        15  8  6;
        20  12 10];
tau_v=[12 15 25]; % (h) time constant (or Residence Time) cannot be shorter than 12 h
niter1=length(tau_v);
niter2=size(VL_v,1);
DX=zeros(niter2,niter1);
FR=zeros(niter2,niter1);
VLmin=zeros(niter,niter1);
% Scanning the whole space of parameters
% ======================================
nMan=.2*20; % to have substrates in excess when scanning the parameters space
for iter1=1:niter1
  for iter2=1:niter2
    VL_2=VL_v(iter2,iter1);
    Fin_2=VL_2/tau_v(iter1);
    % Computation of the state system of the biphasic compounds (same for Rhodo and Spiru)
    % -------------------------------------------------------------
    [A2_2,B2_2,GG1_2,GG2_2] = stasys_4(NG_2, NL_2, Gin_2, Fin_2, VL_2, alpha_2, Kdis_2,
KLa_2);
    % Computation of the max production of active biomass of Spiru
    % ------------------------------------------------------------
    cX0_2 = .01;  % (g/l) Value of biomass at starting of the iterative procedure
    imax=50; % max of iterations
    for ii=1:imax
      % 1. Concentrations at input of Rhodo
      % 1.1. Gas phase (mol/l of CO2 NH3 AcOH BuOH from Lique assumed null) :
      CG0_2 = [0; 0; 0; 0]; % mol/l
      % 1.2. Liquid phase (mol/l of CO2 NH3 AcOH BuOH from Lique only) :
      CC = [Yx1_2(NG_2+[1,2],:) ./ (ones(2,1)*[Yx1_2(3,1),Yx1_2(4,2)])] * Yp_1p(4:5,1); %
(mol/h/man) SO4 PO4 consumed in Rhodo
      CL0_2 = nMan*[Yp_1p(2:5,1)./(1+Kdis_2); CC]/Fin_2; % mol/l of the molecular form CO2 NH3
AcOH BuOH, (SO4 & PO4) in excess
      % 2. Steady state of Rhodo
      [FR0_2, X0_2, Y0_2, dX0_2] = stesta_2(...
        NG_2, NL_2, NO_2, NS_2, NI_2, NX_2, vNB_2, vNM_2, vNS_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, FRmaxc_2, fI_2, RT_2, Ea_2, Es_2, muM_2, KJ_2, EpsJ_2, q_rhod_2, zmin_I_2);
      if (isempty(FR0_2) | isempty(X0_2))
        disp([' FR0_2 or X0_2 empty at iteration ',num2str(ii)])
        break
      end
      % 3. End of iterative computation
      delta = (FRmax_2-FR0_2)/FRmax_2;
      if (abs(delta) < 1e-2), break, end
      cX0_2 = cX0_2*(1+.5*delta); % with relaxation coefficient
    end
    %if (isempty(FR0_2) | isempty(X0_2)), break, end
    if ii == imax,
      disp('*=*=* Iterative procedure for max biomass failed in size_2 *=*=*')
      disp(['Maximum number of iterations (',int2str(imax),') has been exceeded']);
      arret = 1;
    end
    DX(iter2,iter1) = Y0_2(length(Y0_2)) * Fin_2 ;
    FR(iter2,iter1)=FR0_2;
  end
  if idisp, Vol_DX_FR=[VL_v(:,iter1), DX(:,iter1), FR(:,iter1)], end
  if arret==1
    break
  end
```

```
  % Volume function of nMan
  % ========================
  VLmin(:,iter1)=interp1(DX(:,iter1),VL_v(:,iter1),prod_v);
  if idisp
    VLmin
    fen2tr(iter1+1);
    subplot(311)
    plot(nMan_v,VLmin(:,iter1)),grid
    xlabel('ratio of 1 man waste')
    ylabel('volume min (l)')
    title(['Min Liq Volume at ',num2str(FRmax_2),' W/m^2 and RT=',num2str(tau_v(iter1)),' h'])
    subplot(312)
    plot(nMan_v,VLmin(:,iter1)/tau_v(iter1)),grid
    xlabel('ratio of 1 man waste')
    ylabel('Flow rate (l/h)')
    title(['Flow rate for Vol min at RT=',num2str(tau_v(iter1)),' h'])
    %ax1=gca;
    %ax2=axes('Position',get(ax1,'Position'), 'YAxisLocation','right')
    %hl2=line(nMan_v,VLmin/tau_v(iter1),'Parent',ax2)
    subplot(313)
    plot(VL_v(:,iter1),DX(:,iter1)),grid
    xlabel('reactor volume (l)')
    ylabel('XA production (mol/h)')
    texte=['[',num2str(KLa_2),']'];
    title(['XA production for KLa = ',texte,' h^-^1'])
  end
end
if ~idisp
  x=[.3 .3 .3];
  fen2tr(1);
  subplot(211)
  for iter1=1:niter1
    plot(nMan_v,VLmin(:,iter1)),grid
    ind = find((nMan_v>=x(iter1)-eps) & (nMan_v<=x(iter1)+eps));
    y=VLmin(ind,iter1);
    if iter1==2
    text(x(iter1),y,['RT=',num2str(tau_v(iter1)),'
h\rightarrow'],'HorizontalAlignment','right')
    else
    text(x(iter1),y,['\leftarrowRT=',num2str(tau_v(iter1)),' h'])
    end
    hold on
  end
  xlabel('ratio of 1 man waste')
  ylabel('volume min (l)')
  title(['Min Liq Volume for some Residence Times'])
  subplot(212)
  for iter1=1:niter1
    plot(nMan_v,VLmin(:,iter1)/tau_v(iter1)),grid
    ind = find((nMan_v>=x(iter1)-eps) & (nMan_v<=x(iter1)+eps));
    y=VLmin(ind,iter1)/tau_v(iter1);
    if iter1==2
    text(x(iter1),y,['RT=',num2str(tau_v(iter1)),'
h\rightarrow'],'HorizontalAlignment','right')
    else
    text(x(iter1),y,['\leftarrowRT=',num2str(tau_v(iter1)),' h'])
    end
    hold on
  end
  xlabel('ratio of 1 man waste')
  ylabel('flow min (l/h)')
  title(['Min Flow Rate for some Residence Times'])
end
hold off
titre=['Sizing Rhodo; KLa = ',num2str(KLa_2),' 1/h'];
trtitre(gcf,titre,date)

% Rhodo (2) :
% CG0 = [CO2 NH3 AcOH BuOH]
% CL0 = [CO2 NH3 AcOH BuOH SO4 PO4]
% X0  = [CO2 NH3 AcOH BuOH SO4 PO4 XA]
```

## 7.3. Programme for sizing the Spirulina compartment

```
%**********************************************************************
%       Sizing compartment 4A (Spiru)                                 *
%       Version 1     October 2002                                    *
%                                                                     *
%       size_4.m : Main programme to help sizing Spirulina compartment *
%                                                                     *
%**********************************************************************
clear all
idisp=1; % if 1 ==> displaying details

% Two ways of expression of the problem :
express=2; % The required performance of Spiru is expressed in production of oxygen (mol/h)
express=1; % The required performance of Spiru is expressed in production of biomasse XA (g/h)
if express == 1
  prod_v=[.5:.5:1.5]';   % (g/h)   XA production required from Spiru
elseif express == 2
  prod_v=[.04:.01:.1]';  % (mol/h) O2 production required from Spiru
end

% The G flow rate of the Spirulina compart is set to the other compart. excepted Lique and
Rhodo.
Gin_4 = 180;       % incoming gas flow rate (l/h) (from TN 43.110 p.26, UAB)
% The circulating L flow is set to 0.77 l/h (previous value of flow through Spiru).
Fcirc = .77;   % Recirculating L flow rate of the Melissa loop (arbitrary value) (l/h)
Fin_1 = Fcirc; % liquid flow rate through Lique (l/h)
Fin_3 = Fcirc; % liquid flow rate through Nitri(l/h)
Fin_4 = Fcirc; % liquid flow rate through Spiru(l/h)

% Initializing parameters of compart.
% ===================================
Matom = [12;   1;      16;    14;    32;   31];  % C H O N S P atomik mass
i_sim_0
i_sim_1
i_sim_4

% Environment of the study
% ========================
% 'nRat' and 'nMan' in excess to have non limiting substrates
nRat = 3*2;    % number of rats in the consumer compartment
nMan = .2*2;   % ratio of 1 man_waste at input 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); % (mol/h/man) Production (H2 CO2 NH3 AcOH BuOH) for 1
man_waste (faeces + urea)
Yp_1(1,1) = -Yp_1p(1,1)/2;  % (mol/h/man) Lique consumption of O2
Yp_1(2:5,1) = Yp_1p(2:5,1); % (mol/h/man) Lique production of CO2 NH3 AcOH BuOH
% Production rate of CO2 in Consu : 4e-2 mol/h/rat
rCO2_0 = rCO2r_0*nRat;   % mol/h for n rats
% Consumption rate of O2 in Consu : 4.45e-2 mol/h/rat
rO2_0 = rO2r_0*nRat;     % mol/h for n rats
% Consumption rate of O2 in Nitri
lNH3 = nMan*Yp_1p(3,1); % NH3 load (mol/h (NOT mol/l/h) of N total) from human waste
rO2_3 = -1.5*lNH3;      % approximate global stoechio in Nitri : 1.5 O2 + NH3 --> NO3
% Production rate of CO2 in Lique
rCO2_1 = nMan*Yp_1(2);
fm_O2_0  = .21;   %  O2 G (molar fraction of O2 at input of Consu)
fm_CO2_0 = 3e-4;  %  CO2 G (molar fraction of CO2 at input of Consu)

niter=length(prod_v);
% Parameters to be scanned : Volume and Residence Time
% ===================================
VL_v = [30  30  30;
        90  90  90;
        150 150 150];
tau_v=[55 100 150]; % (h) time constant (or Residence Time) cannot be shorter than 55 h
niter1=length(tau_v);
niter2=size(VL_v,1);
DO=zeros(niter2,niter1);
DX=zeros(niter2,niter1);
```

```
FR=zeros(niter2,niter1);
VLmin=zeros(niter,niter1);
for iter1=1:niter1
  for iter2=1:niter2
    VL_4=VL_v(iter2,iter1);
    Fin_4=VL_4/tau_v(iter1);
    % Computation of the state system of the biphasic compounds
    % -------------------------------------------------------
    [A2_4,B2_4,GG1_4,GG2_4] = stasys_4(NG_4, NL_4, Gin_4, Fin_4, VL_4, alpha_4, Kdis_4,
KLa_4);
    % Computation of the max production of active biomass of Spiru
    % ------------------------------------------------------------
    cXA0_4 = 1;  % (g/l) Value of biomass at starting of the iterative procedure
    imax=10; % max of iterations
    for ii=1:imax
      % 1. Concentrations at input of Spiru
      % 1.1. Gas phase
      CG0_4 = [fm_O2_0/VM_0+(rO2_0+rO2_3)/Gin_4; fm_CO2_0/VM_0+rCO2_0/Gin_4];  % O2 CO2
(mol/l)
      % 1.2. Liquid phase
      cNO3 = -1.5*Yx1_4(3,1)*cXA0_4; % Excess of NO3 needs to avoid mineral limitation
      CL0_4 = [0;                                  % O2  (mol/l)
               rCO2_1/(1+Kdis_4(NG_4))/Fin_4;   % CO2 (mol/l)
               cNO3;                               % NO3 (mol/l)
               sum(Yx1_4(4,:))/Yx1_4(3,1)*cNO3; % SO4 (mol/l)
               Yx1_4(5,1)/Yx1_4(3,1)*cNO3];     % PO4 (mol/l)
      % 2. Steady state of Spiru
      [FR0_4, X0_4, Y0_4] = stesta_4( ...
        NG_4, NL_4, NO_4, vNB_4, vNM_4, Fin_4, VL_4, Yx1_4, ...
        A2_4, B2_4, GG1_4, GG2_4, CG0_4, CL0_4, cXA0_4, ...
        FRmin_4, FRmaxc_4, fI_4, zPC_4, zCH_4, ...
        RT_4, Ea_4, Es_4, muM_4, muEPS_4, Kj_4, KjEPS_4, Fmin_4, zmin_I_4, ...
        KSNO3_4, KSSO4_4, KSPO4_4, KSPC_4);
      if (isempty(FR0_4) | isempty(X0_4))
        disp(' FR0_4 or X0_4 empty')
        break
      end
      % 3. End of iterative computation
      delta = (FRmax_4-FR0_4)/(FRmax_4);
      if (abs(delta) < 1e-2), break, end
      cXA0_4 = cXA0_4*(1+.5*delta); % with relaxation coefficient
    end
    if (isempty(FR0_4) | isempty(X0_4)), break, end
    if ii == imax,
      disp('*=*=* Iterative procedure for max biomass failed in size_4 *=*=*')
      disp(['Maximum number of iterations (',int2str(imax),') has been exceeded']);
      arret = 1;
    end
    DO(iter2,iter1) = (Y0_4(1) - CG0_4(1)) * Gin_4 ;
    DX(iter2,iter1) = Y0_4(2*NG_4+NL_4+1) * Fin_4 ;
    FR(iter2,iter1) = FR0_4;
  end
  if idisp, Vol_DO_FR=[VL_v(:,iter1), DO(:,iter1), FR(:,iter1)], end
  if arret==1
    break
  end
  % Volume function of nMan
  % =======================
  if express == 1
    VLmin(:,iter1)=interp1(DX(:,iter1),VL_v(:,iter1),prod_v);% VL min versus XA production
  elseif express == 2
    VLmin(:,iter1)=interp1(DO(:,iter1),VL_v(:,iter1),prod_v);% VL min versus O2 production
  end
  if idisp
    VLmin
    if express == 1
      xtexte='XA production (g/h)';
    elseif express == 2
      xtexte='O2 production (g/h)';
    end
    fen2tr(iter1);
    subplot(311)
```

```
    plot(prod_v,VLmin(:,iter1)),grid
    xlabel(xtexte)
    ylabel('volume min (l)')
    title(['Min Liq Volume at ',num2str(FRmax_4),' W/m^2 and RT=',num2str(tau_v(iter1)),' h'])
    subplot(312)
    plot(prod_v,VLmin(:,iter1)/tau_v(iter1)),grid
    xlabel(xtexte)
    ylabel('Flow rate (l/h)')
    title(['Flow rate for Vol min at RT=',num2str(tau_v(iter1)),' h'])
    subplot(313)
    plot(DO(:,iter1),DX(:,iter1)),grid
    xlabel('O2 production (mol/h)')
    ylabel('XA production (g/h)')
    title(['XA versus O2 at RT=',num2str(tau_v(iter1)),' h'])
  end
end
if ~idisp
  if express == 1
    x1=[1 1 1 ];
    x2=[1 1 1];
    xtexte='required production of XA (g/h)';
  elseif express == 2
    x1=[.08 .07 .07];
    x2=[.07 .07 .07];
    xtexte='required production of O2 (mol/h)';
  end
  gcftr
  subplot(1,1,1); cla,
  subplot(211)
  for iter1=1:niter1
    plot(prod_v,VLmin(:,iter1)),grid
    ind = find((prod_v>=x1(iter1)-eps) & (prod_v<=x1(iter1)+eps));
    y=VLmin(ind,iter1);
    if iter1==3
    text(x1(iter1),y,['\leftarrowRT=',num2str(tau_v(iter1)),' h'])
    else
    text(x1(iter1),y,['RT=',num2str(tau_v(iter1)),'
h\rightarrow'],'HorizontalAlignment','right')
    end
    hold on
  end
  xlabel(xtexte)
  ylabel('volume min (l)')
  title(['Min Liq Volume for some Residence Times'])
  hold off
  subplot(212)
  for iter1=1:niter1
    plot(prod_v,VLmin(:,iter1)/tau_v(iter1)),grid
    ind = find((prod_v>=x2(iter1)-eps) & (prod_v<=x2(iter1)+eps));
    y=VLmin(ind,iter1)/tau_v(iter1);
    if iter1==2
    text(x2(iter1),y,['RT=',num2str(tau_v(iter1)),'
h\rightarrow'],'HorizontalAlignment','right')
    else
    text(x2(iter1),y,['\leftarrowRT=',num2str(tau_v(iter1)),' h'])
    end
    hold on
  end
  xlabel(xtexte)
  ylabel('flow min (l/h)')
  title(['Min Flow Rate for some Residence Times'])
end
hold off
titre=['Sizing Spiru; KLa = ',num2str(KLa_4),' 1/h; fI = ',num2str(fI_4)];
%trtitre(gcf,titre,date)

% Spiru (4) :
% CG0 = [O2 CO2]
% CL0 = [O2 CO2 NO3 SO4 PO4]
% X0  = [O2 CO2 NO3 SO4 PO4 XA XV EPS PC CH]
```