ASSOCIATION POUR LE DÉVELOPPEMENT DE L'ENSEIGNEMENT ET DE LA RECHERCHE EN SYSTÉMATIQUE APPLIQUÉE

MELISSA

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A first approach for the Biomass and nitrite estimators of the nitrifying compartment

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1. INTRODUCTION

The nitrite is a poison for man and, in a less degree, for the biomass of the nitrifying compartment.

The nitrite concentration increases during a transient period that follows an increasing of NH_3 (and not a decreasing one)

As it is difficult to measure the nitrite, it is necessary to estimate it in order to allow an increasing of NH_3, if any, according to a maximum slope corresponding to the maximum admissible content of NO_2^- .

The compounds, whose concentrations can be measured easily enough in real time, are NH_3 and NO_3^- in the liquid phase. The nitrite estimator has to work from these data.

So the first step is to estimate the concentrations of N_s and N_b biomass (by means of a biomass estimator). Then a nitrite estimator, fed with this estimation of biomass and with the measurement of the incoming flow of NH_3, estimates the nitrite concentration in the outgoing flow of the column.

2. BIOMASS ESTIMATOR

The starting point is the state system of the column built in TN 44.2 (whose all the notations are maintained here).

$$\left| \begin{array}{l} \dot{X} = A_e \,.\, X + B_e \,.\, U_o + E \,.\, J \,.\, C_x \\ Y = C_e \,.\, X + D_e \,.\, U_o \end{array} \right. \qquad (1)$$

with, particularly :

$$\left| \begin{array}{l} A_e = A - B(GD + H)^{-1} \,.\, GC \\ C_e = C - D(GD + H)^{-1} \,.\, GC \\ B_e = \text{10 first columns of } B(GD + H)^{-1} \\ D_e = \text{10 first columns of } D(GD + H)^{-1} \end{array} \right.$$

In the case of the biomass estimator, only the 2 compounds which are measured, have to be taken into account : NH_3 and NO_3^- .

The behaviour of these 2 compounds along the column is given by a part of the system (1).

Hereafter, the matrices A_b, B_b, C_b, D_b, E_b, G_b, H_b, J_b and the vectors X_b, U_{ob} have the same meaning as in (1) but their dimensions are reduced to the 2 compounds NH_3 and NO_3^-. The index b means that theses matrices and vectors are associated to the Biomass estimation.

Given $n = N_B + 2$:

$$X_b = \begin{bmatrix} X_1 \\ \vdots \\ X_i \\ \vdots \\ X_n \end{bmatrix} \qquad \text{with :} \qquad X_i = \begin{bmatrix} b_{1i} \\ \\ b_{2i} \end{bmatrix}$$

$$U_{ob} = \begin{bmatrix} d_{G1} \\ \\ d_{L1} \\ \\ d_{L2} \end{bmatrix}$$

index 1 for NH_3
index 2 for NO_3^-

d_{G1} : conc. of NH_3 in gas
d_{L1} : conc. of NH_3 in liquid
d_{L2} : conc. of NO_3^- in liquid

$$A_b = \begin{pmatrix} A_1 & & \mathbf{0} \\ & \ddots & \\ & A_i & \\ & & \ddots \\ \mathbf{0} & & A_n \end{pmatrix} \qquad \text{with : } A_i = \begin{bmatrix} -\frac{1}{\tau_{11i}} & 0 \\ \\ 0 & -\frac{1}{\tau_{L2i}} \end{bmatrix}$$

$$B_b = \begin{pmatrix} B_1 & & \mathbf{0} \\ & \ddots & \\ & B_i & \\ & & \ddots \\ \mathbf{0} & & B_n \end{pmatrix} \qquad \text{with : } B_i = \begin{bmatrix} \frac{G_{21i}}{\tau_{11i}} & \frac{G_{11i}}{\tau_{11i}} & 0 \\ \\ 0 & 0 & \frac{1}{\tau_{L2i}} \end{bmatrix}$$

$$E_b = \begin{pmatrix} E_1 & & \mathbf{0} \\ & \ddots & \\ & E_i & \\ & & \ddots \\ \mathbf{0} & & E_n \end{pmatrix} \qquad \text{with : } E_i = \begin{bmatrix} \frac{G_{3i}}{\tau_{11i}} & 0 \\ 0 & 1 \end{bmatrix}$$

$$C_b = \begin{pmatrix} C_1 & & \mathbf{0} \\ & \ddots & \\ & C_i & \\ & & \ddots \\ \mathbf{0} & & C_n \end{pmatrix} \qquad \text{with : } C_i = \begin{bmatrix} \alpha_4 & 0 \\ 1 & 0 \\ 0 & 1 \end{bmatrix}$$

$$D_b = \begin{pmatrix} D_1 & & \mathbf{0} \\ & \ddots & \\ & D_i & \\ & & \ddots \\ \mathbf{0} & & D_n \end{pmatrix} \qquad \text{with : } D_i = \begin{bmatrix} \alpha_5 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

$G_b =$

1	**2**	**i-1**	**i**	**i+1**	**n-1**	**n**	
	$-\delta(I_3+\beta)$					$-\beta$	**1**
$-(I_3+\delta)$		$-\delta$					**2**
	$-(I_3+\delta)$		$-\delta$				**i-1**
		$-(I_3+\delta)$		$-\delta$			**i**
			$-(I_3+\delta)$		$-\delta$		**i+1**
				$-(I_3+\delta)$		$-\delta$	**n-1**
					$-I_3$		**n**

δ = diag ([f', f, f])
β = diag([R_G, R_L, R_L])

I_3 = identity matrix with dimension 3

1	**2**	**i-1**	**i**	**i+1**	**n-1**	**n**	

H_b =

$(I_3+\delta)(I_3+\beta)$							**1**
	$I_3+2\delta$						**2**
		$I_3+2\delta$					**i-1**
			$I_3+2\delta$				**i**
				$I_3+2\delta$			**i+1**
					$I_3+2\delta$		**n-1**
						I_3	**n**

$$J_b = \begin{pmatrix} J_1 & & & \mathbf{0} \\ & \ddots & & \\ & & J_i & \\ & & & \ddots \\ \mathbf{0} & & & J_n \end{pmatrix} \quad \text{with } J_i = Y_{X12} \,.\, r_{\mu i} \,.\, \mu_m + Y_{m12} \,.\, Klim_i \,.\, m$$

$$Y_{X12} = \begin{pmatrix} -4.5341 & -0.1994 \\ 0 & 15.1714 \end{pmatrix} \quad \text{et} \quad Y_{m12} = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$\mu_m = \begin{pmatrix} 5.7 \,.\, 10^{-2} & 0 \\ 0 & 3.6 \,.\, 10^{-2} \end{pmatrix} \quad \text{et} \quad m = \begin{pmatrix} 3.38 \,.\, 10^{-3} & 0 \\ 0 & 7.92 \,.\, 10^{-3} \end{pmatrix}$$

$Klim_i$, matrix of limiting consumption of substrates, and $r_{\mu i}$,matrix of limiting global growth, are defined in TN 44.2 .

With the new matrices A_{eb} and B_{eb} associated to the 2 compounds NH_3 and NO_3^- only, the system (1) becomes :

$$\dot{X}_b = A_{eb} \,.\, X_b + B_{eb} \,.\, U_{ob} + E_b \,.\, J_b \,.\, C_X \qquad (5)$$

$$\Rightarrow \quad C_X = (E_b \,.\, J_b)^{-1} \,.\, (\dot{X}_b - A_{eb} X_b - B_{eb} U_{ob}) \qquad (6)$$

When X_b, vector of concentrations of NH_3 L and NO_3^- of each tank, is measured, the relation (6) is the biomass estimator.

The software of (6) is tested from the data processing point of view. The figure 1 shows the concentrations of active biomass in each tank simulated by the state system of the column (equation (15) of TN 44.2).

The figure 2 shows the concentrations of biomass estimated (by (6) of the present TN) from the "measurements" (i.e. simulated data) of NH_3 and NO_3^- in each tank.

The estimations of the biomass are quite similar to the values of the column simulation. This good agreement between simulation and estimation is possible because there is no noise in simulation and no mismatch of parameters.

Of course, the robustness of the estimator has to be tested in a further study.

N.B. : J_b varies versus time because of $Klim_i$ and $r_{\mu i}$.

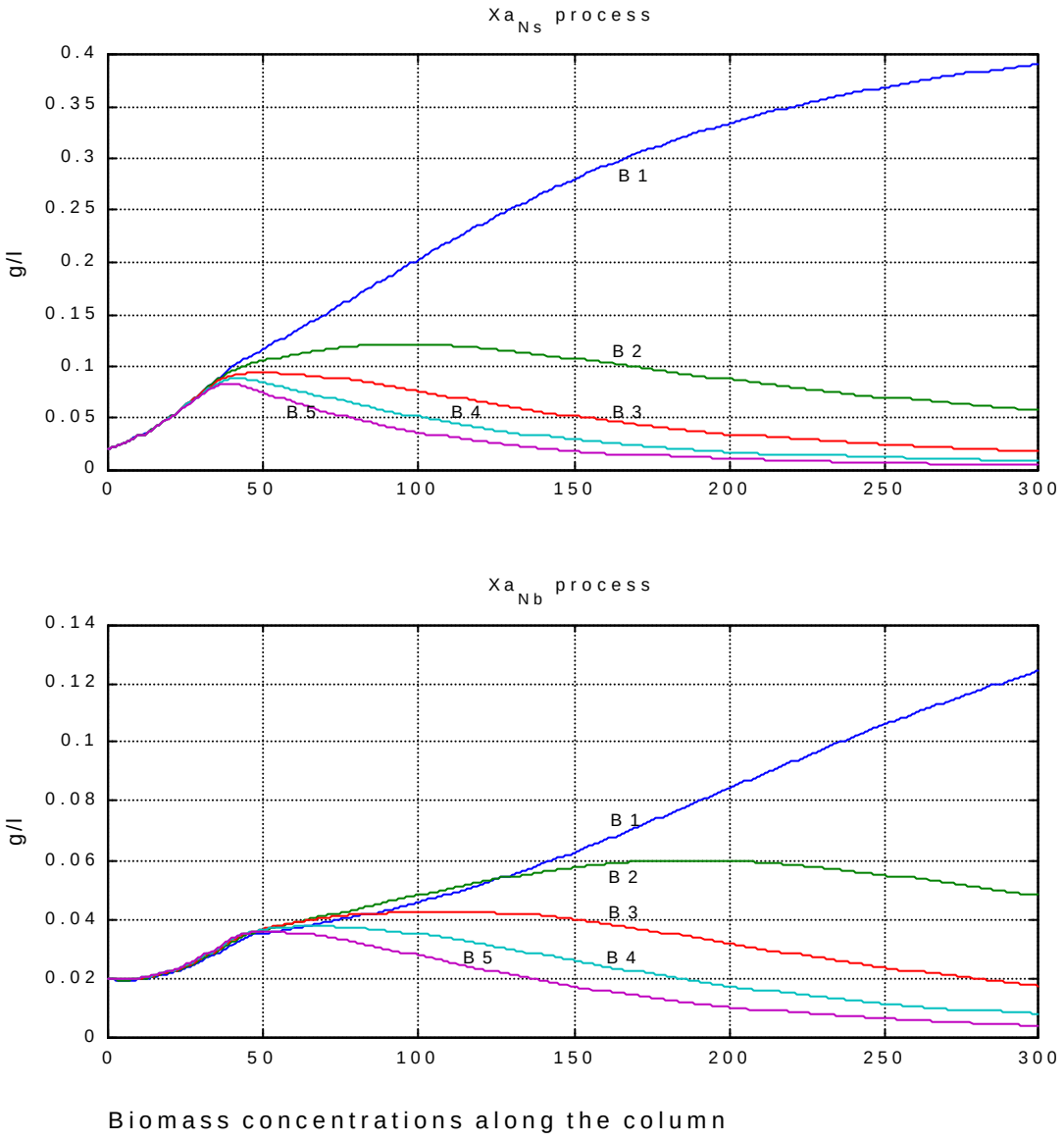


Figure 1 : Biomass in each tank of part B of the column (process)

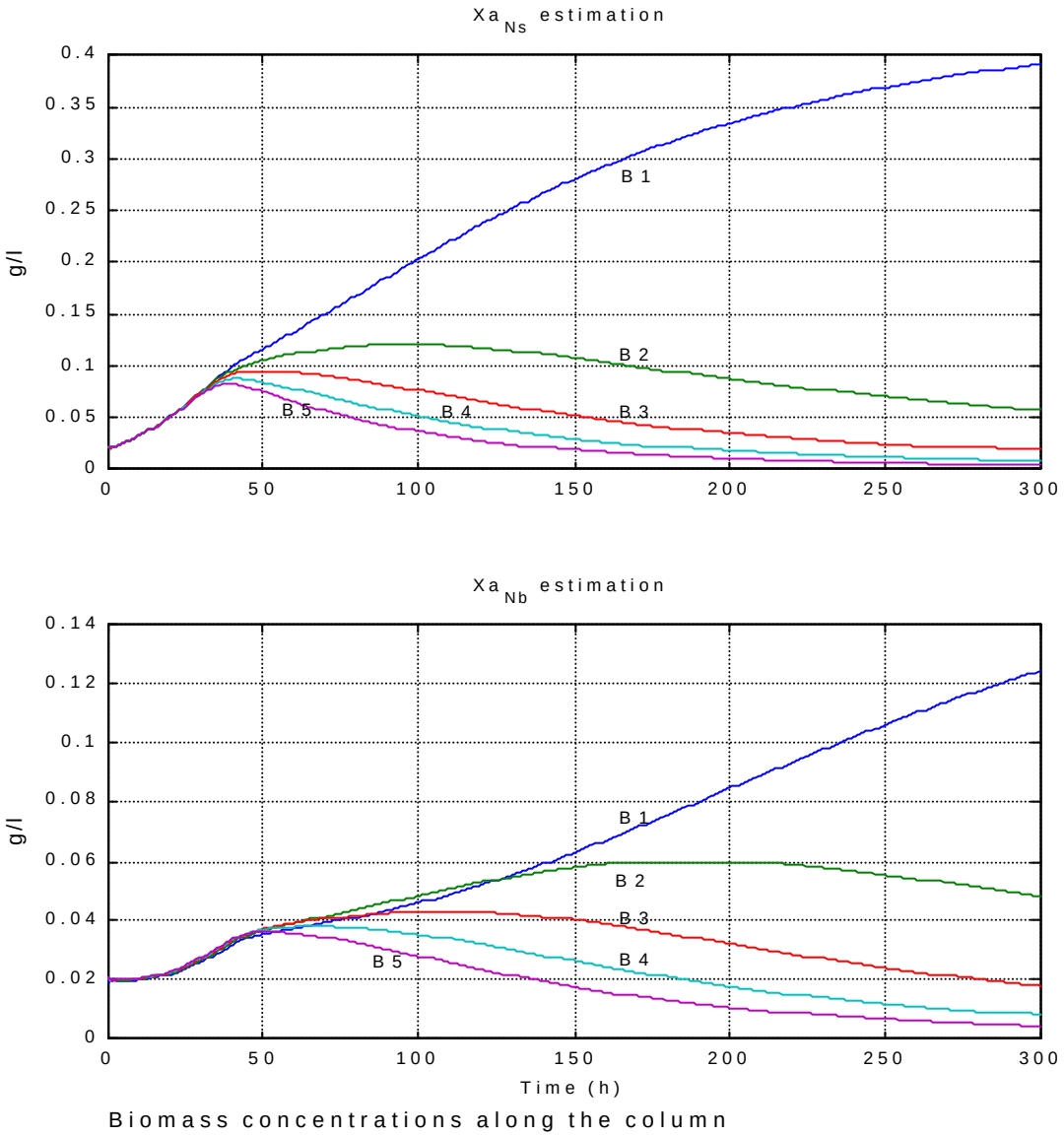


Figure 2 : Estimation of biomass in each tank of part B

3. NITRITE ESTIMATOR

As for the biomass estimator, the starting point is the state system (1) of the column of TN 44.2.

In the case of the nitrite estimator, only one compound is taken into account : NO_2^-.

For each tank i, the matrices and vectors are now :

- $X_i = b_{4i}$ (b_{4i} is the concentration of NO_2^- in tank i)
- $Y_i = X_i$
- $A_i = -\frac{1}{\tau_{L4i}}$
- $B_i = \frac{1}{\tau_{L4i}}$
- $C_i = 1$
- $D_i = 0$
- $E_i = 1$
- $J_i = Y_{X11} \cdot r_{\mu i} \cdot \mu_m + Y_{m11} \cdot Klim_i \cdot m$

$$Y_{X11} = (4.3347 \quad -15.1714)$$
$$Y_{m11} = (1 \quad -1)$$

$r_{\mu i}$, μ_m, $Klim_i$ and m : identical to those of the biomass estimator

The vectors and matrices A_n, B_n, C_n, D_n, E_n, J_n, X_n, U_{on} and C_x are built in the same way as for the biomass estimator (or for the state system of the column). The index n means that these matrices and vectors are associated to the Nitrite estimation.

The matrices G_n and H_n are built in the same way as those of the biomass estimator where :

- I_3 is replaced by 1
- $\delta = f$
- $\beta = R_L$

The vector U_{on} is now :

$U_{on} = d_{L4}$ (d_{L4} is the concentration of NO_2^- of the liquid at the input of the column).

Then, the evolution of the nitrite concentration of the column, X_n, is given by the state system :

$$\left| \begin{array}{l} \dot{X}_n = A_{en} \,.\, X_n + B_{en} \,.\, U_{on} + E_n \,.\, J_n \,.\, C_X \\ J_n = C_{en} \,.\, X_n + D_{en} \,.\, U_{on} \end{array} \right. \qquad (7)$$

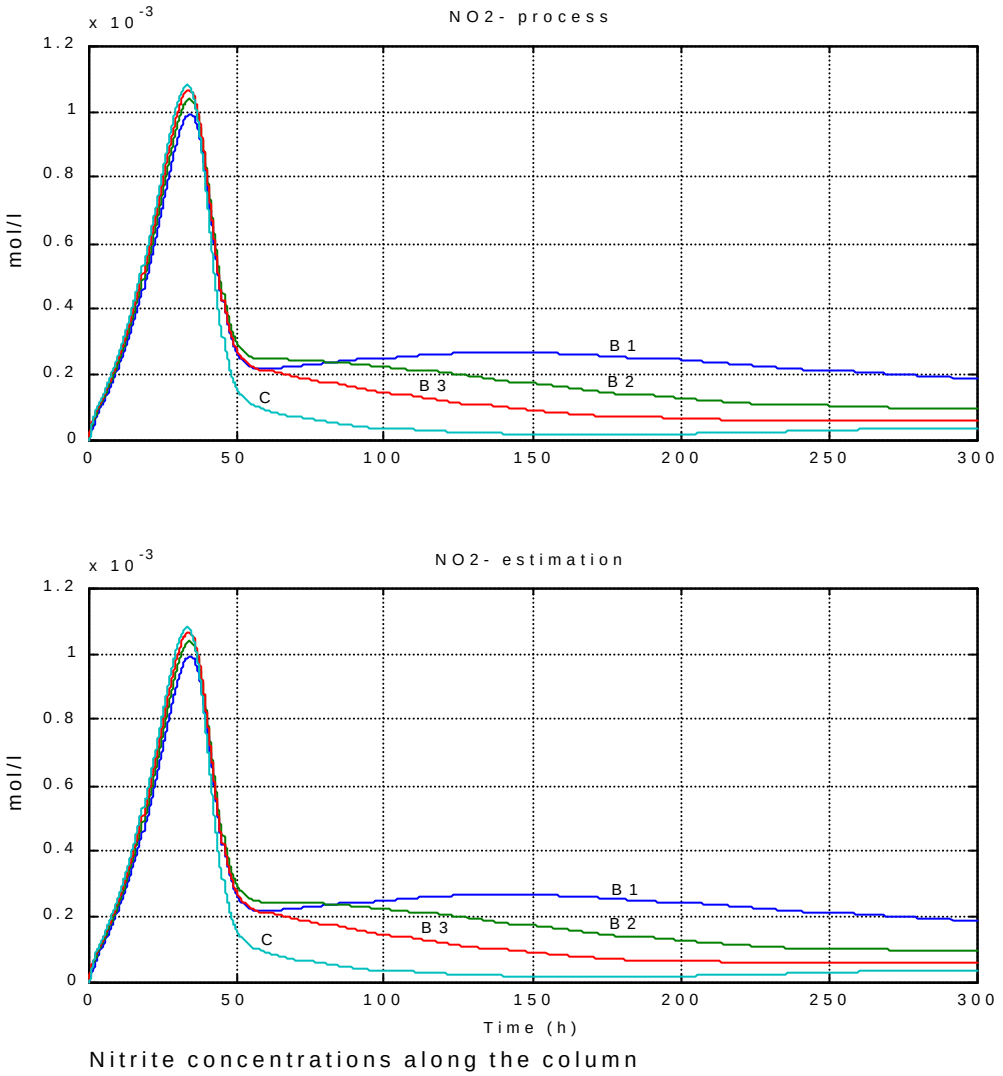
with :

$$\left| \begin{array}{l} A_{en} = A_n - B_n(G_nD_n + H_n)^{-1} \,.\, G_nC_n \\ C_{en} = C_n - D_n(G_nD_n + H_n)^{-1} \,.\, G_nC_n \\ B_{en} = \text{first column of } B_n(G_nD_n + H_n)^{-1} \\ D_{en} = \text{first column of } D_n(G_nD_n + H_n)^{-1} \end{array} \right.$$

The upper graph of figure 3 shows the evolution of the nitrite concentration along the column simulated by the state system of the column (equation (15) of TN 44.2).

The lower graph of the figure 3 shows the nitrite concentrations estimated by the estimators (6) and (7) of the present note.

The estimation of the nitrite is quite similar to the column simulation. This good agreement is due to the fact that the simulation is not noisy and that there no mismatch of parameters between the model of the simulated column and the estimators.



Nitrite concentrations along the column

Figure 3 : Simulation & Estimation of nitrite in each tank of the column

4. CONCLUSION

The relations (6) and (7) are a first step in the way of biomass and nitrite estimators.

Three major problems are not yet solved :

1. The biomass estimator, relation (6), implies, particularly, that $[NH_3\ L]$ and $[NO_3^-]$ are measured in each tank of the column. It is impossible now : there is no sampling holes along the column. Moreover, relation (6) assumes too that the number of tanks of the fixed bed could be determined for a given column.

2. The relation (6) uses the derivative of the state vector X_b, which is dangerous when X_b is noisy. So, a Kalman filter will be necessary.

3. The nitrite estimator, relation (7), is a differential equation whose solution has to be initialised from time to time (because drift will occur with time). So a measure of NO_2^- will be necessary at a given period of time (1 or more days ?), that will depend on the performance and robustness of the estimator.

The relations (6) and (7) are a first step in the way of a nitrite estimator.

5. REFERENCE

LECLERCQ J.-J. : "Numerical simplification of the dynamic model of nitrifying compartment for the elaboration of a nitrite estimator". Contract ESTEC n° 12924/98/NL/MV, 1999, TN 44.2.

ANNEX

```
%************************************************************
%       Biomass and Nitrite estimators                      *
%       Version 2.0     April 1999                          *
%                                                           *
%       State system according to TN 44.3                   *
%          . dissociation of CO2 and NH3                    *
%          . column = linear combination of tanks           *
%                                                           *
%************************************************************

clear
typmes = 0;     % all the needed concentrations are assumed to be known

load simu_e   % data of a simulation of the nitrifying column
load p_estim  % parameters of the estimators

% Computation of the state system of the Biomass estimator
% function 'statesys' is common with the simulator of the column
%-------------------------------------------------------------
  alpha_b = alpha(3); % NH3
  Kdis_b = Kdis(3);   % NH3
  KLa_b = KLa(3);     % NH3
  NG_b = 1;     % number of bi-phasis compound : NH3 (Gas and Liquid phase)
  NL_b = 1;     % number of monophasis compound : NO3 (Liquid phase)

  [Ab,Bb,Cb,Db,Eb] = statesys(NG_b, NL_b, NB, Gin, Fin, RG, RL, fG, fL, ...
                              VA, VnB, VC, epsL, epsG, epsT, ...
                              alpha_b, Kdis_b, KLa_b);

% Computation of the state system of the Nitrite estimator
% function 'statesys' is common with the simulator of the column
%-------------------------------------------------------------
  alpha_n = 0; %not used
  Kdis_n  = 0; %not used
  KLa_n   = 0; %not used
  NG_n = 0;     % number of bi-phasis compound (Gas and Liquid phase)
  NL_n = 1;     % number of monophasis compound : NO2 (Liquid phase)

  [An,Bn,Cn,Dn,En] = statesys(NG_n, NL_n, NB, Gin, Fin, RG, RL, fG, fL, ...
                              VA, VnB, VC, epsL, epsG, epsT, ...
                              alpha_n, Kdis_n, KLa_n);

% Matrices of the stoechiometries
% -------------------------------
  % Matrices of the stoechiometries associated to NH3 and NO3 :
  Yx1_b = [Yx1(3,:) ; Yx1(5,:)]; % stoechio. coef. of biosynthesis for NH3 & NO3
  Ym1_b = [Ym1(3,:) ; Ym1(5,:)]; % stoechio. coef. of maintenance for NH3 & NO3

  % Matrices of the stoechiometries associated to NO2 :
  Yx1_n = [Yx1(4,:)];     % stoechiometric coef. of biosynthesis for NO2-
  Ym1_n = [Ym1(4,:)];     % stoechiometric coef. of maintenance for NO2-

% NH3 and NO3
% -----------
  % Measures of NH3 and NO3
  if typmes == 0  % measures in each tank of the column
    ind = [6,8];
    for ii = 1:NB+1
      ind = [ind, [6,8] + ii*NO];
    end
```

```
  end
  Xb = cisc(:,ind);

  % Derivative of measures of NH3 and NO3
  dXb = diff(Xb) ./ (diff(tempsc)*ones(size(ind)));
  [m,n] = size(tempsc);
  dXb(m,:) = dXb(m-1,:);

  % Measures of the input vector : NH3 G, NH3 L & NO3 conc. at input of column
  if typmes == 0
    Ub = interp1(T,[dG(:,3) , dL(:,3) , dL(:,5)],tempsc);
  end

  % Computation of the (NH3 and NO3-) production/consumption rate
  Rx = Eb \ (dXb' - Ab*Xb' - Bb*Ub');

% NO2
% ---
  % measures of the input vector : NO2- concentration at input of column
  if typmes == 0
    Un = interp1(T,[dL(:,4)],tempsc);  % measure at input of column
  end

% Indices of growth limiting compounds
% ------------------------------------
  ind  = 0:NO:(NB+1)*NO;         % each tank of the column
  iO2  = ind + 4;                % indices of O2  Liquide in each tank
  iNH3 = ind + 6;                % indices of NH3 Liquide in each tank
  iNO2 = ind + 7;                % indices of NO2 in each tank

% Initialization of vectors
% -------------------------
  % Initialization for estimation of biomass concentration in the column
  Cx = zeros(2*(NB+2),m);

  % Initialization for estimation of NO2- concentration in the column
  dtem = diff(tempsc);
  Xn = zeros(NB+2,m);

% Estimation of biomass and nitrite
% ---------------------------------
  for jj = 2:m-1
    [mui,mai,rmu] = irate(cisc(jj,:)',iO2,iNH3,iNO2,KlNs,KlNb,mumax,maint);

    % 1. Computation of matrix Jb (for estimation of Biomass)
    dim = NG_b+NL_b;
    Jb = zeros(dim*(NB+2),NS*(NB+2));
    ind1 = 1:dim;
    ind2 = 1:NS;
    for ii = 1:NB+2
      Ji = Yx1_b*diag(mui(:,ii)) + Ym1_b*diag(mai(:,ii));
      Jb(ind1,ind2) = Ji;
      ind1 = ind1 + dim;
      ind2 = ind2 + NS;
    end

    % 2. Computation of matrix Jn (for estimation of Nitrite)
    dim = NG_n+NL_n;
    Jn = zeros(dim*(NB+2),NS*(NB+2));
    ind1 = 1:dim;
    ind2 = 1:NS;
```

```
    for ii = 1:NB+2
      Ji = Yx1_n*diag(mui(:,ii)) + Ym1_n*diag(mai(:,ii));
      Jn(ind1,ind2) = Ji;
      ind1 = ind1 + dim;
      ind2 = ind2 + NS;
    end

    % 3. Biomass concentration in each tank of the column
    Cx(:,jj) = Jb \ Rx(:,jj);

    % 4. production rate of nitrite in each tank of the column at step jj
    dXn = An * Xn(:,jj) + Bn * Un(jj,:)' + En * Jn * Cx(:,jj);

    % 5. concentration of nitrite in each tank of the column at step jj
    Xn(:,jj+1) = Xn(:,jj) + dXn*dtem(jj,1);
  end
  Cno2 = Xn;      % saving for plotting

% Plot
% ----
  pou = 3;       % plot of the nitrite concentrations (process and estimation)
  t_est
```