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

MELISSA

Memorandum of Understanding
ECT/FG/MMM/97.012

CONTRACT ESA-ESTEC/ADERSA
Purchase Order n° 161 399 of 14/06/1996

TECHNICAL NOTE : 35.2

Numerical simplification of the dynamic model of the nitrifying compartment

Version : 1
Issue : 0

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May 1998

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Document Change Log

Version	Issue	Date	Observation
0	0	April 1998	Draft
1	0	May 1998	Original version

WARNING TO THE READER

This technical note was written by a "non_biochemist" who misuses the registered term "total biomass".

In the present note, when it appears in the figures, the term "total biomass" means, exceptionaly, the biomass produced by the equations of biosynthesis of biomass of TN 27.1 and recalled hereafter, for Nitrosomonas and Nitrobacter, respectively :

$$CO_2 + 0.0089\ H_3PO_4 + 0.0035\ H_2SO_4 + 5.4269\ O_2 + 4.5341\ NH_3 \xrightarrow{r_g^{Ns}}$$

$$CH_{1.6147}\ O_{0.1994}\ S_{0.0035}\ P_{0.0089} + 4.3347\ HNO_2 + 3.8433\ H_2O$$

$$CO_2 + 0.0089\ H_3PO_4 + 0.0035\ H_2SO_4 + 6.5106\ O_2$$

$$+ 15.1714\ HNO_2 + 0.1994\ NH_3 + 0.4914\ H_2O \xrightarrow{r_g^{Nb}}$$

$$CH_{1.6147}\ O_{0.3906}\ N_{0.1994}\ S_{0.0035}\ P_{0.0089} + 15.1714\ HNO_3$$

In the text, the biomass produced by these reactions is called "global biomass" or "X_G".

In the same way, the term "visible biomass" or "X_V" in the figures means "the biomass fixed on the beads". In the text, it is called "active biomass".

TABLE OF CONTENTS

SIMPLIFICATION OF THE DYNAMIC MODEL OF THE NITRIFYING COMPARTMENT

1. INTRODUCTION

The dynamic model built by the University of Clermont Ferrand (TN 27.1 and 27.2) is a "first principles" model based on biology, chemistry and physics. It takes into account a lot of compounds to describe the complexity of the phenomena. The author of this model, L. Poughon, noticed that the computation time was huge when the gas NH_3 is involved in the description of the reactions.

As this paper will show it, this huge computation time is due to very short time constants, particularly for NH_3

The first step of this study is to replace the non linear rigorous law of the gas-liquid equilibrium by an approximate linear one. Then, the system of equations can be solved explicitly and the short time constants removed.

In order to reach this aim, the substrates of the problem are divided into 2 parts :

- those which are present in two phases : O_2, CO_2 and NH_3
- those which are present only in liquid phase : NO_2^-, NO_3^-, $HPO_4^{=}$ and $SO_4^{=}$

N.B. : This work is limited to TN 27.1 and TN 27.2 of 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)
- a biofilm diffusion model (introduced in TN 27.3)
- metabolism and growth of Nitrosomonas and Nitrobacter in presence of organic matter (introduced in TN 32.1)

2. NOTATION

For each substrate of the problem

a : molar concentration in the gas phase
b : molar concentration in the liquid phase
c : molar concentration at the thermodynamical equilibrium
d_G : molar concentration in the incoming gas flow
d_L : molar concentration in the incoming liquid flow
q_G : gas flow rate (1/h)
q_L : liquid flow rate (1/h)
r : production or consumption rate (mol/1/h)
K : volumetric transfer coefficient in liquid phase (notation KLa in TN 27.1)
k : partition coefficient of gas-liquid equilibrium

With this notation, each variable is considered as a vector whose components are the corresponding values of the substrates. For example, a is the vector of the molar concentrations of the substrates (O_2, CO_2 and NH_3)in the gas phase. The product of 2 vectors is a term by term product (and not a vectorial product). All these concentrations are in mol/1.

For each part of the column (A or tank n of B or C) the volumes are :

V_G : volume of gas (beads not included, for part B)
V_L : volume of liquid (beads not included, for part B)

3. SIMPLIFIED SYSTEM OF EQUATIONS OF THE BI-PHASES SUBSTRATES

Considering any part of the column (part A or C or any tank of B) :

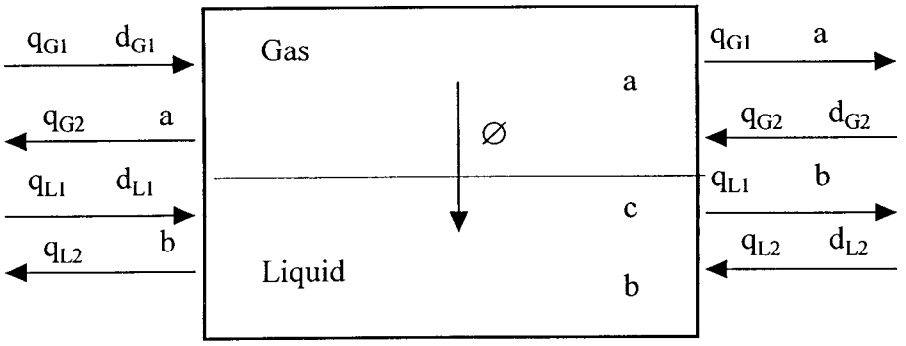


Figure 1 : Concentrations and mass fluxes of any part of the column

The indices 1 and 2 are :

1 : for flow from left to right hand side ;
2 : for flow from right to left hand side.

The process is described by the 4 following equations.

With the assumptions of perfect gases, the gas-liquid equilibrium is written (justification in Annex 1) :

$$a = \alpha \,.\, c \quad \text{with} : \alpha = \frac{k}{n_o \cdot V_M} \tag{1}$$

$n_o = 55.56$ (number of mols in a liter of water)
$V_M = 24.86$ (molar volume under 1 atmosphere and 303 K)

The mass flux, $\varnothing$, from gas to liquid is :

$$\varnothing = K\,(c-b) \tag{2}$$

The mass conservation in the gas is :

$$V_G \cdot \frac{da}{dt} = -\varnothing . V_L + q_{G1}(d_{G1} - a) + q_{G2}(d_{G2} - a) \tag{3}$$

The mass conservation in the liquid is :

$$V_G \cdot \frac{db}{dt} = (r + \varnothing) . V_L + q_{L1}(d_{L1} - b) + q_{L2}(d_{L2} - b) \tag{4}$$

So, given the following new input variables q_G, q_L, d_G and d_L :

$$q_G = q_{G1} + q_{G2}$$

$$q_L = q_{L1} + q_{L2}$$

$$q_G . d_G = q_{G1} \cdot d_{G1} + q_{G2} \cdot d_{G2}$$

$$q_L . d_L = q_{L1} \cdot d_{L1} + q_{L2} \cdot d_{G2}$$

the previous system of equations becomes a system of 4 equations with 4 unknowns (a, b, c and $\varnothing$) :

$$a = \alpha.c \tag{5}$$

$$\varnothing = K\,(c-b) \tag{6}$$

$$V_G \cdot \frac{da}{dt} = -\varnothing \cdot V_L + q_G\,(d_G - a) \tag{7}$$

$$V_L \cdot \frac{db}{dt} = (r+\varnothing)\; V_L + q_L\,(d_L - b) \tag{8}$$

Using Laplace transforms and cancelling a, c and Φ lead to a relation between the inputs of the probrem r, d_G, d_L and the output b (full details in Annexe 2) :

$$(1-\alpha_1\,\alpha_4)\,(1+\tau_1\,p)\,(1+\tau_2\,p)\,.\,b$$

$$= \alpha_2(1+\theta_2\,p)\,.\,r + \alpha_1\,\alpha_5\,.\,d_G + \alpha_3(1+\theta_2\,p)\,.\,d_L \tag{9}$$

where the time constants τ_1, τ_2 and θ_2 and the scalars α_1, α_2, α_3, α_4 and α_5 are functions of the parameters α, K, V_L, V_G, q_L and q_G.

Two simplifications may be done.

First simplification : as figure 2 shows it, $\frac{\theta_2}{\tau_2} \simeq 1$. So $\quad 1 + \tau_2\,.\,p \simeq 1 + \theta_2\,.\,p.$

Second simplification : as figure 3 shows it, the ratio $\frac{\tau_2}{\tau_1}$ is small (the biggest value of this ratio is 0.07). So the second order transfer is nearly equal to a first order transfer :

$$(1+\tau_1\,p)\,(1+\tau_2\,p) \simeq 1 + \tau_1\,.\,p$$

So the relation (9) becomes :

$$(1-\alpha_1\,\alpha_4)\,(1+\tau_1\,p)\,.\,b = \alpha_2\,.\,r + \alpha_1\,.\alpha_5\,.\,d_G + \alpha_3\,.\,d_L \tag{10}$$

A similar expression is obtained for the concentration in the gas phase, a.

Using the inverse Laplace transforms, the derivatives of a or b are :

$$\frac{db}{dt} = \frac{1}{\tau_1}\,(-b + G_1\,.\,d_L + G_2\,.\,d_G + G_3\,.\,r) \tag{11}$$

$$\frac{da}{dt} = \frac{1}{\tau_1} (-a + G'_1 \cdot d_L + G'_2 \cdot d_G + G'_3 \cdot r) \qquad (12)$$

where τ_1, G_1, G_2, G_3, G'_1, G'_2 and G'_3 are functions of the parameters α, K, V_L, V_G, q_L and q_G (full expressions in annexe 2).

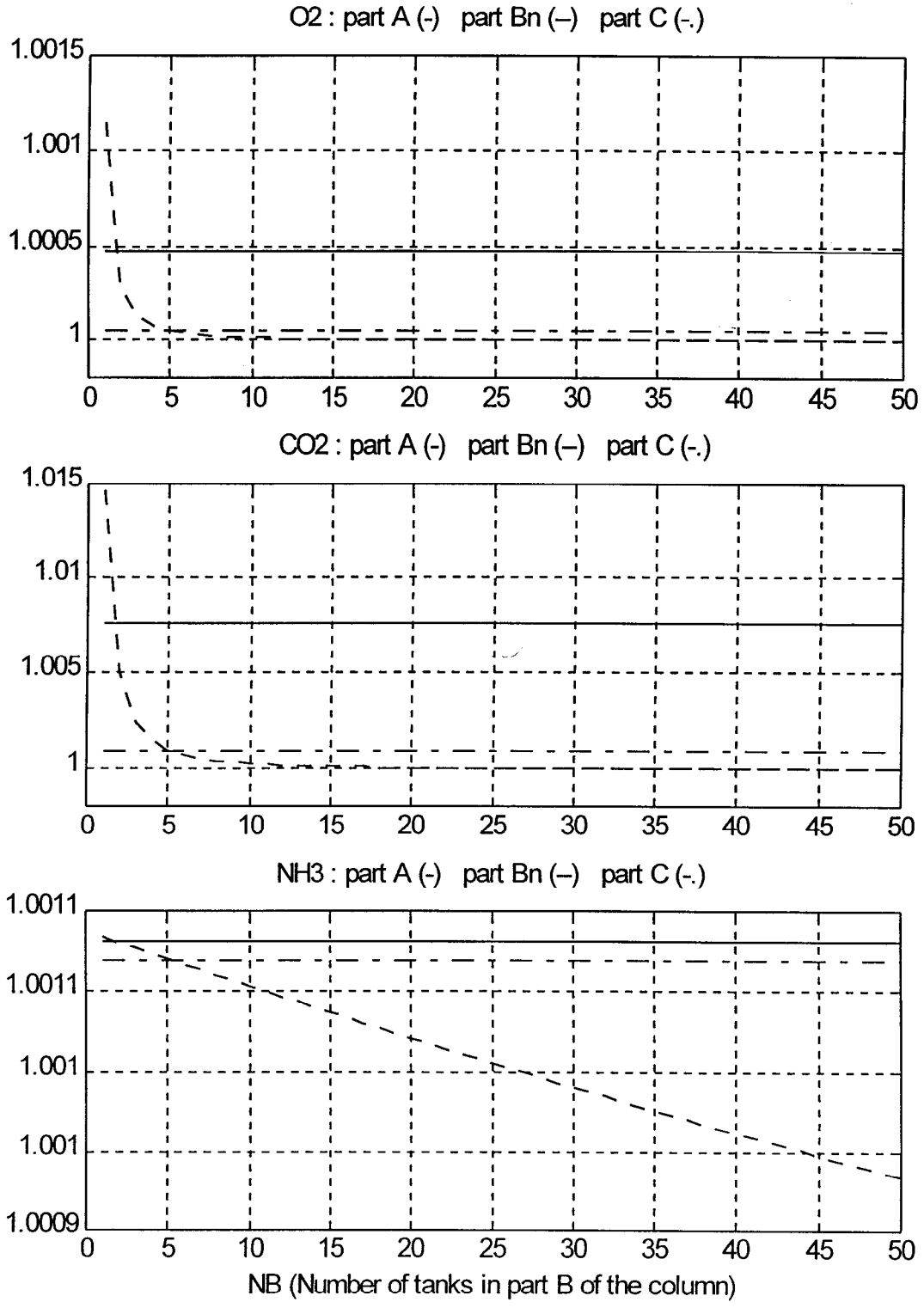


Figure 2 : Time constants ratio $\frac{\theta_2}{\tau_2}$

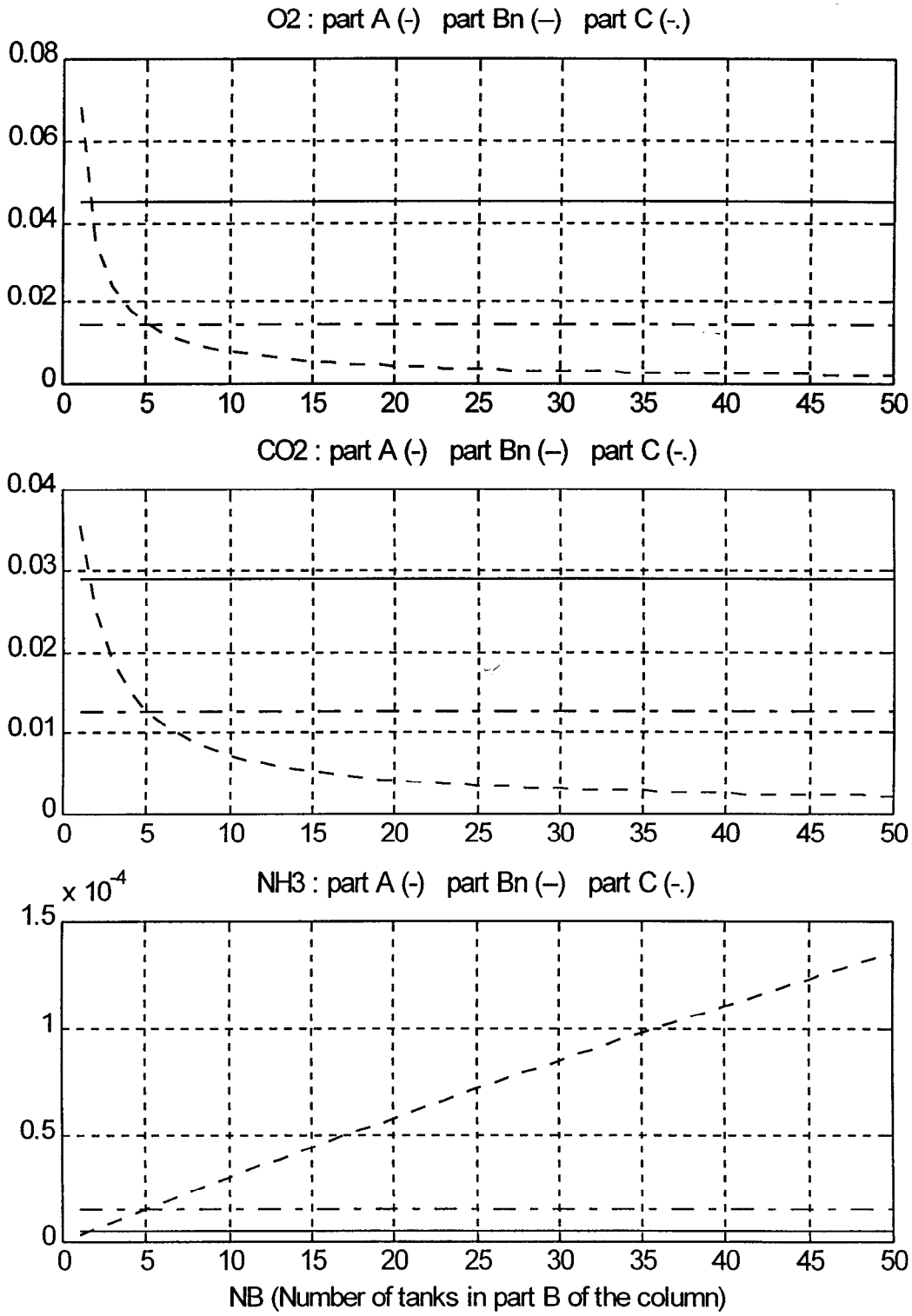


Figure 3 : Time constants ratio $\frac{\tau_2}{\tau_1}$

Computation time and memory allocation

The computation time and memory allocation have been compared for a first order and a second order transfer for the part B of the column with $N_B = 1$.

With this configuration,the ratio $\frac{\tau_2}{\tau_1}$ is maximum for O2 and CO2 and minimum for NH3 (values given in table 1).

Bi-phases compound	τ_1 (h)	τ_2 (h)	$\frac{\tau_2}{\tau_1}$
O_2	$1.97\ 10^{-2}$	$1.35\ 10^{-3}$	$6.85\ 10^{-2}$
CO_2	$2.80\ 10^{-2}$	$9.44\ 10^{-4}$	$3.37\ 10^{-2}$
NH_3	$7.48\ 10^{-1}$	$1.99\ 10^{-6}$	$2.65\ 10^{-6}$

Table 1 : Time constants of part B with $N_B = 1$

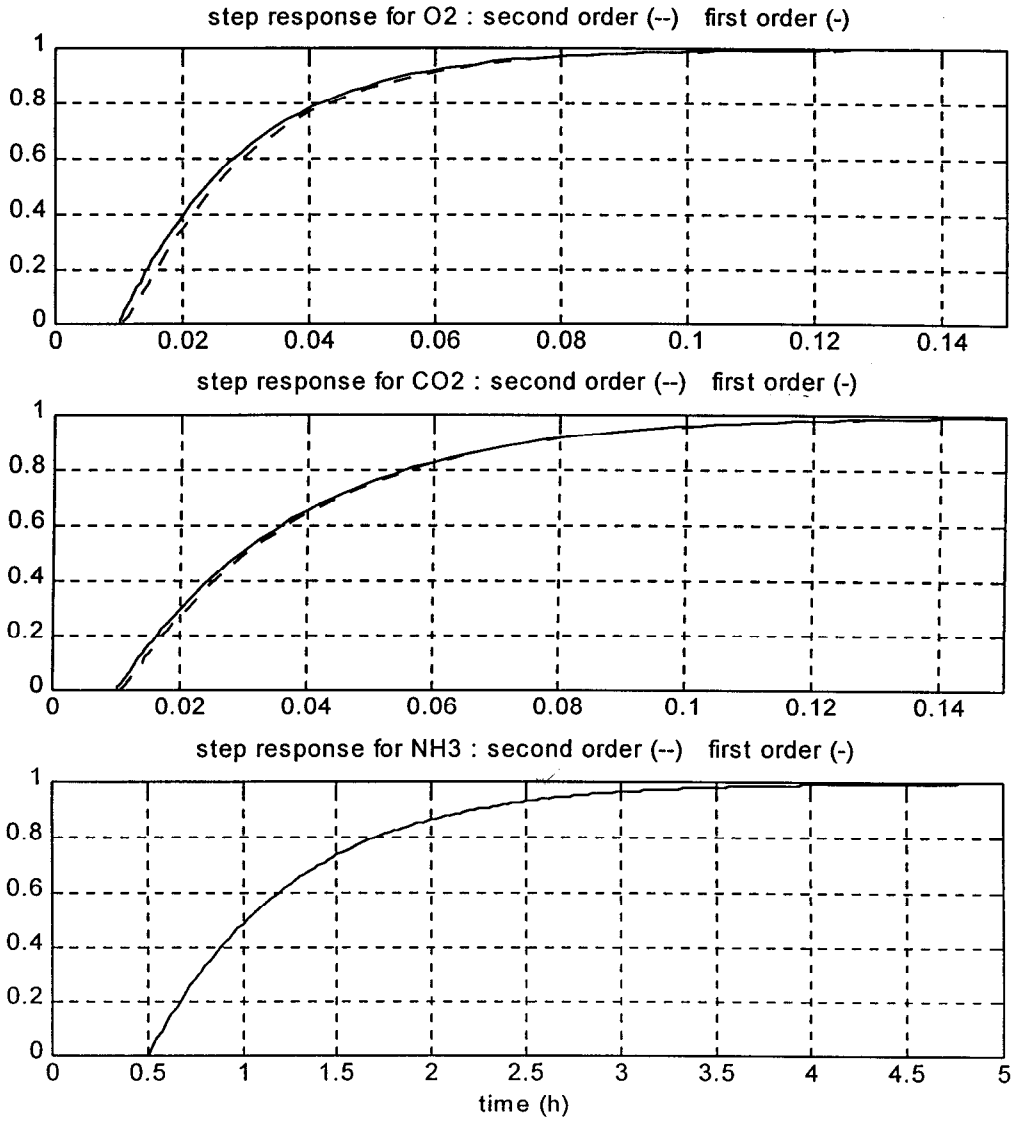
Figure 4 shows the step responses of these 2 transfers. There is a slight difference for O_2 and CO_2 during the transient behaviour, but no difference at all for NH_3. Moreover, for this last compound, the second order transfer needs more than 10 000 times the computation time and the memory allocation of the first order one (table 2).

Bi-phases Compound	First order		Second order		ratio second order versus first one	
	CT1 (s)	MA1	CT2 (s)	MA2	$\frac{CT2}{CT1}$	$\frac{MA2}{MA1}$
O2	5.10^{-2}	66	6.10^{-2}	81	1.2	1.23
CO2	5.10^{-2}	60	6.10^{-2}	75	1.2	1.25
NH3	5.10^{-2}	64	514	684034	10^4	$1.07\ 10^4$

Table 2 : Computation time (CT) and memory allocation (MA) of figure 4.

N.B : The memory allocation is the number of points of the simulation horizon of figure 4 : 0.15 hour for O_2 and CO_2, 5 hours for NH_3.

From this example that covers all the variation range of the ratio τ_2/τ_1, it is clear that the first order transfer is quite equivalent to the second one, for all the bi-phases compounds and for $1 \leq N_B \leq 50$.



Comparison between first order transfer and second order transfer

Figure 4

4. EQUATIONS OF THE MONO-PHASE SUBSTRATES

For the substrates only present in liquid phase (NO_2^- , NO_3^- , $HPO_4^{=}$ and $SO_4^{=}$), the derivative of the concentration is :

$$\frac{db}{dt} = \frac{1}{\tau_L} (-b + \tau_L \cdot r + d_L) \qquad (13)$$

with $\tau_L = \frac{V_L}{q_L}$

Figure 5 shows that, for O_2 and CO_2, and for N_B between 1 and 5, the time constant τ_1 can be neglected versus τ_L. But, in a general way, τ_1 cannot be neglected versus τ_L.

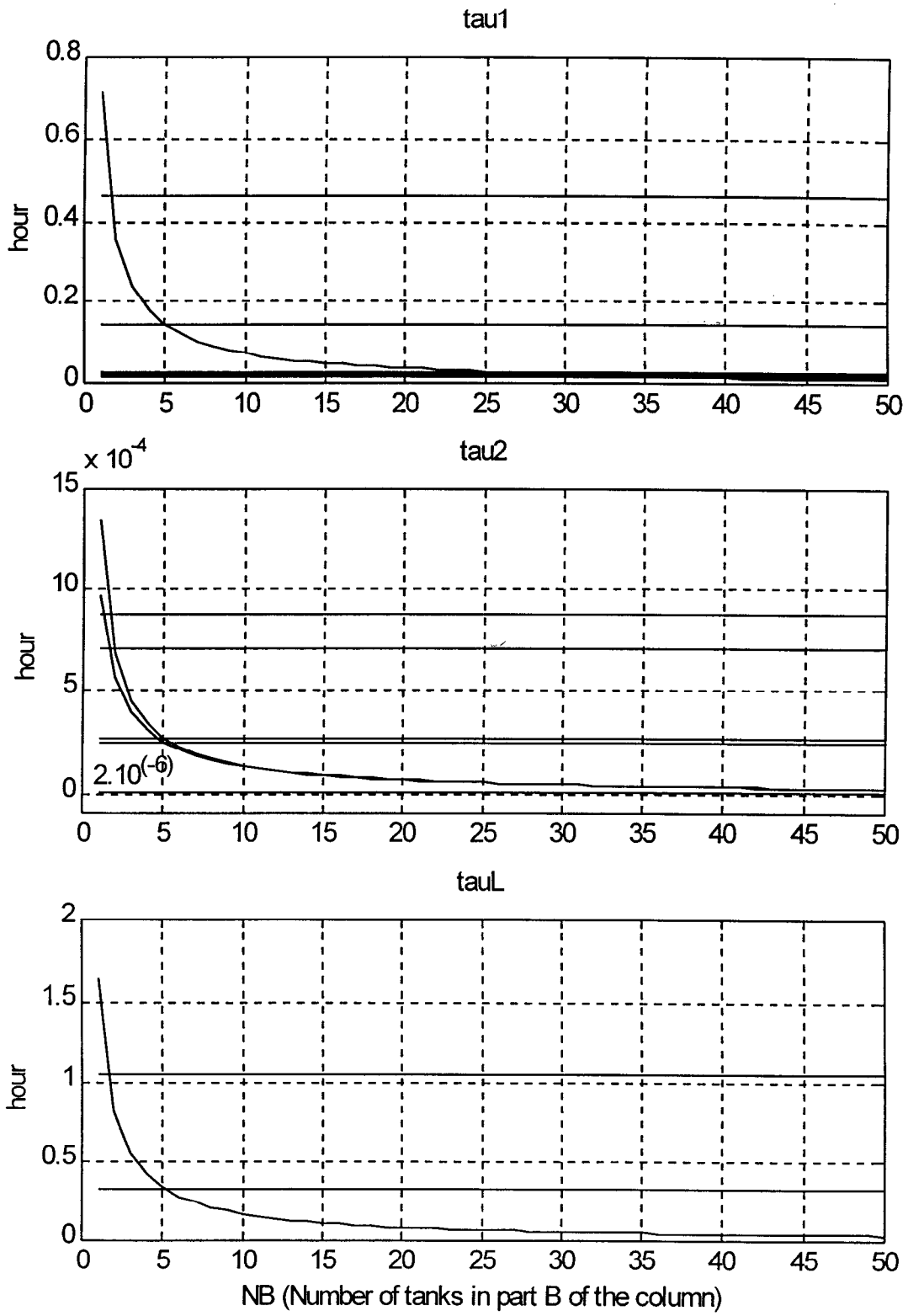


Figure 5 : Time constants τ_1, τ_2, τ_L

5. SIMULATION

5.1. Configuration of the simulation

The configuration of the simulation are those of TN27.2 (L. Poughon, Laboratoire de Génie Chimique Biologique) :

- standard configuration described p.12 and 13 ;
- number of equivalent tanks in the fixed bed : 5
- stoïchiometries p.3 ;
- dissociation constant of CO_2/HCO_3^- p.2 ;
- limiting substrates defined p.4 ;
- no inhibitory substrate ;
- no limitation due to liquid/biofilm transfer
- transfer coefficient $K_La = [51 \quad 51 \quad 500]\ h^{-1}$ for O_2 CO_2 NH_3
- partition coefficient $k = [45990 \quad 1853.1 \quad 11.349]$ for O_2 CO_2 NH_3 (non ionic form)

The compounds involved in the simulation are :

- O_2 G(Gas phase) and L(Liquid phase)
- CO_2 G and L
- NH_3 G and L
- HCO_3^-
- NO_2^-
- NO_3^-
- $HPO_4^=$
- $SO_4^=$
- X_N_s (biomass Nitrosomonas, active and global (active + decay))
- X_N_b (biomass Nitrobacter, active and global (active + decay))

5.2. Results

Figure 6 to 9 are composed of 8 graphs whose the last one (below right hand side) is common to all the figures and shows the average active biomass concentration in the fixed bed. The 7 other graphs are connected to tank 1 (of the fixed bed) in the figures 6 and 8, and to tank 5 (the last one of the fixed bed) in the figures 7 and 9.

The figures 8 and 9 are abscissa zooms of figures 6 and 7, respectively.

The composition of the gaz phase (G notation) is given in molar fraction (mf), the composition of the liquid phase (L notation) is given in mol/l or g/l (for biomass).

■ **Tank 1 of fixed bed :**

During the 29 first hours, no substrate is limiting for biomass N_s and the growth of this biomass is exponential while the concentrations of substrates HCO_3^- O_2 and NH_3 are decreasing exponentially. At the beginning, NO_2^- is limiting for N_b and this biomass is slightly decreasing. After several hours its growth is exponential.

At time t = 29h, the NH_3 concentration (0.4 mmol/l) becomes limiting : the growth of biomass bends, so that the consumption of HCO_3^- is decreasing (CO_2 concentration reachs a minimum). On the contrary, NO_2^- concentration is maximum (2 mmol/l) : the consumption of NO_2^- by N_b becomes greater than its production by N_s.

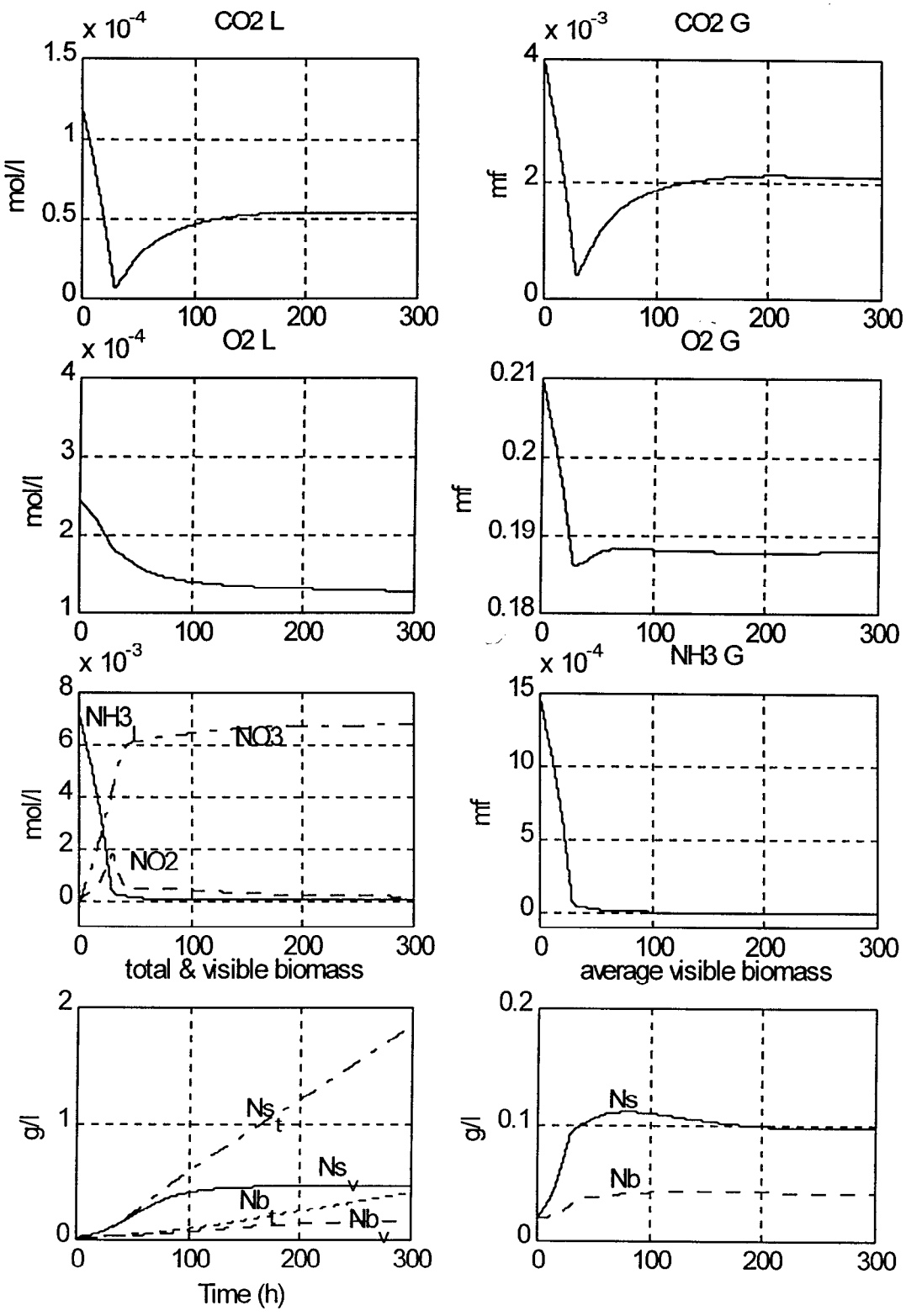
The O_2 concentration goes on decreasing slowly (until 0.125 mmol/l at the end of the simulation) as the active biomass N_s and N_b is nearly becoming stabilized. The NH_3-L and NO_2^- concentrations are nearly stabilized at 0.02 and 0.15 mmol/l. During the last 150 h, NH_3-G is decreasing slowly from 5.10^{-5} to 2.10^{-5} molar fraction.

■ **Tank 5 of fixed bed :**

The 29 first hours are quite similar to those of thank 1. The NH_3 concentration becomes quickly null. The growth rate of global biomass N_s becomes null and the active biomass disappears progressively.

After its maximum at 2 mmol/l, NO_2^- concentration is getting null quickly (10 h). As for N_s, the biomass N_b is nearly null at the end of 300 h.

Remark : the NH_3 and NO_2^- concentrations are null because the consumption rates of these substrates in the maintenance reaction are not limited by a michaelian factor.



Part B1 of the column

Input cst: O2 CO2 NH3 G and L; Growth of biomass

Figure 6

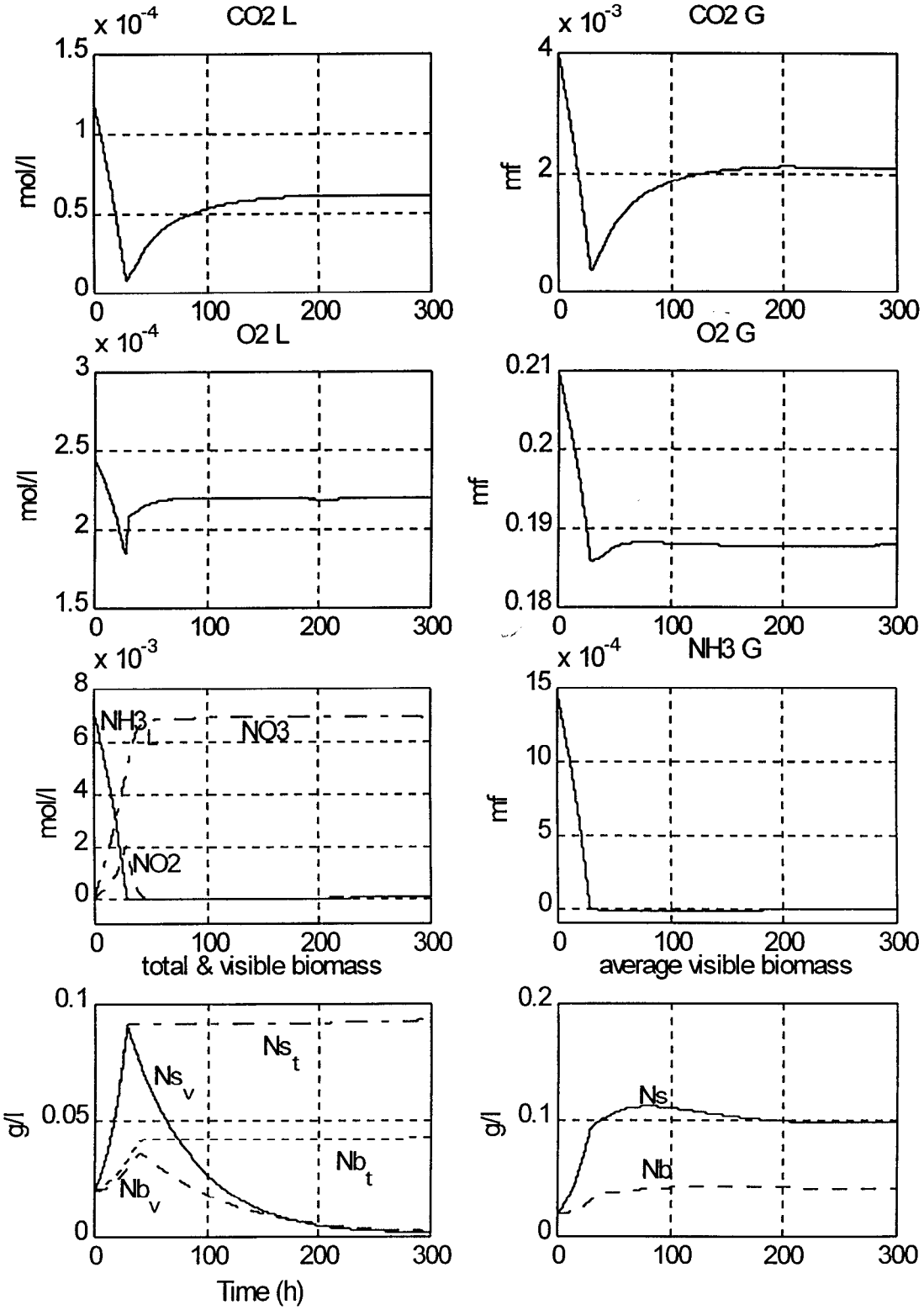

x 10-4
CO2 L
mol/l
x 10-3
CO2 G
mf
x 10-4
O2 L
mol/l
O2 G
mf
x 10-3
NH3
NO3
NO2
mol/l
total & visible biomass
x 10-4
NH3 G
mf
average visible biomass
Nst
Nsv
Nbt
Nbv
g/l
Ns
Nb
g/l
Time (h)
Part B5 of the column
Input cst: O2 CO2 NH3 G and L; Growth of biomass

Figure 7

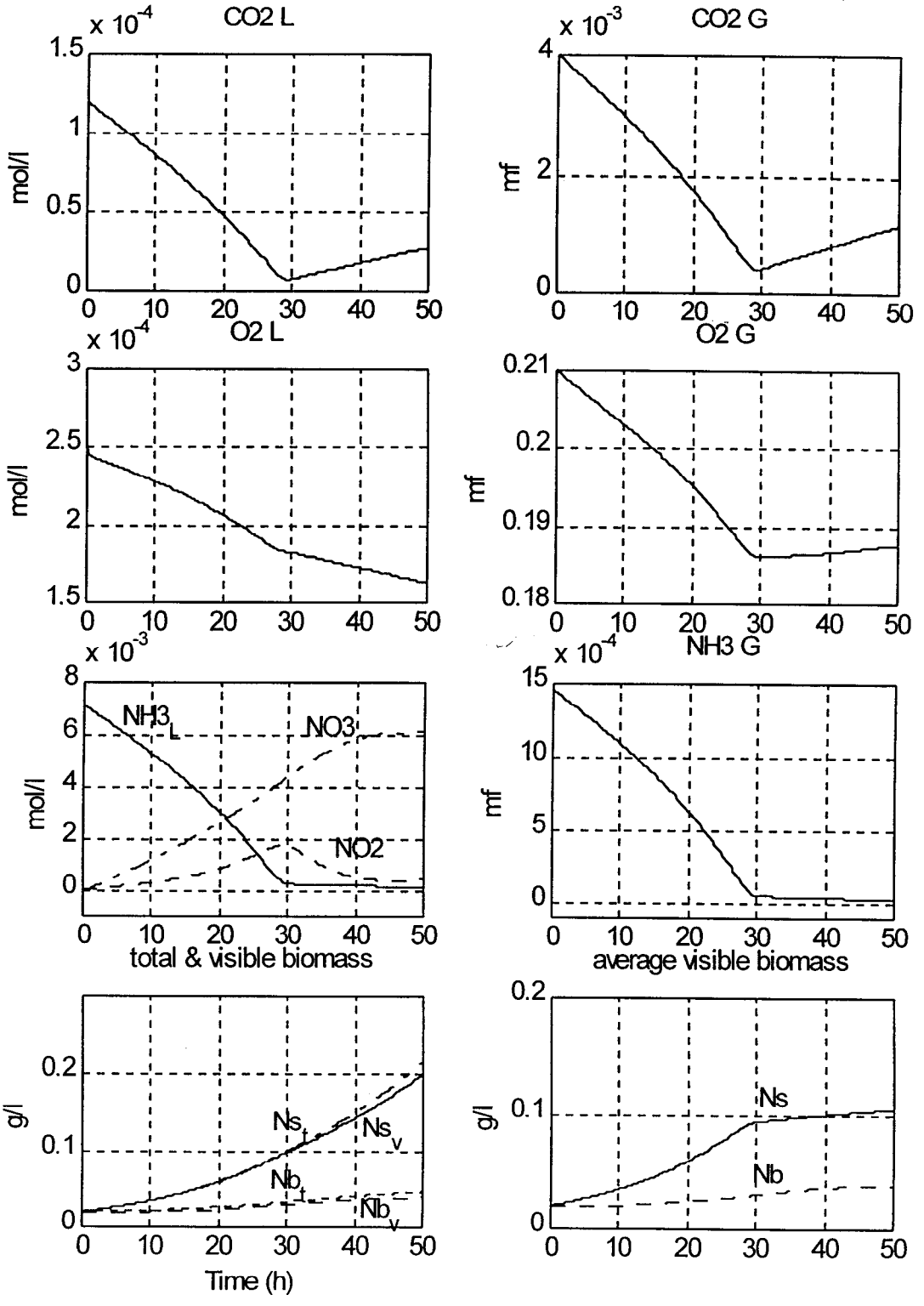

x 10-4
CO2 L
mol/l
x 10-3
CO2 G
mf
x 10-4
O2 L
mol/l
O2 G
mf
x 10-3
NH3L
NO3
NO2
mol/l
total & visible biomass
x 10-4
NH3 G
mf
average visible biomass
Nst
Nsv
Nbt
Nbv
g/l
Time (h)
Ns
Nb
g/l
Part B1 of the column

Figure 8

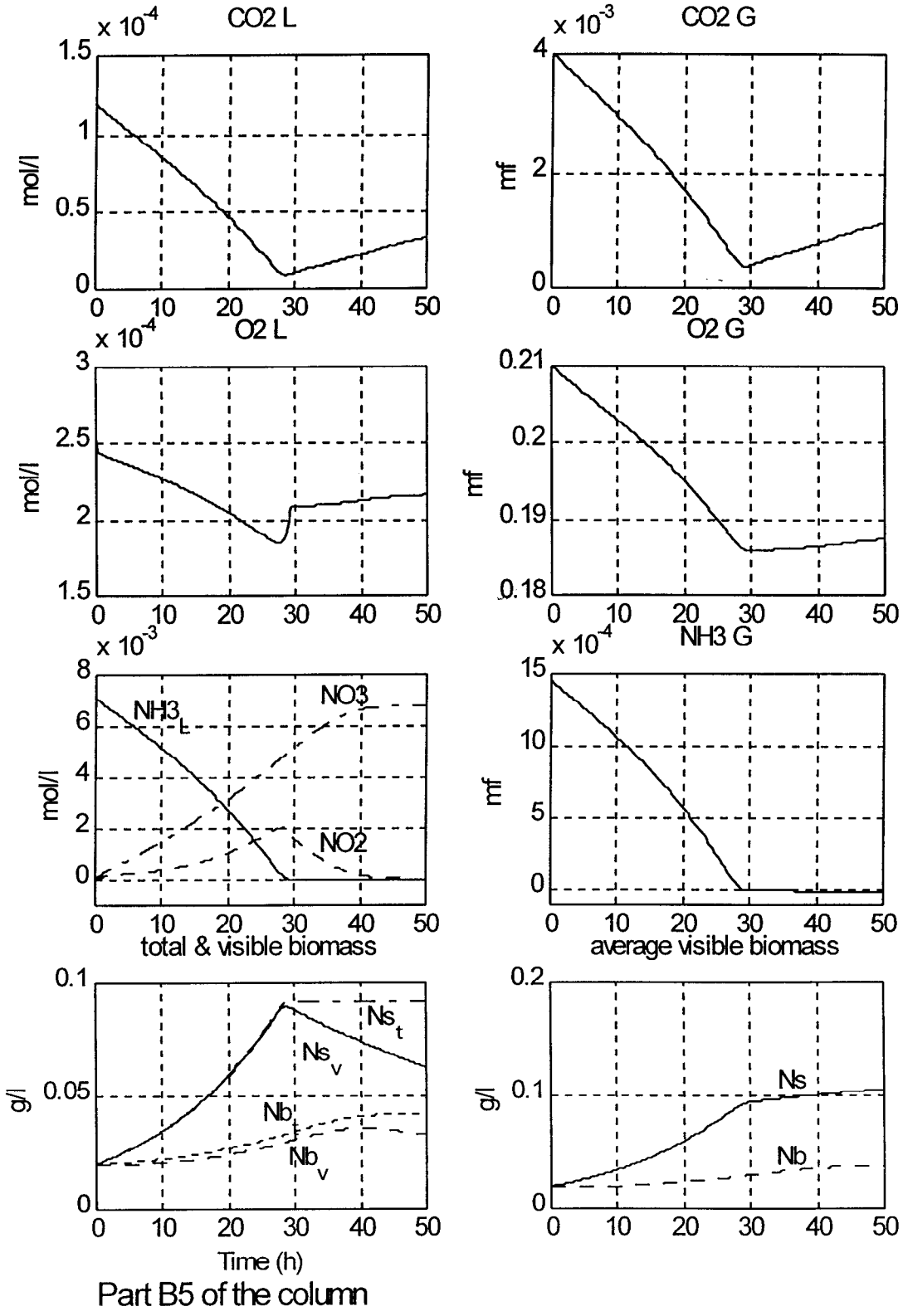

x 10-4
CO2 L
mol/l
x 10-3
CO2 G
mf
x 10-4
O2 L
mol/l
O2 G
mf
x 10-3
NH3 L
NO3
NO2
mol/l
x 10-4
NH3 G
mf
total & visible biomass
average visible biomass
Nst
Nsv
Nbt
Nbv
Ns
Nb
g/l
Time (h)
Part B5 of the column

Figure 9

6. CHECKING THE MASS BALANCE

To test the software simulating the column, the mass balance of atom N is used : the incoming rate of N is compared to the sum of outgoing rate of N and of stocking rate of N in the column (parts A, B and C).

The top graph of figure 10 shows 2 temporal curves :

- the dash dotted curve is the incoming rate of N (NH_3 G and L) ;
- the continuous curve is the sum of the outgoing rate of N and of the derivative of the total amount of N in the column (NH_3 G and L, NO_2^-, NO_3^-, global (active + decay) biomass).

The distance between these 2 curves is distributed on 2 different scales : it is about 0,4 % during the exponential growth and nearly null otherwise.

7. CHECKING THE APPROXIMATION OF THE GAS/LIQUID EQUILIBRIUM

In order to estimate the error that is done when the non linear law of gas/liquid equilibrium is replaced by the linear relation (1), one need only to compare for each compound i the partition coefficient k_i to the ratio.

$$z_i = \frac{y_i}{x_i}$$

with :

$$y_i = \frac{a_i}{\sum a_i}$$

$$x_i = \frac{c_i}{\sum c_i}$$

where : a_i is the molar concentration in the gas phase

c_i is the molar concentration in the liquid phase at thermodynamical equilibrium

An other expression of z_i is :

$$z_i = \frac{k_i}{n_{lo} \cdot V_M} \cdot \frac{\Sigma c_i}{\Sigma a_i}$$

With the legitimate approximation $\Sigma c_i = n_{lo}$

$$z_i = \gamma \cdot k_i \quad \text{where} \quad \gamma = \frac{1}{V_M \cdot \Sigma a_i}$$

γ is independent of compound i.

The 3 bottom graphs of figure 10 show the evolution of γ all along the simulation for part A, tank 1 of the fixed bed and part C.

The mean value of γ is about 1.03, which means that the right partition coefficient k_i is overestimate of about 3 %. In order to compensate this overestimation, one only need to reduce of 3 % the right value of k_i in the simulations.

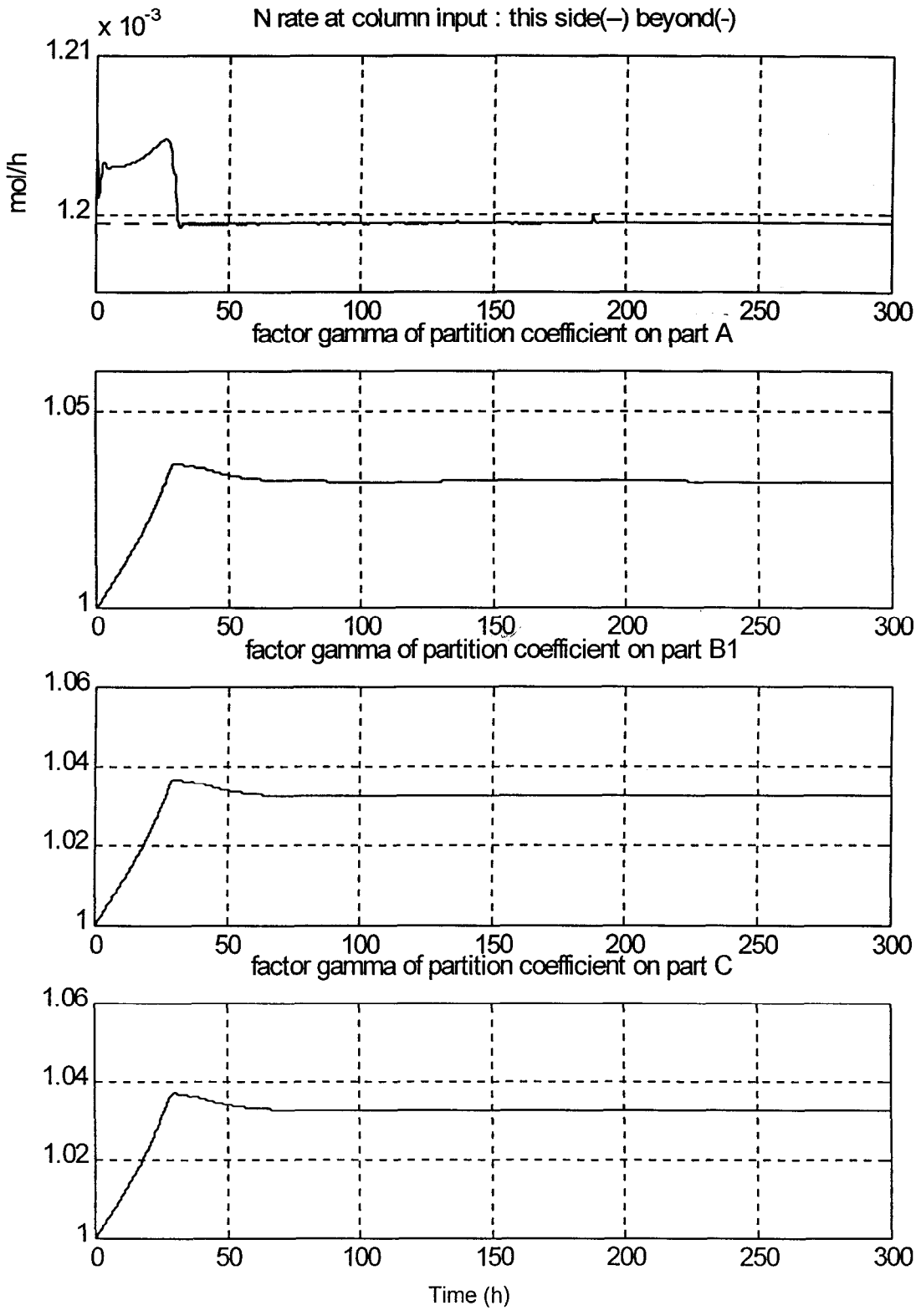


Figure 10 : Standard configuration

8. CONCLUSION

The equations (11), (12) and (13) are used to simulate the behaviour of the nitrifying column.

The smallest time constant of the initial system (equations (1) to (4)) is seen for NH_3, whatever N_B, and is $\tau_2 = 2.10^{-6}$ hour (figure 5). The smallest time constant of the simplified system (equations (11) and (12)) is $\tau_1 = 10^{-2}$ hour. So, the computation time is divided by about 5000 when the simplified system is used. It could be still reduced for small value of the number of equivalent tanks of part B of the column, N_B ($N_B \leq 5$) : in that case, τ_1 could be neglected versus τ_L for O_2 and CO_2.

This work shows that the bio-physical complexity of the dynamical model buit by LGCB, is not responsible of the huge time computation. Indeed this complexity, which makes the wealth of the model should be preserved. That is possible thanks to the mathematical simplification proposed here.

This simplification includes 3 aspects :

1. the substitution of the non linear law of the gas / liquid equilibrium by a linear approximative one (relation (1)). This substitution is equivalent to a non linear law where the partition coefficient would be increased of about 3 %. This over-estimation can be eliminated in reducing of 3 % the right values of the partition coefficient in the simplified model.

2. the elimination of the smaller time constant versus the bigger one. This simplification is quite legitimate and is invisible in the numerical results.

3. the Laplace transforms, used to explicitly solved the set of differential equations, needs the assumption of constant gaz and liquid flow rates at the input of the column.

This last aspect of the simplification involves a too restrictive assumption. An other way of simplification has to be looked for in a further study.

REFERENCES

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.

POUGHON L. "Description of the nitrifying column model and first simulations". ESTEC contract PRF 151739, May 1996, TN27.2

ANNEX 1

APPROXIMATIVE RELATION FOR GAS/LIQUID EQUILIBRIUM

The gas/liquid equilibrium of each compound i is haracterized by the partition coefficient k_i :

$$k_i = \frac{y_i}{x_i}$$

where y_i = molar fraction of compound i in gas phase
x_i = molar fraction of compound i in liquid phase

Here, the compounds involved are O_2 CO_2 NH_3 H_20 and N_2.

Given : V_g volume of gas (in l)
V_l volume of liquid (in l)
n_{gi} number of mol of compound i in gas phase
n_{li} number of mol of compound i in liquid phase
V_M molar volume at pression and temperature of the column
a_i molar concentration of compound i in gas phase
c_i molar concentration of compound i in liquid phase at thermodynamical equilibrium

Assumptions :

1. The total number of mols in liquid is the number of mols of water :

$$\sum_i n_{li} = n_{l0} \cdot V_l \quad \text{with} \quad n_{l0} = \frac{1000}{18} = 55.56 \text{ mol/l}$$

2. The gas are perfect :

$$\sum_i n_{gi} = \frac{V_g}{V_M}$$

Molar fraction and concentration are related by :

$$y_i = \frac{n_{gi} \cdot V_M}{V_g} = a_i \cdot V_M$$

$$x_i = \frac{n_{li}}{n_{l0} \cdot V_l} = \frac{c_i}{n_{l0}}$$

$$\Rightarrow a_i = \alpha_i \cdot c_i \quad \text{with} \quad \alpha_i = \frac{k_i}{n_{l0} \cdot V_M}$$

This last relation is the equation (1) of the system of the bi-phases substrates.

ANNEX 2

SIMPLIFICATION OF THE EQUATIONS SYSTEM OF THE BI-PHASES SUBSTRATES

The starting point of the resolution is the following set of equations (relations (5) to (8) of paragraph 3).

$$a = \alpha \cdot c$$

$$\phi = K(c - b)$$

$$V_L \cdot \frac{db}{dt} = (r + \phi) \cdot V_L + q_L \cdot d_L - q_L \cdot b$$

$$V_G \cdot \frac{da}{dt} = -\phi \cdot V_L + q_G \cdot d_G - q_G \cdot a$$

Cancellation of c and ϕ gives :

$$(K \cdot V_L + q_L)\, b + V_L \cdot \frac{db}{dt} = \frac{K \cdot V_L}{\alpha} \cdot a + V_L \cdot r + q_L \cdot d_L$$

$$\left(\frac{K \cdot V_L}{\alpha} + q_G\right) a + V_G \cdot \frac{da}{dt} = K \cdot V_L \cdot b + q_G \cdot d_G$$

Using the Laplace transforms :

$$(1 + \theta_1 p) \cdot b = \alpha_1 \cdot a + \alpha_2 \cdot r + \alpha_3 \cdot d_L \qquad \text{(A2.1)}$$

$$(1 + \theta_2 p) \cdot a = \alpha_4 \cdot b + \alpha_5 \cdot d_G \qquad \text{(A2.2)}$$

with :

$$\theta_1 = \frac{V_L}{K \cdot V_L + q_L}$$

$$\theta_2 = \frac{V_G}{\frac{K \cdot V_L}{\alpha} + q_G}$$

$$\alpha_1 = \frac{K \cdot V_L}{\alpha(K \cdot V_L + q_L)}$$

$$\alpha_2 = \frac{V_L}{K \cdot V_L + q_L}$$

$$\alpha_3 = \frac{q_L}{K \cdot V_L + q_L}$$

$$\alpha_4 = \frac{K \cdot V_L}{\frac{K \cdot V_L}{\alpha} + q_G}$$

$$\alpha_5 = \frac{q_G}{\frac{K \cdot V_L}{\alpha} + q_G}$$

p : the Laplace variable

Although the notations have not been changed with the Laplace transformation, the functions a, b, r, d_L and d_G are now functions of the Laplace variable p. (Before the transformation, they were functions of time).

Cancellation of a in (A2.1) and (A2.2) :

$$a = \frac{\alpha_4}{1 + \theta_2 p} b + \frac{\alpha_5}{1 + \theta_2 p} \cdot d_G \qquad \text{(A2.3)}$$

gives :

$$(1-\alpha_1 \alpha_4)(1 + \beta_1 p + \beta_2 p^2) \cdot b = \alpha_2(1 + \theta_2 p) \cdot r + \alpha_1 \alpha_5 d_G + \alpha_3 (1 + \theta_2 p) \cdot d_L \qquad \text{(A2.4)}$$

with :

$$\beta_1 = \frac{\theta_1 + \theta_2}{1 - \alpha_1 \cdot \alpha_4}$$

$$\beta_2 = \frac{\theta_1 \cdot \theta_2}{1 - \alpha_1 \cdot \alpha_4}$$

Study of $y = 1 + \beta_1 p + \beta_2 p^2$:

Given :

$$y = \beta_2\left(p^2 + \frac{\beta_1}{\beta_2} p + \frac{1}{\beta_2}\right)$$

Given p_1 and p_2 the roots of $p^2 + \frac{\beta_1}{\beta_2} p + \frac{1}{\beta_2}$.

$$\Rightarrow \quad \left| \begin{array}{l} y = \beta_2(p - p_1)(p - p_2) \\ \text{and } p_1 \cdot p_2 = \frac{1}{\beta_2} \end{array} \right.$$

Given $\tau_1 = -\frac{1}{p_1}$ et $\tau_2 = -\frac{1}{p_2}$ such as $\tau_1 > \tau_2$.

The expression of y becomes :

$$y = \frac{\beta_2}{p_1 \cdot p_2} \cdot (1 + \tau_1 p)(1 + \tau_2 p)$$

$$\Rightarrow \quad y = (1 + \tau_1 p)(1 + \tau_2 p) \qquad \text{(A2.5)}$$

So (A2.4) becomes :

$$(1-\alpha_1 \alpha_4)(1 + \tau_1 p)(1 + \tau_2 p) \cdot b = \alpha_2(1 + \theta_2 p) \cdot r + \alpha_1 \alpha_5 d_G + \alpha_3 (1 + \theta_2 p) \cdot d_L \qquad \text{(A2.6)}$$

As previously said in paragraph 3, for the compounds O_2, CO_2 and NH_3 and for $1 \leq N_B \leq 50$, the two following approximations can be done :

$$\left| \begin{array}{l} 1 + \tau_2 p = 1 + \theta_2 p \\ (1 + \tau_1 p)(1 + \tau_2 p) = 1 + \tau_1 p \end{array} \right.$$

The relation (A2.6) becomes :

$$b = \frac{G_1}{1 + \tau_1 p} \cdot d_L + \frac{G_2}{1 + \tau_1 p} \cdot d_G + \frac{G_3}{1 + \tau_1 p} \cdot r \qquad \text{(A2.7)}$$

with :

$$G_1 = \frac{\alpha_3}{1 - \alpha_1 \cdot \alpha_4}$$

$$G_2 = \frac{\alpha_1 \cdot \alpha_5}{1 - \alpha_1 \cdot \alpha_4}$$

$$G_3 = \frac{\alpha_2}{1 - \alpha_1 \cdot \alpha_4}$$

In the same way (A2.3) gives :

$$a = \frac{G'_1}{1 + \tau_1 p} \cdot d_L + \frac{G'_2}{1 + \tau_1 p} \cdot d_G + \frac{G'_3}{1 + \tau_1 p} \cdot r \qquad \text{(A2.8)}$$

with :

$$G'_1 = \alpha_4 \cdot G_1$$

$$G'_2 = \alpha_5 + \alpha_4 \cdot G_2$$

$$G'_3 = \alpha_4 \cdot G_3$$

The relations (A2.7) and (A2.8), binding the inputs r, d_G and d_L, of the one part, and the outputs, a and b, of the other part, are first order transfers with the time constant τ_1.

The inverse Laplace transforms allow to express the derivatives of a and b :

$$\frac{db}{dt} = \frac{1}{\tau_1}\left(-b + G_1 \cdot d_L + G_2 \cdot d_G + G_3 \cdot r\right) \qquad \text{(A2.9)}$$

$$\frac{da}{dt} = \frac{1}{\tau_1}\left(-a + G'_1 \cdot d_L + G'_2 \cdot d_G + G'_3 \cdot r\right) \qquad \text{(A2.10)}$$

Although the notations have not been changed with the Laplace transformation, the functions a, b, r, d_L and d_G are functions of time again, as they were before resolution through Laplace transforms.

The relations (A2.9) and (A2.10) are the relations (11) and (12) given in paragraph 3.

ANNEX 3

SOFTWARE OF THE SIMULATOR OF THE NITRIFYING COLUMN

The software is written in Matlab® language and is composed of the following programmes :

. i_sim.m : initialization of the simulation (duration, configuration ...)
. column.m : derivative equations of the column
. calmu.m : calculation of μ, taking into account the limiting substrates.

It is saved in the directory :

c:\melissa\nitri\colonne5

```
%*************************************************************
%       Nitrifying column                                     *
%       Version 1.0     April 1998                            *
%       Simplified equations set according to TN 35.2         *
%                                                             *
%                                                             *
%       i_sim.m   Initialization of the simulation            *
%                                                             *
%*************************************************************


 clear all

global NL NG NS NB NX
global AA2 BA2 AB2 BB2 AC2 BC2 BA1 BB1 BC1
global Gin RG fG Fin RL fL
global KCO2
global mumax maint Kl In Yx Nls Nis Yx1 Ym1

arret = 0;
% Simulation parameters
        tdeb=0;
        tmin=1e-8;
        tmax=.1;
        prec=1e-6;      % necessary precision to avoid too big numerical noise
        tfin=10;
        nbptx=ceil(1.2*tfin/tmin);
        nbptx = 100000;

% Simulation horizon
        dt = .25;        % simulation period of the inputs
        T = [0:dt:tfin]';
        [m,n] = size(T);

% type of test
% ------------
typtst = 2;     titre = 'Input cst:O2 CO2 NH3 G and L; No biomass';
typtst = 4;     titre = 'Impulse response of the column; No biomass; SO4=';
typtst = 5;     titre = 'Impulse response of the column; No biomass; NO2-';
typtst = 1;     titre = 'Input step:O2 CO2 Gas, NH3 L; No biomass';
typtst = 3;     titre = 'Input cst:O2 CO2 NH3 G and L; Checking the steady state';
typtst = 6;     titre = 'Input cst:O2 CO2 NH3 G and L; Growth of biomass';
                %At starting : G/L thermodynamical equilibrium inside the column
                %Incoming G : O2 CO2; incoming L : NH3 HPO4 SO4

% general parameters
% ------------------
        NL = 4;         % number of mono-phase substrates in the liquid phase
        NG = 3;         % number of bi-phases substrates (in the L and G phases)
        NS = 2;         % number of strains of bacteria (Ns and Nb)
        NX = 2*NG + NL + 2*NS;  % nb of coef of state vector Xi for any tank i

% Column parameters
%------------------
        NB = 5;         % 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

        VnB = VB / NB;  % volume of an equivalent stirred tank
        epsT = epsG + epsL;

% 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))

        Kl =    [6.625e-5   1e-30  ;     % limiting substrate : NH3   (mol/l)
                 1e-30      3.6e-4 ;     % limiting substrate : NO2-  (mol/l)
                 5.05e-6    1.7e-5 ;     % limiting substrate : O2    (mol/l)
                 1e-10      1e-10 ];     % limiting substrate : HCO3-(mol/l)

        In =    [1e30       1e30   ;     % inhibitory substrate : NO2-  (mol/l)
                 1e30       1e30]  ;     % inhibitory substrate : NO3-  (mol/l)

                                          % inverse of yield of biosynthesis :
                                          % (mol substr./mol biomass)
        Yx1  =  [-5.4269   -6.5106 ;     % O2
                 -1        -1       ;     % HCO3- or CO2
                 -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 = [51; 51; 500];    % O2 CO2 NH3   (1/h)

% partition coefficients (apparent value for weak electrolyte)
% -------------------------------------------------------------
        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 H3PO4)
% -----------------------------------
        Ka = 6.166e-8;          % (at T=298K, from TN 27.2,LGCB)
        xx = 1e-8/Ka;   KPO4 = 1+xx;       %[PO4]total = f([HPO4=])

% initial concentrations in the column
% ------------------------------------
  %1. Gas phase :
        fm_O2_0  = .21;         % O2  (molar fraction)
        fm_CO2_0 = .004;        % CO2 (molar fraction)
        fm_H2O_0 = 4.129e-2;    % H2O (molar fraction)
    if typtst == 1
        fm_NH3_0 = 0;           % NH3 (molar fraction)
    elseif typtst == 2
        fm_NH3_0 = 7.14e-3*kpartN(3)/55.56;      % NH3 (molar fraction)
    elseif typtst == 3
        fm_NH3_0 = 1*7.14e-3*kpartN(3)/55.56;      % NH3 (molar fraction)
    elseif (typtst == 4 | typtst == 5)
        fm_O2_0  = 0;           % O2  (molar fraction)
        fm_CO2_0 = 0;           % CO2 (molar fraction)
        fm_H2O_0 = 0;           % H2O (molar fraction)
        fm_NH3_0 = 0;           % NH3 (molar fraction)
    elseif typtst == 6
        fm_NH3_0 = 1*7.14e-3*kpartN(3)/55.56;      % NH3 (molar fraction)
    end
    fm_N2_0 = 1 - fm_O2_0 - fm_CO2_0 - fm_NH3_0 - fm_H2O_0;     % N2
    % conc. in gas phase (perfect gases at T=303 K and P=1 atm)
    VM = 22.4 * 303 / 298;  % molar volume (l/mol)
    CG0 = [fm_O2_0; fm_CO2_0; fm_NH3_0] / VM;        % mol/l
    CN2 = fm_N2_0 / VM;         % mol/l
    CH2O = fm_H2O_0 / VM;       % mol/l
  %2. Liquid phase :
        C_O2_0   = fm_O2_0 / kpartN(1) * 55.56;       % mol/l
        C_CO2_0  = fm_CO2_0/kpartN(2)*55.56;          % mol/l (CO2 solvated)
        C_NH3_0  = 7.14e-3;                           % mol/l (NH3 solvated)
        C_NO2_0  = 0;                                 % mol/l
        C_NO3_0  = 0;                                 % mol/l
        C_PO4_0  = 1e-4;                              % mol/l (HPO4--)
        C_SO4_0  = 1e-4;                              % mol/l (SO4--)
        C_XNs_0  = 1*2e-2;                              % g/l
        C_XNb_0  = 1*2e-2;                              % g/l

        CL0 = [C_O2_0; C_CO2_0; C_NH3_0; C_NO2_0; C_NO3_0; C_PO4_0; C_SO4_0];
        CX0 = [C_XNs_0; C_XNb_0; C_XNs_0; C_XNb_0];
    if typtst == 1
        CL0 = [0; 0; 1; 0; 0; 0; 0] .* CL0;
        CX0 = [0; 0; 0; 0] .* CX0;
    elseif typtst == 2
        CL0 = [1; 1; 1; 0; 0; 0; 0] .* CL0;
    elseif typtst == 3
        CL0 = [1; 1; 1; 1; 1; 1; 1] .* CL0;
        CX0 = [0; 0; 0; 0] .* CX0;
    elseif (typtst == 4 | typtst == 5)
        CL0 = [0; 0; 0; 0; 0; 0; 0] .* CL0;
        CX0 = [0; 0; 0; 0] .* CX0;
    elseif typtst == 6
```

```
        CG0 = [1; 1; 0] .* CG0;
        CL0 = [0; 0; 1; 1; 1; 1; 1] .* CL0;
    end

%Temporal input :
%----------------
    if 0 % calcul de R_0 inutile depuis colonne5 (utile pour mu et muX event)
    CHCO3 = CL0(2) * KCO2;          % concentration of HCO3-
    C = [CL0(3); CL0(4); CL0(1); CHCO3];    % NH3 NO2 O2 HCO3 in Liquid phase
    [mu,muX] = calmu(C)
    rg = mu.*[C_XNs_0;C_XNb_0];     % global (active + decay) growth rate of biomass Ns and N
    rm = maint.*[C_XNs_0;C_XNb_0];  % maintenance rate of biomass Ns and Nb
    R_0 = Yx1 * rg + Ym1 * rm;      % consum/production rate of substrates
    end

    if typtst == 1
        dG_0 = 0 * CG0;
        dL_0 = 0 * CL0;
    elseif typtst == 2
        dG_0 = 1 * CG0;
        dL_0 = 1 * CL0;
    elseif typtst == 3
        dG_0 = 1 * CG0;
        dL_0 = 1 * CL0;
    elseif (typtst == 4 | typtst == 5)
        dG_0 = 0 * CG0;
        dL_0 = 0 * CL0;
    elseif typtst == 6
        dG_0 = [fm_O2_0; fm_CO2_0; fm_NH3_0] ./ VM;        % mol/l
        dL_0 = [C_O2_0; C_CO2_0; C_NH3_0; C_NO2_0; C_NO3_0; C_PO4_0; C_SO4_0];
    end

    if typtst == 1
        t0 = .100;
    elseif typtst == 2
        t0 =-1.00;
    elseif typtst == 3
        t0 =-1.00;
    elseif (typtst == 4 | typtst == 5)
        t0 = .100;
    elseif typtst == 6
        t0 =-1.00;
    end
    dG = ones(size(T))*CG0';     % incoming gas [O2,CO2,NH3] conc (mol/l)
    dL = ones(size(T))*CL0';     % incoming liq [O2,CO2,NH3,NO2,NO3,HPO4,SO4] conc (mol/l)
    ind = find(T<=t0);
    if (~isempty(ind))
        dG(ind,:) = ones(size(ind)) * dG_0';
        dL(ind,:) = ones(size(ind)) * dL_0';
    end

% Initialization of the state matrices for each tank of the column
%-----------------------------------------------------------------

        Gin = .03*60;     % incoming gas volumic rate (l/h)
        Fin = .0028*60;   % incoming liq volumic rate (l/h)
        RG = 1*99.0;       % recycling ratio of gas
        RL = 1*6.42;       % recycling ratio of liquid
       %RL = 45/2.8;       % 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)
        qG = Gin * (1+RG) * (1+fG);
```

```
    qL = Fin * (1+RL) * (1+fL);
    alpha = kpartN / 55.56 / VM;

for ii = 1:3
    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) * (1+fL);
      qG = Gin * (1+RG) * (1+fG);
    elseif ii == 2     % Tank n of the part B of the column
      VL = VnB*epsL;         % volume of liquid
      VG = VnB*epsG;         % volume of gas
      qL = Fin * (1+RL) * (1+2*fL);
      qG = Gin * (1+RG) * (1+2*fG);
    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) * (1+fL);
      qG = Gin * (1+RG) * (1+fG);
    end

   %% Direct computation of teta1 teta2 beta1 beta2
   %teta1 = 1 ./ (KLa + qL/VL);
   %teta2 = VG./(qG + VL*(KLa ./ alpha));
   %num = VG*KLa + qL*VG/VL + qG + VL*(KLa./alpha);
   %den = qG*KLa + qL*qG/VL + qL*(KLa./alpha);
   %beta1 = num ./ den;
   %beta2 = VG ./ den;
    % Indirect computation of teta1 teta2 beta1 beta2
    den1 = KLa*VL + qL;
    den2 = (KLa ./ alpha)*VL + qG;
    teta1 = VL ./ den1;
    teta2 = VG ./ den2;
    alpha1 = VL * (KLa ./ alpha) ./ den1;
    alpha2 = VL ./ den1;
    alpha3 = qL ./ den1;
    alpha4 = VL * (KLa ./ den2);
    alpha5 = qG ./ den2;
    den3 = 1 - alpha1 .* alpha4;
    beta1 = (teta1 + teta2) ./ den3;
    beta2 = (teta1 .* teta2) ./ den3;

    xx1 = roots([1 beta1(1)/beta2(1) 1/beta2(1)]);
    xx2 = roots([1 beta1(2)/beta2(2) 1/beta2(2)]);
    xx3 = roots([1 beta1(3)/beta2(3) 1/beta2(3)]);
    taux(:,1) = -1 ./ xx1;       % time constants for O2
    taux(:,2) = -1 ./ xx2;       % time constants for CO2
    taux(:,3) = -1 ./ xx3;       % time constants for NH3
    if ~all((taux(1,:) ./ taux(2,:)) < .07)
      message = 'The approximation of first order is not justified.';
      message = [message ' Loop : ' num2str(ii)]
      tau2_tau1 = taux(1,:) ./ taux(2,:)
      arret = 1;
    end
    tau = taux(2,:)';
   %tau1 = taux(2,:)
    if ~all((teta2 ./ tau) < .07)
      message = 'The approximation of first order is not justified.';
      message = [message ' Loop : ' num2str(ii)]
      teta2_tau1 = (teta2 ./ tau)'
      arret = 1;
    end
```

```
        G1 = alpha3 ./ den3;                                % Gain of b/dL
        G2 = alpha1 .* alpha5 ./ den3;                      % Gain of b/dG
        G3 = alpha2 ./ den3;                                % Gain of b/r
        Gp1 = alpha4 .* G1;                                 % Gain of a/dL
        Gp2 = alpha4 .* G2 + alpha5;                        % Gain of a/dG
        Gp3 = alpha4 .* G3;                                 % Gain of a/r
        As = [-1 ./ tau .* ones(NG,1);
              -1 ./ tau .* ones(NG,1)];
        Bs = [diag(G1./tau)  ,diag(G2./tau)  ,diag(G3./tau)  ;
              diag(Gp1./tau) ,diag(Gp2./tau) ,diag(Gp3./tau)];

        % 1_ bi-phases substrates :
        % -------------------------
        if ii == 1          % Part A of the column
          AA2 = As;       BA2 = Bs;
        elseif ii == 2      % Tank n of the part B of the column
          AB2 = As;       BB2 = Bs;
        elseif ii == 3      % Part C of the column
          AC2 = As;       BC2 = Bs;
        end

        % 2_ mono-phase substrates :
        % --------------------------
        %ts1 = VL/qL
        if ii == 1          % Part A of the column
          BA1 = qL/VL .* ones(NL,1);
        elseif ii == 2      % Tank n of the part B of the column
          BB1 = qL/VL .* ones(NL,1);
        elseif ii == 3      % Part C of the column
          BC1 = qL/VL .* ones(NL,1);
        end

    end

% Initialization of the state vector
%-----------------------------------
        X0 = [dL_0(1:NG); dG_0; dL_0(NG+1:NG+NL); 0; 0; 0; 0];
        for ii = 1:NB
          X0 = [X0; dL_0(1:NG); dG_0; dL_0(NG+1:NG+NL); CX0];
        end
        X0 = [X0; dL_0(1:NG); dG_0; dL_0(NG+1:NG+NL); 0; 0; 0; 0];
        if typtst == 4 % computation of Impulse Response with SO4
          X0(10) = 1/VA/epsL*epsT;
        elseif typtst == 5 % computation of Impulse Response with NO2
          X0(7) = 1/VA/epsL*epsT;
        end

if arret
% break
end
disp(' *** End of initialization ***')
```

```
%*****************************************************************
%        Nitrifying column                                        *
%        Version 1.0      April 1998                              *
%        Simplified equations set according to TN 35.2            *
%                                                                 *
%                                                                 *
%        column.m  Computation of the derivatives                 *
%                                                                 *
%*****************************************************************

  function [sys,x0]=column(tn,x,u,flag,X0)

% COLUMN        S-Function for simulation of the nitrifying column
%
% Synopsis
%       [sys,x0]=column(tn,x,u,flag,X0)
%
% Parameters
%       X0      initial state vector
%
% State vector x
%       Length of the state vector : NX * (NB + 2)
%         with : NX = 2*NG + NL + 2*NS
%                NG = number of bi-phases substrates (present in Gas and Liquid)
%                NL = number of mono-phase substrates (present in Liquid only)
%                NS = number of strains (Nitrosomonas and Nitrobacter)
%                NB = number of equivalent tanks in part B of the column
%       The state vector is composed of the concentrations of the compounds
%       of the column
%       Indices of the compounds in the state vector :
%         For a compartment i (i between 1 and NB+2)
%         Indice                          Compound
%         (i-1)*NX + 1                    O2     in Liquid phase
%         (i-1)*NX + 2                    CO2    in Liquid phase
%         (i-1)*NX + 3                    NH3    in Liquid phase
%         (i-1)*NX + NG + 1               O2     in Gas phase
%         (i-1)*NX + NG + 2               CO2    in Gas phase
%         (i-1)*NX + NG + 3               NH3    in Gas phase
%         (i-1)*NX + 2*NG + 1             NO2
%         (i-1)*NX + 2*NG + 2             NO3
%         (i-1)*NX + 2*NG + 3             HPO4
%         (i-1)*NX + 2*NG + 4             SO4
%         (i-1)*NX + 2*NG + NL + 1        Xv_Ns  active Nitrosomonas biomass
%         (i-1)*NX + 2*NG + NL + 2        Xv_Nb  active Nitrobacter biomass
%         (i-1)*NX + 2*NG + NL + NS + 1   Xt_Ns  global Nitrosomonas biomass
%         (i-1)*NX + 2*NG + NL + NS + 2   Xt_Nb  global Nitrobacter biomass
% Inputs
%       The inputs vector is composed of the concentrations of the compounds
%       of the incoming liquid and gas flows.
%       Indices of the compounds in the inputs vector :
%         Indice      Compound
%         1           O2     in the incoming liquid flow (flow rate : Fin)
%         2           CO2    in the incoming liquid flow (flow rate : Fin)
%         3           NH3    in the incoming liquid flow (flow rate : Fin)
%         NG + 1      O2     in the incoming gas flow (flow rate : Gin)
%         NG + 2      CO2    in the incoming gas flow (flow rate : Gin)
%         NG + 3      NH3    in the incoming gas flow (flow rate : Gin)
%         2*NG + 1    NO2    in the incoming liquid flow (flow rate : Fin)
%         2*NG + 2    NO3    in the incoming liquid flow (flow rate : Fin)
```

```
%          2*NG + 3    HPO4   in the incoming liquid flow (flow rate : Fin)
%          2*NG + 4    SO4    in the incoming liquid flow (flow rate : Fin)
%
% Outputs
%       x        state vector (concentrations in liquid or gas phase)
%

global NL NG NS NB NX
global AA2 BA2 AB2 BB2 AC2 BC2 BA1 BB1 BC1
global KCO2
global Gin RG fG Fin RL fL
global NI
global mumax maint Kl In Yx Nls Nis Yx1 Ym1

%> Sizes array and Initial conditions ----------------------------------------

if flag==0,
   NI = 2*NG + NL;
   sys = [
        NX*(NB+2)    % continuous states
        0            % discrete states
        NX*(NB+2)    % outputs
        NI           % inputs
        0            % discontinuous ...
        0            % direct feedthrough
        ];

   x0 = [X0];

%> Continuous state (computation of derivatives) -----------------------------
elseif abs(flag)==1,
  % The concentrations cannot be negative
    ind = find(x<0);
    x(ind) = zeros(size(ind));

  %1_ part A of the column
  %-----------------------
    rX = zeros(NS,1);           % active growth rate of biomass Ns and Nb null
    rg = zeros(NS,1);           % global   growth rate of biomass Ns and Nb null
    ri = zeros(NG+NL,1);        % consum/production rate of substrates null

    % derivatives of concentrations of bi-phases substrates
    ind2La = NX*(NB+1) + [1:NG];
    ind2Lp = NX + [1:NG];
    ind2Ga = ind2La + NG;
    ind2Gp = ind2Lp + NG;
    dL = (u(1:NG) + RL*x(ind2La) + fL*(1+RL)*x(ind2Lp)) / (1+RL) / (1+fL);
    dG = (u(NG+1:2*NG) + RG*x(ind2Ga) + fG*(1+RG)*x(ind2Gp)) / (1+RG) / (1+fG);
    ee = [dL; dG; ri(1:NG)];
    ind2 = [1:2*NG];
    sys(ind2) = AA2 .* x(ind2) + BA2 * ee;

    % derivatives of concentrations of mono-phase substrates
    ind1La = NX*(NB+1) + 2*NG + [1:NL];
    ind1Lp = NX + 2*NG + [1:NL];
    dL = (u(2*NG+1:2*NG+NL) + RL*x(ind1La) + fL*(1+RL)*x(ind1Lp)) / (1+RL) / (1+fL);
    ind1 = 2*NG + [1:NL];
    sys(ind1) = BA1 .* (dL - x(ind1)) + ri(NG+1:NG+NL);

    % biomass growth rate
    indX = [NX-3:NX];
    sys(indX) = [rX; rg];
```

```
%2_ part B of the column
%-----------------------
ind2La = -NX + [1:NG];
ind2Ga = ind2La + NG;
ind1La = -NX + 2*NG + [1:NL];
for ii = 2:NB+1
  ix = (ii-1)*NX;
  iy = ix + 2*NG + 1;
  CHCO3 = x(ix+2) * KCO2;   % concentration of HCO3-
  C = [x(ix+3); x(iy); x(ix+1); CHCO3];    % NH3 NO2 O2 HCO3 in Liquid phase
  [mu,muX] = calmu(C);
  ind = NX*ii - [3,2];        % indices of biomass conc. in state vector
  rX = muX .* x(ind);         % active growth rate of biomass Ns and Nb
  rg = mu .* x(ind);          % global (active + decay) growth rate of biomass Ns and Nb
  C1 = [x(ix+3); x(ix+1)];    % NH3 O2 in Liquid phase
  C2 = [x(ix+7); x(ix+1)];    % NO2 O2 in Liquid phase
  Klim = [all(C1>0); all(C2>0)]; %limiting coef when conc. C1 C2 null
  rm = Klim .* maint .* x(ind);  % maintenance rate of biomass Ns and Nb
  ri = Yx1 * rg + Ym1 * rm;   % consum/production rate of substrates

  % derivatives of concentrations of bi-phases substrates
  ind2La = ind2La + NX;
  ind2Lp = ind2Lp + NX;
  ind2Ga = ind2Ga + NX;
  ind2Gp = ind2Gp + NX;
  dL = ((1+fL)*x(ind2La) + fL*x(ind2Lp)) / (1+2*fL);
  dG = ((1+fG)*x(ind2Ga) + fG*x(ind2Gp)) / (1+2*fG);
  ee = [dL; dG; ri(1:NG)];
  ind2 = ind2 + NX;
  sys(ind2) = AB2 .* x(ind2) + BB2 * ee;

  % derivatives of concentrations of mono-phase substrates
  ind1La = ind1La + NX;
  ind1Lp = ind1Lp + NX;
  dL = (x(ind1La) + fL*x(ind1Lp)) / (1+fL);
  ind1 = ind1 + NX;
  sys(ind1) = BB1 .* (dL - x(ind1)) + ri(NG+1:NG+NL);

  % biomass growth rate
  indX = indX + NX;
  sys(indX) = [rX; rg];

end

%3_ part C of the column
%-----------------------
  rX = zeros(NS,1);           % active growth rate of biomass Ns and Nb null
  rg = zeros(NS,1);           % global   growth rate of biomass Ns and Nb null
  ri = zeros(NG+NL,1);        % consum/production rate of substrates null

  % derivatives of concentrations of bi-phases substrates
  ind2La = ind2La + NX;
  ind2Ga = ind2Ga + NX;
  dL = x(ind2La);
  dG = x(ind2Ga);
  ee = [dL; dG; ri(1:NG)];
  ind2 = ind2 + NX;
  sys(ind2) = AC2 .* x(ind2) + BC2 * ee;

  % derivatives of concentrations of mono-phase substrates
  ind1La = ind1La + NX;
```

```
    dL = x(ind1La);
    ind1 = ind1 + NX;
    sys(ind1) = BC1 .* (dL - x(ind1)) + ri(NG+1:NG+NL);

    % biomass growth rate
    indX = indX + NX;
    sys(indX) = [rX; rg];

%> Outputs ----------------------------------------------------------------------

elseif flag==3,
    sys = x;

%> ----------------------------------------------------------------------------
else
   sys = [];
end
```

```
%*****************************************************************
%       Nitrifying column                                        *
%       Version 1.0     April 1998                               *
%       Simplified equations set according to TN 35.2            *
%                                                                *
%                                                                *
%       calmu.m Calculation of mu (limiting substrates only)     *
%                                                                *
%*****************************************************************

function [mu,muX] = calmu(C)

global mumax maint Kl In Yx Nls Nis

% components of C :
%       1 : NH3
%       2 : NO2-
%       3 : O2
%       4 : HCO3-

  % 1_ Computation of rmu = mu/mumax :
  aa1 = C(1) * C(3) * C(4) / (Kl(1,1)+C(1)) / (Kl(3,1)+C(3)) / (Kl(4,1)+C(4));
  aa2 = C(2) * C(3) * C(4) / (Kl(2,2)+C(2)) / (Kl(3,2)+C(3)) / (Kl(4,2)+C(4));
  rmu = [aa1; aa2] ;
  % 2_ computation of mu and muX :
  mu = rmu.*mumax;
  muX = rmu.*mumax + (1-rmu).*maint.*Yx;
```