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Nitrite control of the Nitrifying compartment

SIMPLIFICATION OF THE STATE SYSTEM OF THE INTERNAL MODEL

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0	0	April 2003	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
solv. : solvated = molecular form (not total form)
PC : Personal Computer
PLC : Programmable Logical Computer
CV : Controlled Variable
MV : Manipulated Variable
CST : Completely Stirred Tank

1. INTRODUCTION

The state system of the internal model of the control is identical to the one of the simulated process, except the fact that the fixed bed of the model is considered as only one CST (Completely Stirred Tank) instead of a series of several CST's.
So, at the beginning of the study related to the control (elaboration, tuning of performance and robustness), it seemed natural to re-use the algorithm of the process itself and to apply it to the control. All the study was done with a controller written with Matlab® code. At the end the Matlab® code was translated into C language for its implementation in the computer of the pilot plant at UAB. But when tests of the C software were done on several compilers, it appeared that one of them (Watcom 10.6 compiler) was unable to allocate enough memory to run correctly the computation : the algorithm involves multiplication and inversion of rather huge matrices that needs more than 64 K-octet of contiguous memory.
So as the column of the internal model is composed of 3 tanks only (parts A, B or fixed bed, and C of the column), it was decided to adapt the algorithm of the internal model to this specific case so that less memory is needed. Another advantage is a shorter computation time. The disadvantage is that the algorithm is not general and strictly devoted to a column with 3 tanks.

2. NEW ALGORITHM OF THE STATE SYSTEM

2.1. Case of the mono-phasis compounds

It is recalled that the mono-phasis compounds are the compounds only solvated in the liquid phasis and not present in the gas phasis : NO_2, NO_3, SO_4 and PO_4.
The column of the internal model is represented by a series of 3 CST's where the dynamic behaviour is described by a first order transfer (figure 1). The back mixing ratios f_L of the 3 tanks are assumed null in the internal model.

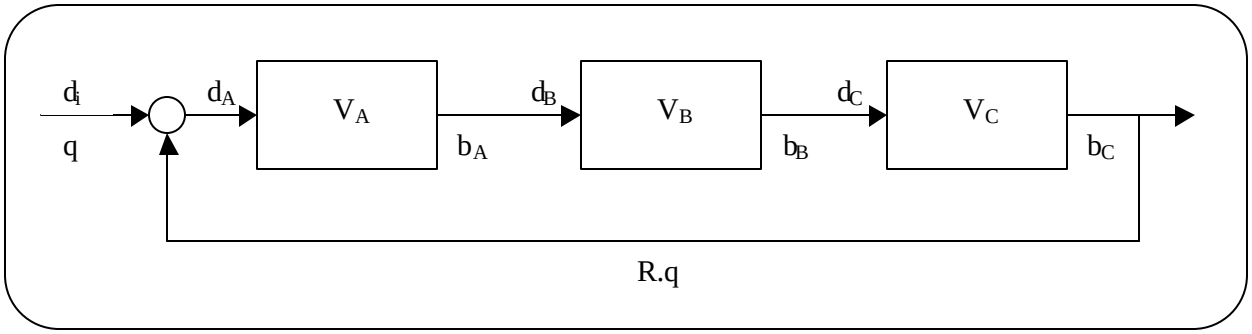

Figure 1 : Scheme of the column for the mono-phasis compounds
A,B,C : indices of the 3 parts
d : concentration of a compound at input of a tank
d_i : concentration of a compound at input of the column
b : concentration of a compound at output of a tank
q : liquid flow rate
R : re-circulating ratio
V : volume

Given $\theta = \frac{(1+R)\cdot q}{V}$ for any tank A, B or C.

Given r the variation rate of a compound.

The mass conservation implies the following set of equations for each mono-phasis compound :

$$\begin{aligned}
\dot{b}_A &= -\theta_A \cdot b_A + \theta_A \cdot d_A + r_A \\
\dot{b}_B &= -\theta_B \cdot b_B + \theta_B \cdot d_B + r_B \\
\dot{b}_C &= -\theta_C \cdot b_C + \theta_C \cdot d_C + r_C \\
(1+R)\cdot d_A &= d_i + R \cdot b_C \\
d_B &= b_A \\
d_C &= b_B
\end{aligned} \qquad (1)$$

Given the state vector X for a mono-phasis compound :

$$X = \begin{bmatrix} b_A \\ b_B \\ b_C \end{bmatrix}$$

The system (1) becomes :

$$\dot{X} = M_{AL} \cdot X + M_{BL} \cdot d_i + M_{EL} \cdot r_B \qquad (2)$$

with

$$M_{AL} = \begin{bmatrix} -\theta_A & 0 & \theta_A \cdot \frac{R}{1+R} \\ \theta_B & -\theta_B & 0 \\ 0 & \theta_C & -\theta_C \end{bmatrix} \qquad M_{BL} = \begin{bmatrix} \theta_A \cdot \frac{1}{1+R} \\ 0 \\ 0 \end{bmatrix} \qquad M_{EL} = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}$$

In the relation (2) :

- X is the vector of concentrations of a mono-phasis compound (NO_2, NO_3, SO_4 or PO_4) in the 3 tanks (A, B and C) of the column.
- the matrices M_{AL} and M_{BL} are independent of compound.
- r_B is the variation rate in the fixed bed B and depends on the growth and maintenance law of Ns and Nb biomass. Its way of computation is unchanged in this study. The variation rates r_A and r_C are zero.

2.2. Case of the bi-phasis compounds

The bi-phasis compounds are the compounds present both in the liquid phasis and in the gas phasis : O_2, CO_2 and NH_3.

2.2.1. Recall of the mass conservation in one CST

The dynamic behaviour in a tank (figure 2) is described by a first order transfer in the gas and liquid volumes.

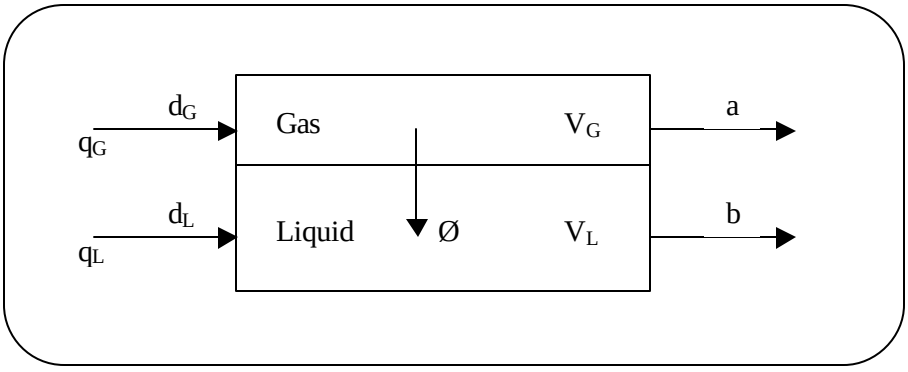

Figure 2 : Scheme of a tank for a bi-phasis compound

The mass conservation implies the following set of equations :

$$a = \alpha \cdot c$$

$$\Phi = K \cdot (c - b)$$

$$V_G \cdot \dot{a} = -\Phi \cdot V_L + q_G \cdot (d_G - a)$$

$$V_L \cdot \dot{b} = (r + \Phi) \cdot \frac{V_L}{1+k} + q_L \cdot (d_L - b)$$

with α : G/L equilibriu m constant (3)

$K : K_{La}$ (G/L tranfer)

k : dissociati on constant

c : concentrat ion at thermod ynamical equilibriu m

r : volumetri c variation rate

The solution has been established in relations (9) and (10) of TN 44.2 :

$$\dot{b} = -\theta \cdot b + \theta_L \cdot d_L + \theta_G \cdot d_G + \theta_r \cdot r$$

$$a = \alpha_4 \cdot b + \alpha_5 \cdot d_G \quad (4)$$

$$\text{with : } \theta = \frac{1}{\tau_1} \qquad \theta_L = \frac{G_1}{\tau_1} \qquad \theta_G = \frac{G_2}{\tau_1} \qquad \theta_r = \frac{G_3}{\tau_1}$$

The expressions of $G_1, G_2, G_3, \alpha_4, \alpha_5, \tau_1$ are given in (A2.2) (A2.8) of TN 44.2 .
The parameters $\theta, \theta_L, \theta_G$ and θ_r of (4) depend on tank (A, B or C) and on compound.

2.2.2. Mass conservation in the column

The column of the internal model is represented by a series of 3 CST's (figure 3). The back mixing ratios f_G and f_L are assumed null in the internal model.

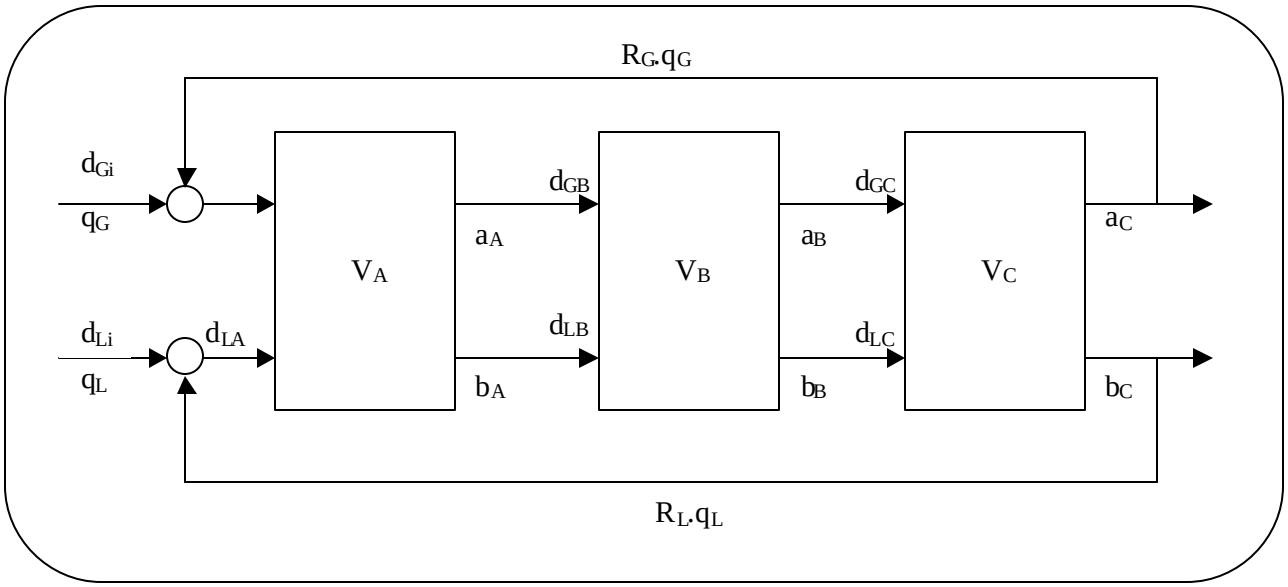

Figure 3 : Scheme of the column for the bi-phasis compounds
A,B,C : indices of the 3 parts
G, L = indices for Gas and Liquid phasis
d : concentration of a compound at input of a tank
d_i : concentration of a compound at input of the column
a : concentration of a G phasis compound at output of a tank
b : concentration of a L phasis compound at output of a tank
q : liquid flow rate
R : re-circulating ratio
V : volume

Applying (4) to each tank A, B and C leads to the 3 sets of equations (5), (6) and (7) :

$$\begin{aligned}
&\dot{b}_A = -\theta_A \cdot b_A + \theta_{LA} \cdot d_{LA} + \theta_{GA} \cdot d_{GA} + \theta_{rA} \cdot r_A \\
&a_A = \alpha_{4A} \cdot b_A + \alpha_{5A} \cdot d_{GA} \\
&(1+R_L) \cdot d_{LA} = d_{Li} + R_L \cdot b_C \\
&(1+R_G) \cdot d_{GA} = d_{Gi} + R_G \cdot a_C
\end{aligned} \qquad (5)$$

$$\begin{aligned}
&\dot{b}_B = -\theta_B \cdot b_B + \theta_{LB} \cdot d_{LB} + \theta_{GB} \cdot d_{GB} + \theta_{rB} \cdot r_B \\
&a_B = \alpha_{4B} \cdot b_B + \alpha_{5B} \cdot d_{GB} \\
&d_{LB} = b_A \\
&d_{GB} = a_A
\end{aligned} \qquad (6)$$

$$\begin{aligned} \dot{b}_C &= -\theta_C \cdot b_C + \theta_{LC} \cdot d_{LC} + \theta_{GC} \cdot d_{GC} + \theta_{rC} \cdot r_C \\ a_C &= \alpha_{4C} \cdot b_C + \alpha_{5C} \cdot d_{GC} \\ d_{LC} &= b_B \\ d_{GC} &= a_C \end{aligned} \qquad (7)$$

Given the intermediate parameters :

$$\alpha_{5G} = 1 - \alpha_{5A} \cdot \alpha_{5B} \cdot \alpha_{5C} \cdot \frac{R_G}{1+R_G}$$

$$p_1 = \frac{\alpha_{4A} \cdot \alpha_{5B} \cdot \alpha_{5C}}{\alpha_{5G}} \cdot \frac{R_G}{1+R_G}$$

$$p_2 = \frac{\alpha_{4B} \cdot \alpha_{5C}}{\alpha_{5G}} \cdot \frac{R_G}{1+R_G} \qquad (8)$$

$$p_3 = \frac{\alpha_{4C}}{\alpha_{5G}} \cdot \frac{R_G}{1+R_G}$$

$$p_4 = \frac{1}{\alpha_{5G}} \cdot \frac{1}{1+R_G}$$

It has to be noted that a_{5G} is strictly positive because $R_G \geq 0$ and $0 < \alpha_5 < 1$ for A, B and C.

Given the state vector X and the vector of inputs U for a bi-phasis compound :

$$X = \begin{bmatrix} b_A \\ b_B \\ b_C \end{bmatrix} \qquad U = \begin{bmatrix} d_{Gi} \\ d_{Li} \end{bmatrix}$$

The system (5) (6) (7) becomes (for a bi-phasis compound) :

$$\dot{X} = M_{AG} \cdot X + M_{BG} \cdot d_i + M_{EG} \cdot r_B \qquad (9)$$

with

$$M_{AG} = \begin{bmatrix} -\theta_A + \theta_{GA} \cdot p_1 & \theta_{GA} \cdot p_2 & \theta_{LA} \cdot \frac{R_L}{1+R_L} + \theta_{GA} \cdot p_3 \\ \theta_{LB} + \theta_{GB} \cdot (\alpha_{4A} + \alpha_{5A} \cdot p_1) & -\theta_B + \theta_{GB} \cdot \alpha_{5A} \cdot p_2 & \theta_{GB} \cdot \alpha_{5A} \cdot p_3 \\ \theta_{GC} \cdot \alpha_{5B} \cdot (\alpha_{4A} + \alpha_{5A} \cdot p_1) & \theta_{LC} + \theta_{GC} \cdot (\alpha_{4B} + \alpha_{5A} \cdot \alpha_{5B} \cdot p_2) & -\theta_C + \theta_{GC} \cdot \alpha_{5A} \cdot \alpha_{5B} \cdot p_3 \end{bmatrix}$$

$$M_{BG} = \begin{bmatrix} \theta_{GA} \cdot p_4 & \theta_{LA} \cdot \frac{1}{1+R_L} \\ \theta_{GB} \cdot \alpha_{5A} \cdot p_4 & 0 \\ \theta_{GC} \cdot \alpha_{5A} \cdot \alpha_{5B} \cdot p_4 & 0 \end{bmatrix} \qquad M_{EG} = \begin{bmatrix} 0 \\ \theta_{rB} \\ 0 \end{bmatrix}$$

In the relation (9) :

- X is the vector of concentrations of a bi-phasis compound (O_2, CO_2 or NH_3) in the 3 tanks (A, B and C) of the column.

- the matrices M_{AG} , M_{BG} and M_{EG} depend on compound through the thermodynamic constants.
- r_B is the variation rate in the fixed bed B and depends on the growth and maintenance law of Ns and Nb biomass. Its way of computation is unchanged in this study. The variation rates r_A and r_C are zero.

2.3. Checking the algorithm

The new algorithm (annex) has been validated versus the previous one. There is no gap between the results of the 2 algorithms :

2.3.1. Mono-phasis compounds

```
Gap between the 2 matrices A of mono-phasis compounds (MAL and As) :
            0            0 -2.2204e-016
            0            0            0
            0            0            0

Gap between the 2 matrices B of mono-phasis compounds (MBL and Bs) :
     0
     0
     0
```

2.3.2. Bi-phasis compounds

```
------ Compound O2  ---------------------------------------------
Gap between the 2 matrices A of bi-phasis compounds (MAG and As) :
            0 -7.1054e-015 -1.7764e-015
 -3.5527e-015 -2.8422e-014 -8.8818e-016
 -5.3291e-015 -7.1054e-015            0

Gap between the 2 matrices B of bi-phasis compounds (MBG and Bs) :
 -1.7764e-015            0
 -8.8818e-016            0
 -1.7764e-015            0

Gap between the 2 matrices E of bi-phasis compounds (MEG and Es) :
     0
     0
     0

------ Compound CO2 ---------------------------------------------
Gap between the 2 matrices A of bi-phasis compounds (MAG and As) :
            0 -3.3307e-016            0
            0 -4.4409e-016            0
            0            0            0

Gap between the 2 matrices B of bi-phasis compounds (MBG and Bs) :
 -5.5511e-017            0
 -5.5511e-017            0
 -5.5511e-017            0

Gap between the 2 matrices E of bi-phasis compounds (MEG and Es) :
     0
     0
     0
```

```
------ Compound NH3 ------------------------------------------------
Gap between the 2 matrices A of bi-phasis compounds (MAG and As) :
            0 -8.6736e-019            0
            0            0 -4.3368e-019
            0            0            0

Gap between the 2 matrices B of bi-phasis compounds (MBG and Bs) :
            0            0
 -6.9389e-018            0
            0            0

Gap between the 2 matrices E of bi-phasis compounds (MEG and Es) :
     0
     0
     0
```

3. CONCLUSION

The general algorithm for the computation of the state system has been established in relation (15) of TN 44.2 and is recalled hereafter :

$$\left| \begin{array}{l} \dot{X} = A_e \,.\, X + B_e \,.\, U_0 + E \,.\, J \,.\, C_x \\ Y = C_e \,.\, X + D_e \,.\, U_0 \end{array} \right. \qquad (10)$$

with :

$A_e = A - B(G \,.\, D + H)^{-1} \,.\, GC$

$C_e = C - D\,(G \,.\, D + H)^{-1} \,.\, GC$

$B_e = \left(2 \cdot N_G + N_L\right)$ first columns of $B(G \,.\, D + H)^{-1}$

$D_e = \left(2 \cdot N_G + N_L\right)$ first columns of $D(G \,.\, D + H)^{-1}$

So, as it can be seen, the previous algorithm involved multiplication and inversion of matrices for the computation of A_e and B_e. In the new algorithm, the components of the matrices M_{AG}, M_{AL}, M_{BG} and M_{BL} are computed directly from the parameters of the internal model by means of relations (2) and (8).

Now concerning the memory allocation :

The size of the square matrix A_e was $3 \cdot \left(N_G + N_L\right) \times 3 \cdot \left(N_G + N_L\right)$ where N_G and N_L are the number of bi and mono-phasis compounds (N_G=3 and N_L=4).

The size of B_e is $3 \cdot \left(N_G + N_L\right) \times \left(2 \cdot N_G + N_L\right)$.

In the new algorithm :

- A_e is replaced by N_G matrices M_{AG} and 1 matrix M_{AL} whose sizes are 3x3. It implies that the total number of components is about 12 times as small.
- B_e is replaced by N_G matrices M_{BG} of size 3x2 and 1 matrix M_{BL} of size are 3x1. It implies that the total number of components is divided by ten.

Then the size of arrays allocated in the memory of the computer for these matrices M_{AG}, M_{AL}, M_{BG} and M_{BL} is reduced considerably.

Moreover the matrices corresponding to the previous C_e and D_e need not to be computed because the concentrations in the gas are not necessary for the control.

4. REFERENCE

LECLERCQ J.-J. : "Numerical simplification of the dynamic model of the nitrifying compartment ". Contract ESTEC n° 12924/98/NL/MV of July 10th 1998; May 1999; TN 44.2.

5. ANNEX : SOFTWARE OF COMPUTATION OF THE STATE SYSTEM

Source file of the Matlab® programme :

```
%*****************************************************************
%       Nitrifying column control                                *
%       Version 1.0     March 2003                               *
%                                                                *
%       State system according to TN 73.4                        *
%                                                                *
%       stasysim.m : Computation of the state system matrices    *
%                    of the internal model of the control        *
%                                                                *
%*****************************************************************
function [MAG,MAL,MBG,MBL,MEG,MEL] = stasysim(NG, Gin, Fin, VA, VB, VC, epsG, epsL, ...
                                        epsT, RG, RL, KLa, Kdis, alpha)

% Computation of the matrices 'A' and 'B' dedicated to the biphasis compounds
G1=zeros(1,NG);
G2=zeros(1,NG);
G3=zeros(1,NG);
a4=zeros(1,NG);
a5=zeros(1,NG);
tau=zeros(1,NG);
NT=3; % Number of compartments of the column (case of internal model)
MAG=zeros(NT,NT,NG);
MBG=zeros(NT,2,NG); % 2=number of phases (G and L for the bi-phases compounds)
MEG=zeros(NT,NG);
for j=1:NG; % for biphasis compounds O2 CO2 and NH3
  for ii = 1:NT  % for the differents parts of the column (case of internal model)
    if ii == 1        % Part A of the column
      VL = VA*epsL/epsT;    % volume of liquid
      VG = VA*epsG/epsT;    % volume of gas
      qL = Fin * (1+RL);
      qG = Gin * (1+RG);
    elseif ii == 2    % Part B of the column
      VL = VB*epsL;         % volume of liquid
      VG = VB*epsG;         % volume of gas
      qL = Fin * (1+RL);
      qG = Gin * (1+RG);
    elseif ii == 3    % Part C of the column
      VL = VC*epsL/epsT;    % volume of liquid
      VG = VC*epsG/epsT;    % volume of gas
      qL = Fin * (1+RL);
      qG = Gin * (1+RG);
    end

    % Computation of the gains G1, G2 ...
    [G1(ii),G2(ii),G3(ii),a4(ii),a5(ii),tau(ii),arret] = ...
      transbi(VG,VL,qG,qL,KLa(j),Kdis(j),alpha(j),ii);
  end

  t=1./tau;
  tL=G1./tau;
  tG=G2./tau;
  a5G=1-a5(1)*a5(2)*a5(3)*RG/(1+RG);
  % Intermediate parameters
  p1=a4(1)*a5(2)*a5(3)/a5G*RG/(1+RG);
  p2=a4(2)*a5(3)/a5G*RG/(1+RG);
  p3=a4(3)/a5G*RG/(1+RG);
  p4=1/(a5G*(1+RG));
  % Computation of the matrix 'A' dedicated to the biphasis compounds(matrix named 'MAG'
hereafter)
```

```
  MAG(:,:,j)=[-t(1)+tG(1)*p1,               tG(1)*p2,
tL(1)*RL/(1+RL)+tG(1)*p3;
              tL(2)+tG(2)*(a4(1)+a5(1)*p1), -t(2)+tG(2)*a5(1)*p2,
tG(2)*a5(1)*p3;
              tG(3)*a5(2)*(a4(1)+a5(1)*p1), tL(3)+tG(3)*(a4(2)+a5(1)*a5(2)*p2), -
t(3)+tG(3)*a5(1)*a5(2)*p3];

  % Computation of the matrix 'B' dedicated to the biphasis compounds(matrix named 'MBG'
hereafter)
  MBG(:,:,j)=[tG(1)*p4,             tL(1)/(1+RL);
              tG(2)*a5(1)*p4,       0;
              tG(3)*a5(1)*a5(2)*p4, 0];

  % Computation of the matrix 'E' dedicated to the biphasis compounds(matrix named 'MEG'
hereafter)
  MEG(:,j)=[0;           % coef set to 0 because variation rate of compound is 0 in part A
            G3(2)/tau(2);% number 2 --> fixed bed (part B)
            0];          % coef set to 0 because variation rate of compound is 0 in part C
end

VL=[VA*epsL/epsT;    % volume of liquid of A
    VB*epsL;        % volume of liquid of B
    VC*epsL/epsT];   % volume of liquid of C

% Computation of the matrix 'A' dedicated to the monophasis compounds (matrix named 'MAL'
hereafter)
t=Fin*(1+RL)./VL;
MAL=[-t(1),     0, t(1)*RL/(1+RL);
      t(2), -t(2),             0;
         0,  t(3),          -t(3)];

% Computation of the matrix 'B' dedicated to the monophasis compounds (matrix named 'MBL'
hereafter)
MBL=[t(1)/(1+RL); 0; 0];

% Computation of the matrix 'E' dedicated to the monophasis compounds (matrix named 'MEL'
hereafter)
MEL=[0; 1; 0];

if arret == 1, disp('*** Subroutine transbi called by stasysim ***'), end
```