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

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TECHNICAL NOTE : 48.1

Nitrite and Biomass Predictors of the Nitrifying Compartment
Phase I : Mathematical inferred variable

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1. INTRODUCTION

The function of the nitrifying compartment is the transformation of ammonia into nitrate. Its behaviour is critical because it should not produce nitrite, which is a poison for man and a lot of bacteria. As the on line measurement of nitrite is impossible (a sensor is not yet available), it is necessary to infer a mathematical measurement of this compound.

Starting from the First Principles model of University of Clermont Ferrand (TN's 27.1 and 27.2), it has been shown in a previous study (TN 44.3) that the behaviour of the nitrifying compartment can be explicitly expressed under the classical form of a state system :

$$\dot{C}_x = F \cdot C_x$$
$$\dot{X} = A \cdot X + B \cdot U + E \cdot C_x$$
$$Y = C \cdot X + D \cdot U$$

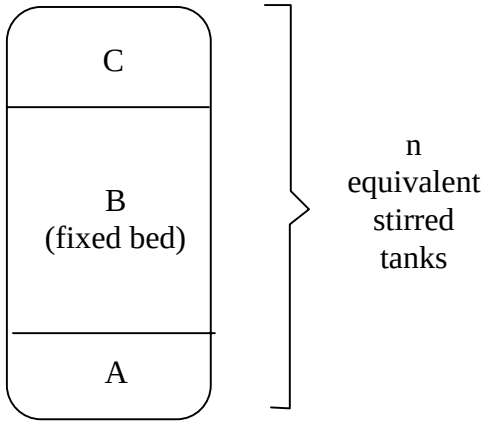


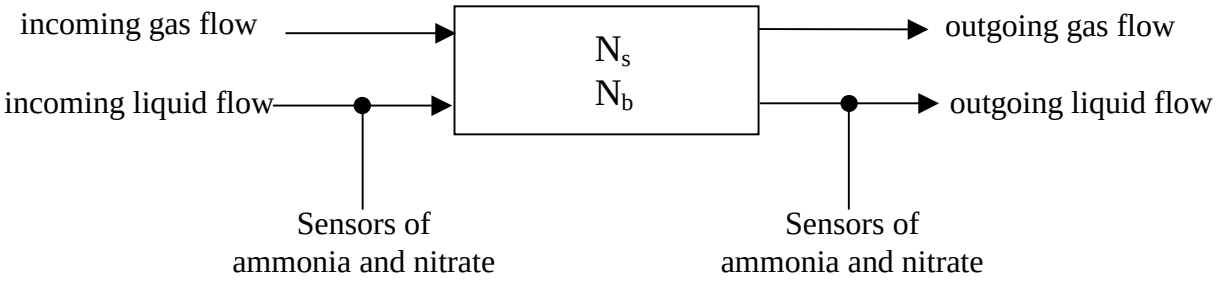
Figure 1 : State system and Scheme of the nitrifying compartment
(in the state system : A, B and C are matrices;
in the nitrifying compartment : A, B and C are the different parts of the column)

This system can be used to estimate the nitrite concentration at column output.
Unfortunately this approach requires a lot of sensors : when the column can be modelled with n tanks, n+1 sensors of nitrate and as many sensors of ammonia are needed. As a good value for n is at least 7, the huge number of sensors and the heavy identification work associated make the approach unfeasible.
So another approach is proposed now. Three simplified models of the column are studied in order to compare their respective advantages and disadvantages and to choose the best one in defined conditions.
This Technical Note (phase I) establishes the formula of the predictors and the next one (phase II) will compare them on their behaviours and robustness

2. THE STUDIED PREDICTORS AND THE PROTOCOL OF TEST

First simplified model (predictor 1) :

In the model of the predictor 1, the column is considered as only one tank in which the strains are equally distributed throughout the volume of liquid. The corresponding model is a first order. Only 2 sensors of nitrate and 2 ones of ammonia are needed (1 at each end of the column).



N_s : Nitrosomonas
N_b : Nitrobacter

Figure 2 : Simplified column for predictor 1

Second simplified model (predictor 2) :

In the model of the predictor 2, the column is assumed to be composed of 2 tanks in each of which the strains are equally distributed and at different concentrations (greater in the first tank than in the second one). The corresponding model is a block of 2 successive first order. Therefore 3 sensors of nitrate and 3 ones of ammonia are needed (1 at each end and 1 in the middle of the column).

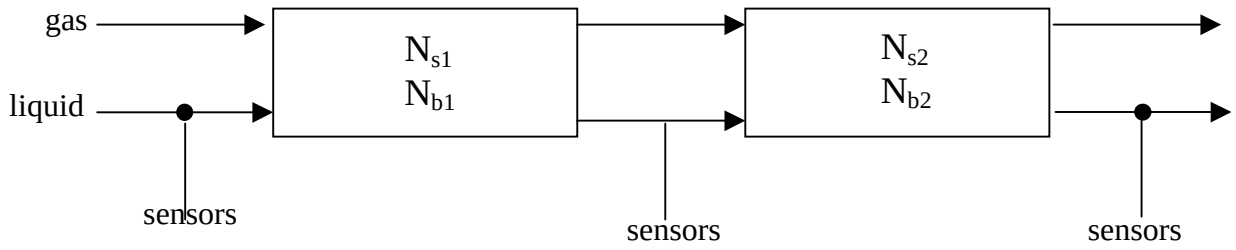


Figure 3 : Simplified column for predictor 2

Third simplified model (predictor 3) :

In the model of the predictor 3, the column is a combination of the 2 previous models. It is still parted into 2 tanks but the biomass is presumed to be present only in the first one and null in the second one. This hypothesis lies on the fact that, in the long run, the strains migrate towards the input of the column where the concentrations of substrates are the highest. The corresponding model is a second order. Only 2 sensors of nitrate and 2 ones of ammonia are needed (1 at each end of the column).

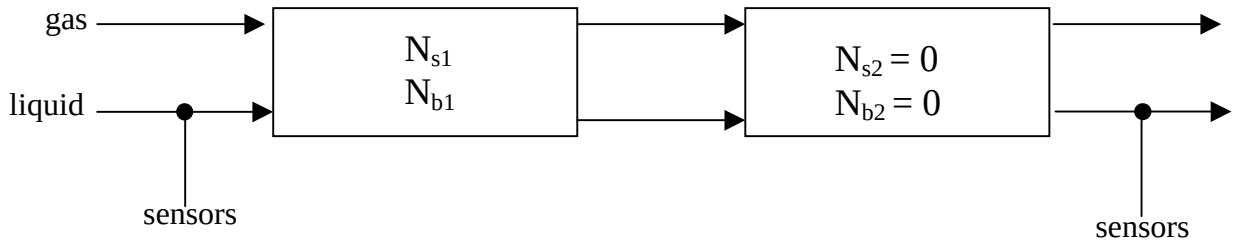


Figure 4 : Simplified column for predictor 3

Protocol of the tests :

In order to illustrate the behaviour of each of these predictors, a protocol of test is designed and the data (ammonia and nitrate concentrations) are obtained from a column simulated in standard conditions.

The simulated experiment is composed of 2 parts :

- the first part of 150 hours (about 6 days functioning) represents a starting column : at the beginning, the strains are equally distributed throughout the fixed bed;
- during this first period, the strains migrate towards the input of the column and the second part of the test (another 150 h period of time) is assumed to represent the long term functioning of the column.

The simulation of the column is done in the standard conditions defined by Clermont:

- the biomass concentrations are standard at the start;
- the concentrations of substrates in the incoming flow are standard. At the beginning of the second part of the simulation, a step of ammonia concentration is realized by doubling the concentration of the first part;
- the number of equivalent tanks of the fixed bed is set to 5.

3. NITRITE PREDICTORS

As the predictor models are simplified models of the column, none of them have the same behaviour as the column (none of them are able to estimate the exact nitrite concentration obtained from the simulated column). This appears in the figure 5 where each graph represents the nitrite concentration of the column (solid or blue line) and of the predictor (dotted or green line).

On the first part of the simulation (150 first hours), the behaviours of the predictors 1 and 2 are very close of the one of the column because the hypothesis of the predictors are those of the column (the strains are equally distributed throughout the liquid volume), and the behaviour of the predictor 3 is far from the column because its hypothesis is that there is no bacteria in the second tank (which is not true at the start of the simulated experiment).
In the second part of the simulation, the strains have migrated towards the column input and the predictors 2 and 3 are adapted to the behaviour of the column.

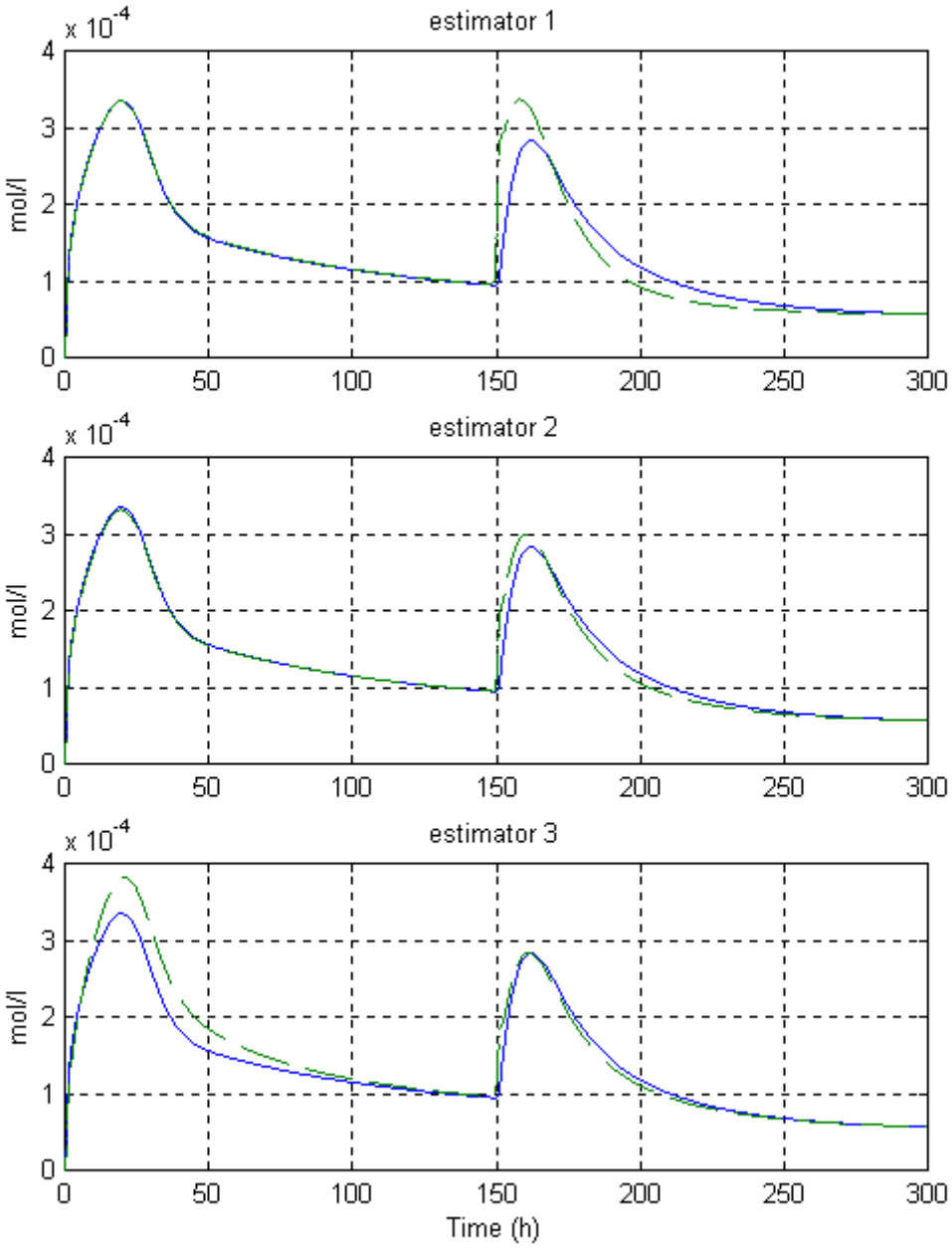


Figure 5 : Behaviour of the nitrite predictors (no noise , no mismatch)

4. BIOMASS PREDICTORS

As demonstrated in annex, the biomass which can be estimated is the quantity represented by the multiplication of the active biomass and of the limiting factor. It represents the part of the biomass which consumes substrates and makes the products. The figure 6 shows that the behaviours of the biomass predictors are near each other(as demonstrated in annex) and near the behaviour of the column when there is no noise of measurement.

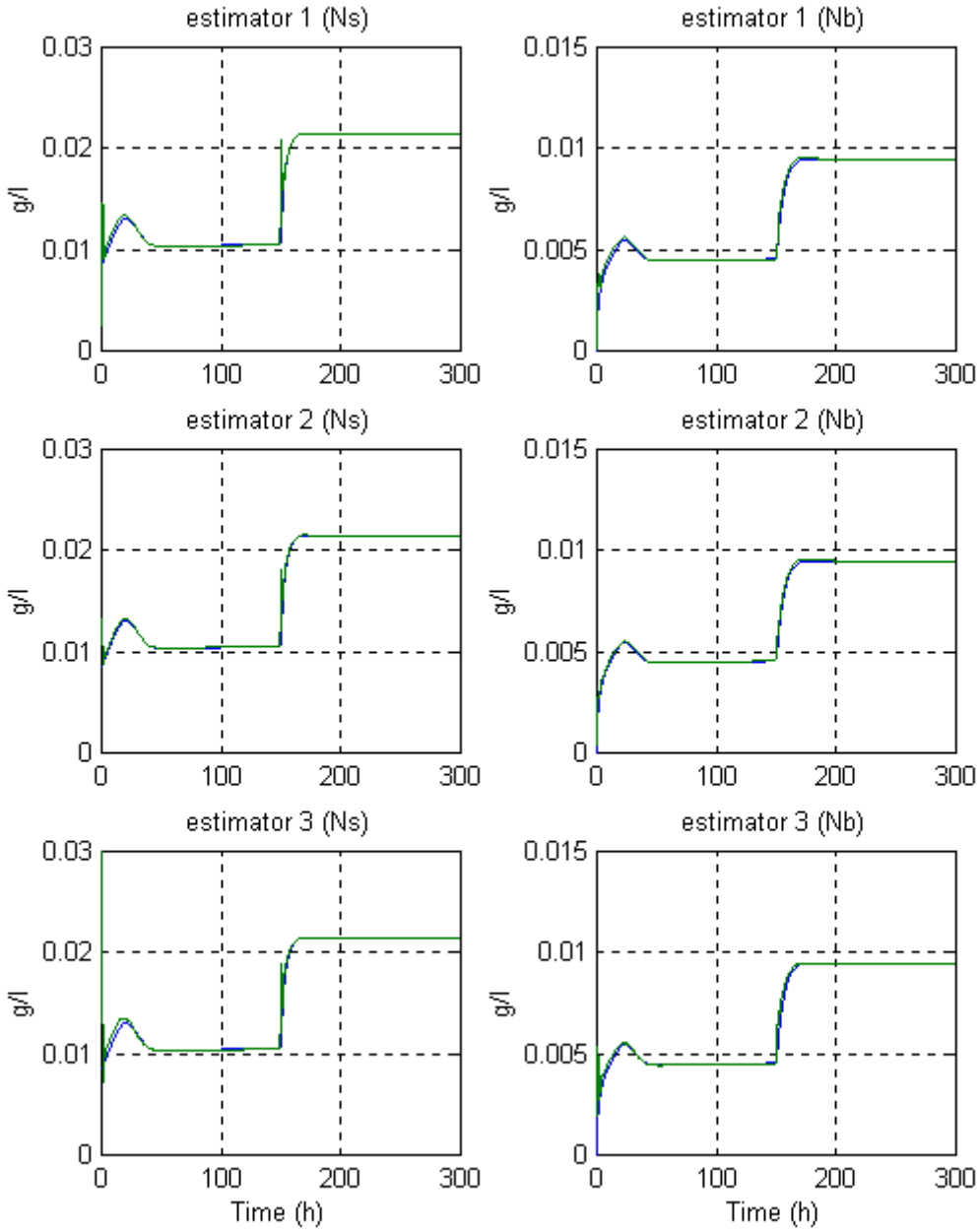


Figure 6 : Behaviour of the Ns and Nb biomass predictors (no noise, no mismatch) (column : solid or blue line | predictors : dotted or green line)

5. CONCLUSION

Three models of predictors have been proposed in order to express the concentrations of nitrite and of Nitrosomonas and Nitrobacter biomass. Their expressions are more or less complex and their accuracy and appropriate usage will be studied in TN 48.2 .

6. 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

LECLERCQ J.-J. : "A first approach for the biomass and nitrite estimators of the nitrifying compartment". Contract ESTEC n° 12924/98/NL/MV, 1999, TN 44.3.

ANNEX

MATHEMATICAL INFERRED VARIABLES

A.1. INTRODUCTION

A.1.1. Notation

The notation is the one of TN 44.2 and is recalled hereafter, for each substrate of the problem and for each tank of the column :

a : molar concentration in the gas phase

b : molar concentration in the liquid phase of the molecular form

c : molar concentration at the thermodynamic equilibrium

d_G : molar concentration in the incoming gas flow

d_L : molar concentration in the incoming liquid flow of the molecular form

q_G : gas flow rate (1/h)

q_L : liquid flow rate (1/h)

r : mean volumetric production or consumption rate (mol/1/h)

K : volumetric transfer coefficient in liquid phase (notation K_{La} in TN 27.1)

k : dissociation constant of acid/base equilibrium

In the liquid phase, the concentration of a molecular form, x, and the one of its ionic form x' are linked by the relation which implies the dissociation constant k :

$$x' = k \cdot x$$

with $k = \dfrac{K_b . [H^+]}{K_e}$ for NH_3 solvated

$k = 0$ for the other compounds

A.1.2. Recall of general equations for a tank of the column

The following equations have been established in the Technical Note 44.2 related to the nitrifying compartment.

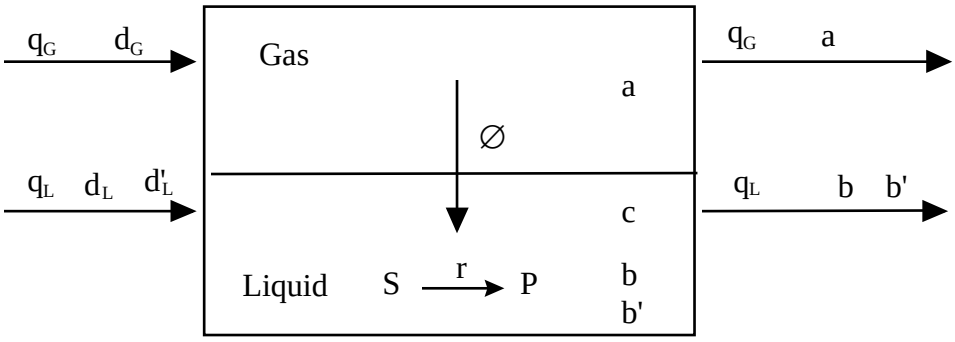


Figure A.1 : General flow sheet of a tank
(S = substrate , P = product)

For a mono-phase substrate, the mass conservation law, in the liquid phase of an ideally stirred tank, leads to :

$$(1 + \tau_L \cdot p)\, b = \tau_L \cdot r + d_L \qquad (A.1)$$

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

p : Laplace variable

For a bi-phase substrate, the mass conservation law, in the liquid and gas phases of an ideally stirred tank, leads to (relations A2.7 and A2.8 of TN 44.2) :

$$(1 + \tau_1.p)\, b = G_1 \cdot d_L + G_2 \cdot d_G + G_3 \cdot r \qquad (A.2)$$

$$a = \alpha_4 \cdot b + \alpha_5 \cdot d_G \qquad (A.3)$$

Considering that, for ammonia, the numerical values of the expressions

$$\frac{(1+k)\cdot q_L}{K \cdot V_L} \quad \text{and} \quad \frac{\alpha \cdot q_G}{K \cdot V_L}$$

are small (but not neglected) compared to 1 (Table A.1),
the static gains and the time constant in (A.2) and (A.3) are :

$$G_1 = \frac{1}{1+\chi} \qquad G_2 = \frac{1}{\alpha} \cdot \frac{1}{1+\frac{1}{\chi}} \qquad G_3 = \frac{\tau_L}{(1+k)}.G_1 \qquad (A.4)$$

with $\chi = \dfrac{\alpha \cdot q_G}{(1+k)\cdot q_L}$

$$\alpha_4 = \alpha \frac{1}{1+\frac{\alpha \cdot q_G}{K \cdot V_L}} \qquad \alpha_5 = \frac{1}{1+\frac{K \cdot V_L}{\alpha \cdot q_G}} \tag{A.5}$$

$$\tau_1 = \tau_L \frac{1}{1+\chi} \tag{A.6}$$

Remark 1 :

The following relation that will be used hereafter can be easily checked :

$$G_1 + \alpha \cdot G_2 = 1 \tag{A.7}$$

Remark 2 :

As (for ammonia, always) $\alpha_5 \cong \frac{\alpha \cdot q_G}{K \cdot V_L}$, which represents a static gain small versus 1 (Table A.1), it can be deduced from (A.3) that the effect of the input 'd_G' (concentration in the incoming gas flow) on the output 'a' (concentration in the outgoing gas flow) is very weak and is negligible.

Expressions	$q_G = G_{in} = 1.8$ l/h $q_L = F_{in} = 0.168$ l/h	$q_G = (1+R_G) \cdot G_{in} = 180$ l/h $q_L = (1+R_L) \cdot F_{in} = 1.20$ l/h
$\frac{(1+k) \cdot q_L}{K \cdot V_L}$	$2.3\ 10^{-3}$	$1.7\ 10^{-2}$
$\frac{\alpha \cdot q_G}{K \cdot V_L}$	$1.6\ 10^{-5}$	$1.6\ 10^{-3}$
χ	10^{-2} $(=\chi_0)$	10^{-1}

Table A.1 : Numerical values of expressions used for approximations

A.1.3. Expression of the variation rate of the nitrite versus the variation rates of ammonia and nitrate

The term *variation* has a general meaning : it means production rate of a compound if the sign is positive and consumption rate of a substrate if negative.

Given :

- μ_1 and μ_2 : maximum growth rates of Nitrosomonas and Nitrobacter, respectively;
- m_1 and m_2 : maintenance coefficients of Nitrosomonas and Nitrobacter, respectively;

- y_{G1} and y_{G2} : stoechiometric coefficient of a considered substrate of the growing reaction for Nitrosomonas and Nitrobacter, respectively;
- y_{M1} and y_{M2} : stoechiometric coefficient of a considered substrate of the maintenance reaction for Nitrosomonas and Nitrobacter, respectively;
- K_{G1j} and K_{G2j} : half maximum growth rate saturation constant of Nitrosomonas and Nitrobacter, respectively, for a substrate j ;
- K_{M1j} and K_{M2j} : half maximum maintenance rate saturation constant of Nitrosomonas and Nitrobacter, respectively, for a substrate j ;

According to TN 27.1 of LGCB, the limiting factor of the Nitrosomonas growth is :

$$\nu_{G1} = \prod_j \frac{S_j}{K_{G1j} + S_j} \qquad \text{(A.8)}$$

where S_j is the concentration of a limiting substrate j : O_2 and NH_3 .

In the same way, the limiting factor of the Nitrobacter growth is :

$$\nu_{G2} = \prod_j \frac{S_j}{K_{G2j} + S_j} \qquad \text{(A.9)}$$

where S_j is the concentration of a limiting substrate j : O_2 and NO_2^- .

Similarly, the limiting factors of the Nitrosomonas and Nitrobacter maintenance can be expressed in function of the saturation constants K_{M1j} and K_{M2j} and for the same substrates O_2, NH_3 and NO_2^- . These factors are designed ν_{M1} and ν_{M2}.
Given C_{X1} and C_{X2}, the concentrations of active biomass Nitrosomonas and Nitrobacter, respectively.
The variation rate, r, of any compound is, according to the pre-quoted TN 27.1 :

$$\begin{aligned} r = \; & y_{G1} \cdot \nu_{G1} \cdot \mu_1 \cdot C_{X1} + y_{M1} \cdot \nu_{M1} \cdot m_1 \cdot C_{X1} \\ & + y_{G2} \cdot \nu_{G2} \cdot \mu_2 \cdot C_{X2} + y_{M2} \cdot \nu_{M2} \cdot m_2 \cdot C_{X2} \end{aligned} \qquad \text{(A.10)}$$

Assuming that, for each strain, the growth limiting factor and the maintenance limiting factor are identical :

$\nu_{G1} = \nu_{M1}$ (Hypothesis *H1*)

$\nu_{G2} = \nu_{M2}$

it becomes :

$$r = \sum_k \sigma_k \cdot c_{Xk} \qquad \text{(A.11)}$$

where $\sigma_k = y_{Gk} \cdot \mu_k + y_{Mk} \cdot m_k$

and $c_{Xk} = \nu_{Gk} \cdot C_{Xk}$

index k = 1 or 2 for Nitrosomonas and Nitrobacter, respectively

In this expression (A.11), the quantity c_X represents the part of the active biomass that produces or consumes compounds. It is referred to as 'productive' biomass in this study.

The relation (A.11) is true for each ideally stirred tank of the column and for each substrate j :

$$r_j = \sum_k \sigma_{jk} \cdot c_{Xk} \qquad \text{(A.12)}$$

where $\sigma_{jk} = y_{Gjk} . \mu_k + y_{Mjk} . m_k$
and particularly for the substrates NH_3 , NO_3^- and NO_2^- .

Given the indices 1, 2 and 3 affected to the variation rates, r_1, r_2 and r_3 of the compounds NH_3, NO_3^- and NO_2^-, respectively.
The variation rate of the nitrite can be expressed versus the variations rates of ammonia and nitrate :

$$r_3 = \beta_1 . r_1 + \beta_2 . r_2 \qquad \text{(A.13)}$$

$$\text{where } \beta_1 = \frac{\sigma_{22} \cdot \sigma_{31} - \sigma_{21} \cdot \sigma_{32}}{D}$$

$$\beta_2 = \frac{\sigma_{11} \cdot \sigma_{32} - \sigma_{12} \cdot \sigma_{31}}{D}$$

$$D = \sigma_{11} . \sigma_{22} - \sigma_{12} . \sigma_{21}$$

Remark :

Under the above hypothesis *H1*, the coefficients β_1 and β_2 of the relation (A.13) are constant independent on the tank. If this hypothesis were not justified, this relation (A.13) would be still true excepted that β_1 and β_2 would depend on the growth and maintenance limiting factors that are dependent on time and on tank. As β_1 and β_2 interfere in the formula of the nitrite predictors (see further), then it would be necessary to know the values of the saturation constant of the maintenance and to measure the O_2 concentration in the liquid phase in order to compute the growth and maintenance limiting factors ν_{Gk} and ν_{Mk} for each strain k, at any moment.

A.1.4. Expression of the biomass concentrations versus the variation rates of ammonia and nitrate

From (A.12) it comes, for each strain k (k=1,2 for Nitrosomonas and Nitrobacter, respectively) :

$$c_{xk} = \delta_{k1} . r_1 + \delta_{k2} . r_2$$

$$\text{where} \quad \delta_{11} = \frac{\sigma_{22}}{D} \qquad \delta_{12} = -\frac{\sigma_{12}}{D} \qquad \text{(A.14)}$$

$$\delta_{21} = -\frac{\sigma_{21}}{D} \qquad \delta_{22} = \frac{\sigma_{11}}{D}$$

$$D = \sigma_{11} \cdot \sigma_{22} - \sigma_{12} \cdot \sigma_{21}$$

The coefficients σ_{jk} are defined in (A.12).

Recall : r_1 and r_2 are the variation rates of NH_3 and NO_3^- , respectively, and are deduced from (A.2) and (A.1) :

$$r_1 = \frac{1}{G_3} \cdot \left((1 + \tau_1 \cdot p) \cdot b_1 - G_1 \cdot d_{L1} - G_2 \cdot d_{G1} \right)$$
$$r_2 = \frac{1}{\tau_L} \cdot \left((1 + \tau_L \cdot p) \cdot b_2 - d_{L2} \right) \qquad \text{(A.15)}$$

Remark :

Under the above hypothesis *H1*, the coefficients δ_{kj} of the relation (A.14) are constant independent on the tank. If this hypothesis were not justified, the same precaution has to be taken as in the case of the coefficients β of the nitrite predictor.

A.1.5 Expression of the nitrite concentration at output of an ideally stirred tank seeded with bacteria

The above general equations, from (A.1) to (A.7) have to be adapted in order to describe the relations between ammonia, nitrate and nitrite. In the following system, the indices 1, 2 and 3 for the concentrations (d_L , d_G) and the production/consumption rates (r) are affected respectively to ammonia, nitrate and nitrite.

Adaptation of (A.2) to ammonia:

$$(1 + \tau_1 . p) . b_1 = G_1 . d_{L1} + G_2 . d_{G1} + G_3 . r_1 \qquad \text{(A.16)}$$

Adaptation of (A.1) to nitrate:

$$(1 + \tau_L . p) . b_2 = d_{L2} + \tau_L . r_2 \qquad \text{(A.17)}$$

Adaptation of (A.1) to nitrite:

$$(1 + \tau_L . p) . b_3 = d_{L3} + \tau_L . r_3 \qquad \text{(A.18)}$$

Relation between rates of ammonia, nitrate and nitrite (A.13):

$$r_3 = \beta_1 . r_1 + \beta_2 . r_2$$

Cancelling the unknowns r_1, r_2 and r_3, the nitrite concentration at tank output, b_3, is a function of the ammonia, nitrate and nitrite concentrations at input of the tank (d_{L1},d_{G1},d_{L2} and d_{L3}, respectively), and of the ammonia and nitrate concentrations at output of the tank (b_1 and b_2, respectively) :

$$b_3 = s_2 - s_1 \qquad \text{(A.19)}$$

with $\quad s_2 = \beta_2 . b_2 + \frac{\beta_1 . \tau_L}{G_3} . \frac{1 + \tau_1 . p}{1 + \tau_L . p} . b_1$

$$s_1 = \frac{1}{1+\tau_L.p}.e$$

$$e = -d_{L3} + \beta_2.d_{L2} + \frac{\beta_1\tau_L}{G_3}\cdot(G_1.d_{L1} + G_2 d_{G1})$$

A.2. MODEL OF THE PREDICTOR 1

A.2.1 Introduction

According to the hypothesis of the predictor 1, the column is considered as only one tank in which the 2 bacteria strains are equally distributed throughout the volume of liquid. The corresponding model is a mere first order. Only 2 pairs of sensors of nitrate and ammonia are needed (1 at each end of the column).

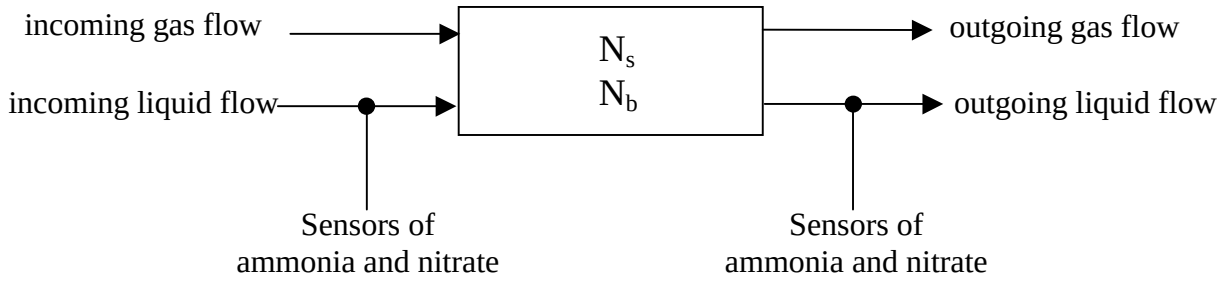


Figure A.2 : Simplified column for predictor 1
(N_s : Nitrosomonas; N_b : Nitrobacter)

A.2.2 Expression of the nitrite concentration

In the case of this predictor 1 where the variable χ (in A.6) is equal to 10^{-2} (Table A.1) and is negligible versus 1) the following simplification is legitimate:

$\tau_1 = \tau_L = \frac{V_L}{F_{in}}$ (F_{in} : 'fresh' incoming liquid flow rate defined in TN27.1)

So,

- taking into account the expressions of G_1, G_2 and G_3 in (A.4);
- considering that the variables q_L and q_G are, here, the incoming liquid and gas F_{in} and G_{in} defined in TN 27.1;
- using the notations d_{Lj0} to clearly indicate that these variables, where j = 1,2 or 3 for NH_3, NO_3^- and NO_2^-, represent the concentrations in the 'fresh' incoming liquid flow;
- assuming that the gas/liquid thermodynamic equilibrium of ammonia is reached in the 'fresh' incoming flow (i.e. $d_{G10} = \alpha \cdot d_{L10}$);

the expression of b3 in (A.19) becomes:

$$b_3 = s_2 - s_1 \qquad \text{(A.20)}$$

with $s_2 = \beta_1\left(1 + k + \alpha.\frac{G_{in}}{F_{in}}\right).b_1 + \beta_2.b_2$

$$s_1 = \frac{1}{1+\tau_L.p}.e$$

$$e = \beta_1\left(1 + k + \alpha.\frac{G_{in}}{F_{in}}\right).d_{L10} + \beta_2.d_{L20} + d_{L30}$$

$$\tau_L = \frac{V_L}{F_{in}}$$ V_L : liquid volume (without beads) of the column

Here is an equivalent expression of the nitrite concentration from (A.20) where the nitrite is assumed null in the 'fresh' incoming liquid flow ($d_{L30} = 0$) :

$$b_3 = \beta_1\left(1 + k + \alpha\frac{G_{in}}{F_{in}}\right)\cdot\left(b_1 - \frac{1}{1+\tau_L.p}.d_{L10}\right) + \beta_2\left(b_2 - \frac{1}{1+\tau_L.p}d_{L20}\right) \qquad \text{(A.21)}$$

where :

- d_{L10} and d_{L20} are, respectively, ammonia and nitrate concentrations in the (fresh' incoming liquid flow of the column (whose flow rate is F_{in});
- b_1 and b_2 are, respectively, ammonia and nitrate concentrations at output of the column.

A.2.3 Expression of the biomass concentration

Assuming, as for the nitrite predictor, that the gas/liquid thermodynamic equilibrium of ammonia is reached in the incoming flow (i.e. $d_{G10} = \alpha \cdot d_{L10}$) and taking into account (A.4) and (A.7), the expression of r_1 in (A.15) becomes :

$$r_1 = \frac{1}{\tau_L}\cdot\left(1 + k + \alpha\cdot\frac{G_{in}}{F_{in}}\right)\cdot\left((1+\tau_1\cdot p)\cdot b_1 - d_{L10}\right) \qquad \text{(A.22)}$$

In the same way as for the nitrite concentration : $\tau_1 = \tau_L = \frac{V_L}{F_{in}}$.

So, the expressions of the mean 'productive' biomass concentrations are :

$$c_{x1} = \delta_{11}.r_1 + \delta_{12}.r_2$$
$$c_{x2} = \delta_{21}.r_1 + \delta_{22}.r_2$$

where
$$r_1 = \frac{F_{in}}{V_L} \cdot \left(1 + k + \alpha \cdot \frac{G_{in}}{F_{in}}\right) \cdot \left(\left(1 + \frac{V_L}{F_{in}} \cdot p\right) \cdot b_1 - d_{L10}\right) \qquad (A.23)$$
$$r_2 = \frac{F_{in}}{V_L} \cdot \left(\left(1 + \frac{V_L}{F_{in}} \cdot p\right) \cdot b_2 - d_{L20}\right)$$

in which d_{L10}, d_{L20}, b_1 and b_2 have the same meaning as in (A.21).

A.3. MODEL OF THE PREDICTOR 2

A.3.1 Introduction

According to the hypothesis of the predictor 2, the column is assumed to be composed of 2 tanks in each of which the strains are equally distributed and at different concentrations (greater in the first tank than in the second one, generally). The corresponding model is a block of 2 successive predictors 1.

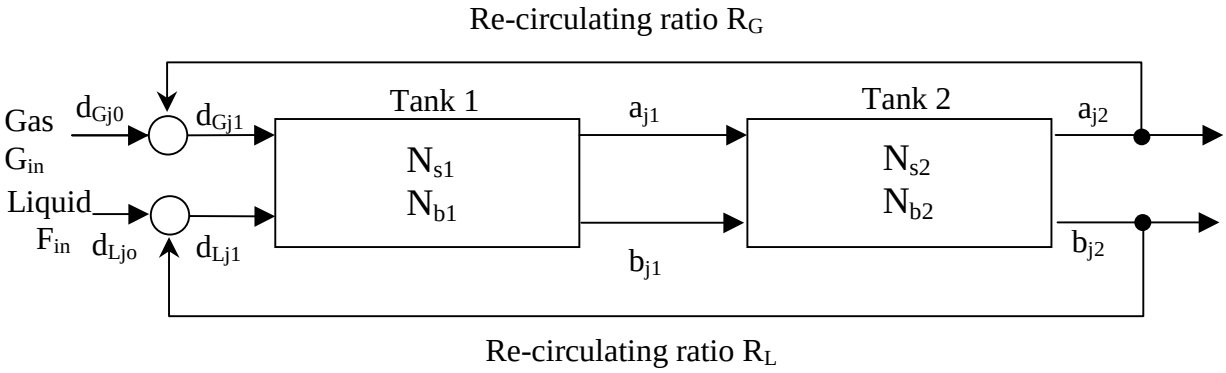


Figure A.3 : Simplified column for predictor 2
(N_s : Nitrosomonas; N_b : Nitrobacter)
Substrate j : NH_3, NO_3^- or NO_2^-

A.3.2 Expression of the nitrite concentration

Then the global model of the predictor 2 is composed of 2 predictors 1 put in series whose relation is deduced from (A.19) where the index i is associated to the tank i (i = 1 or 2) :

$$b_{3i} = s_{2i} - s_{1i} \qquad (A.24)$$

with
$$s_{2i} = \beta_2 \cdot b_{2i} + \frac{\beta_1 \cdot \tau_{Li}}{G_{3i}} \cdot \frac{1 + \tau_{1i}.p}{1 + \tau_{Li}.p} \cdot b_{1i}$$

$$s_{1i} = \frac{1}{1+\tau_{Li}.p} \cdot e_i$$

$$e_i = -d_{L3i} + \beta_2 \cdot d_{L2i} + \frac{\beta_1 \cdot \tau_{Li}}{G_{3i}} \cdot \left(G_{1i} \cdot d_{L1i} + G_{2i} \cdot d_{G1i}\right)$$

The time constants τ_{Li} and τ_{1i} are deduced from (A.1) and (A.6) :

$$\tau_{Li} = \frac{V_{Li}}{(1+R_L) \cdot F_{in}} \tag{A.25}$$

$$\tau_{1i} = \tau_{Li} \cdot \frac{1}{1+\frac{\alpha \cdot (1+R_G) \cdot G_{in}}{(1+k) \cdot (1+R_L) \cdot F_{in}}} \tag{A.26}$$

where :

- R_G and R_L are the volumetric gas and liquid flow rate ratios defined in TN27.1 ;
- G_{in} and F_{in} are the volumetric flow rates of the 'fresh' incoming gas and liquid defined in TN27.1.

The static gains G_{1i}, G_{2i} and G_{3i} are expressed in (A.4) taking into account the characteristics of each tank i.

The non measured input variables of (A.24) have the following expressions (from (A.27) to (A.30) :

$$d_{Lj1} = \frac{d_{Lj0} + R_L \cdot b_{j2}}{1+R_L} \tag{A.27}$$

where :

- j (j=1,2 or 3) is the index associated to the substrates NH_3, NO_3^- and NO_2^-, respectively ;
- R_L is the volumetric liquid flow rate ratio defined in TN27.1 ;
- b_{12} and b_{22} are the measurements of ammonia and nitrate at column output ;
- b_{32} is the estimation of nitrite at column output at previous moment ;
- d_{L10} and d_{L20} are measurements of ammonia and nitrate in the incoming liquid ;
- d_{L30} represents the nitrite concentration in the incoming liquid, if not null.

$$d_{Lj2} = b_{j1} \tag{A.28}$$

where :

- b_{11} and b_{21} are the measurements of ammonia and nitrate at tank 1 output ;
- b_{31} is the estimation of nitrite at tank 1 output at previous moment.

$$d_{G11} = \frac{d_{G10} + R_G \cdot a_{12}}{1 + R_G} \qquad (A.29)$$

where :

- R_G is the volumetric gas flow rate ratio defined in TN27.1 ;
- a_{12} is the estimation of ammoniac in gas phase at column output (in fact, it can be neglected versus ammoniac in the 'fresh' incoming gas flow d_{G10}) ;
- $d_{G10} = \alpha \cdot d_{L10}$ (the gas/liquid thermodynamic equilibrium of ammonia is assumed reached in the 'fresh' incoming flow).

$$d_{G12} = \alpha_{41} \, . \, b_{11} + \alpha_{51} \, . \, d_{G11} \qquad (A.30)$$

where :

- b_{11} is the measurement of ammonia at tank 1 output ;
- d_{G11} is given by (A.29) ;
- α_{41} and α_{51} are the coefficients of (A.3) adapted to the characteristics of tank 1.

A.3.3 Expression of the biomass concentration

For each tank i of the model of the predictor 2, the biomass concentrations c_{x1i} and c_{x2i} are obtained from the relations (A.14) and (A.15) adapted to any tank i :

$$c_{x1i} = \delta_{11} . r_{1i} + \delta_{12} . r_{2i}$$
$$c_{x2i} = \delta_{21} . r_{1i} + \delta_{22} . r_{2i}$$
$$\text{where} \quad r_{1i} = \frac{1}{G_{3i}} \cdot \left((1 + \tau_{1i} \cdot p) \cdot b_{1i} - G_{1i} \cdot d_{L1i} - G_{2i} \cdot d_{G1i} \right) \qquad (A.31)$$
$$r_{2i} = \frac{1}{\tau_{Li}} \cdot \left((1 + \tau_{Li} \cdot p) \cdot b_{2i} - d_{L2i} \right)$$

The unknown variables of this relation (A.31) has already been detailed in (A.27) to (A.30).

A.4. MODEL OF THE PREDICTOR 3

A.4.1 Introduction

In this case, the column is a combination of the 2 previous models. It is still parted into 2 tanks but the biomass is presumed to be present only in the first one and null in the second one. This hypothesis lies on the fact that, in the long run, the strains migrate towards the input of the column where the concentrations of substrates are the highest. The corresponding model is a second order. Only 2 sensors of nitrate and 2 ones of ammonia are needed (1 at each end of the column).

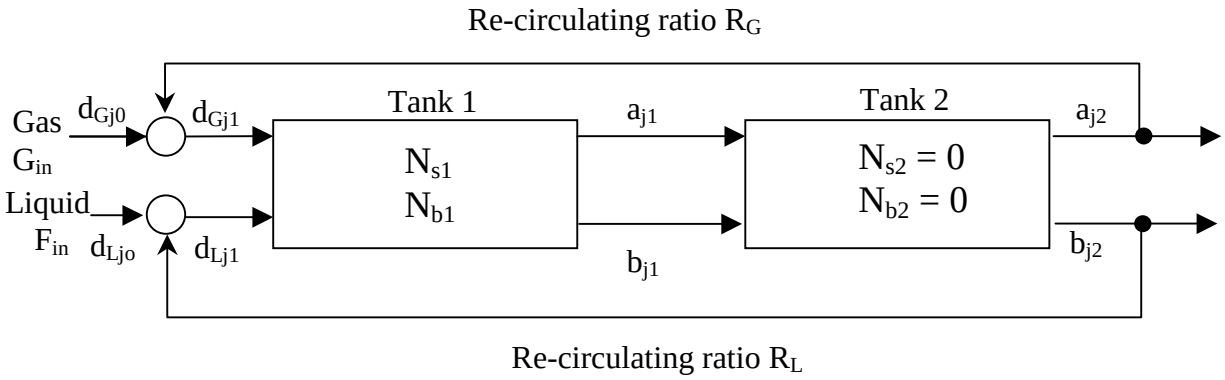


Figure A.4 : Simplified column for predictor 3
(N_s : Nitrosomonas; N_b : Nitrobacter)
Substrate j : NH_3, NO_3^- or NO_2^-

A.4.2 Expression of the nitrite concentration

So, the model of the predictor 3 is composed of the 2 following set of equations (A.32) and (A.33). The relation (A.32) is deduced from (A.24) only applied to the tank i = 1. The relation (A.33) traduces the dilution phenomenon in an ideally stirred tank for each compound j (j = 1 to 3 for the substrates NH_3, NO_3^- and NO_2^-, respectively).

$$b_{31} = s_{21} - s_{11} \tag{A.32}$$

with $$s_{21} = \beta_2 \cdot b_{21} + \frac{\beta_1 \cdot \tau_{L1}}{G_{31}} \cdot \frac{1+\tau_{11}.p}{1+\tau_{L1}.p} \cdot b_{11}$$

$$s_{11} = \frac{1}{1+\tau_{L1}.p} \cdot e_1$$

$$e_1 = -d_{L31} + \beta_2 \cdot d_{L21} + \frac{\beta_1 \cdot \tau_{L1}}{G_{31}} \cdot \left(G_{11} \cdot d_{L11} + G_{21} \cdot d_{G11}\right)$$

$$b_{j2} = \frac{1}{1+\tau_{L2} \cdot p} \cdot b_{j1} \qquad j = 1, 2 \text{ or } 3 \tag{A.33}$$

The non measured input variables of (A.32) have the same expressions as (A.27) to (A.30).

Cancelling the unknowns b_{j1} leads to :

$$z_1 + z_2 + z_3 = 0 \qquad \text{(A.34)}$$

where :

$$z_1 = -b_{32} + I_1 \cdot \left(\frac{1}{1+R_L} \cdot d_{L30} + \frac{R_L}{1+R_L} \cdot b_{32} \right)$$

$$z_2 = \beta_2 \cdot \left(b_{22} - I_1 \cdot \left(\frac{1}{1+R_L} \cdot d_{L20} + \frac{R_L}{1+R_L} \cdot b_{22} \right) \right)$$

$$z_3 = \frac{\beta_1 \cdot \tau_{L1}}{G_{31}} \cdot \left(I_2 \cdot b_{12} - I_1 \cdot G_{11} \cdot \left(\frac{1}{1+R_L} \cdot d_{L10} + \frac{R_L}{1+R_L} \cdot b_{12} \right) - I_1 \cdot G_{21} \cdot \left(\frac{1}{1+R_G} \cdot d_{G10} + \frac{R_G}{1+R_G} \cdot a_{12} \right) \right)$$

$$I_1 = \frac{1}{(1+\tau_{L1} \cdot p) \cdot (1+\tau_{L2} \cdot p)}$$

$$I_2 = \frac{(1+\tau_{11} \cdot p)}{(1+\tau_{L1} \cdot p)}$$

Assuming that, for ammonia, the liquid and gas phases have reached their thermodynamic equilibrium, in the incoming flow and at column output :
$d_{G10} = \alpha \cdot d_{L10}$ and $a_{12} = \alpha \cdot b_{12}$
and taking into account (A.7),
the expression of z_3 becomes :

$$z_3 = \frac{\beta_1 \cdot \tau_{L1}}{G_{31}} \cdot (I_2 \cdot b_{12} - I_1 \cdot (\xi \cdot d_{L10} - (1-\xi) \cdot b_{12})) \qquad \text{(A.35)}$$

with $\xi = G_{11} \cdot \frac{1}{1+R_L} + \alpha \cdot G_{21} \cdot \frac{1}{1+R_G}$

Given the following Laplace functions :

$$H_1 = \frac{I_1}{1+R_L \cdot (1-I_1)} \quad , \quad I_3 = \frac{I_2}{1+R_L \cdot (1-I_1)} \quad \text{and} \quad H_2 = \frac{1}{\xi} \cdot (I_3 - (1-\xi) \cdot H_1) - 1$$

the relation (A.34) leads to :

$$b_{32} = H_1 \cdot d_{L30} + \beta_2 \cdot (b_{22} - H_1 \cdot d_{L20}) + \frac{\beta_1 \cdot \tau_{L1} \cdot \xi \cdot (1+R_L)}{G_{31}} \cdot ((1+H_2) \cdot b_{12} - H_1 \cdot d_{L10}) \qquad \text{(A.36)}$$

$\Leftrightarrow$

$$b_{32} = H_1 \cdot e + \beta_2 \cdot b_{22} + \frac{\beta_1 \cdot \tau_{L1} \cdot \xi \cdot (1+R_L)}{G_{31}} \cdot (1+H_2) \cdot b_{12} \qquad \text{(A.37)}$$

with $e = d_{L30} - \beta_2 \cdot d_{L20} - \frac{\beta_1 \cdot \tau_{L1} \cdot \xi \cdot (1+R_L)}{G_{31}} d_{L10}$

and H_1 and H_2 detailed in (A.40) and (A.44) hereafter.

Expressions of the Laplace transfers H_1 and H_2

1. Expression of $Y = 1+R_L(1-I_1)$

In (A.34), I_1 is defined by :

$$I_1 = \frac{1}{(1+\tau_{L1} \cdot p) \cdot (1+\tau_{L2} \cdot p)}$$

So, it can be shown easily that Y is expressed by :

$$Y = \frac{(1+\theta_1 \cdot p) \cdot (1+\theta_2 \cdot p)}{(1+\tau_{L1} \cdot p) \cdot (1+\tau_{L2} \cdot p)} \qquad \text{(A.38)}$$

with

$$\theta_1 + \theta_2 = (1+R_L) \cdot (\tau_{L1} + \tau_{L2}) = \frac{V_L}{F_{in}}$$

$$\theta_1 \cdot \theta_2 = (1+R_L) \cdot \tau_{L1} \cdot \tau_{L2} = \frac{V_{L1} \cdot V_{L2}}{(1+R_L) \cdot F_{in}^2}$$

where V_{L1} and V_{L2} are the volumes of liquid (without beads) of the 2 tanks ($V_{L1} + V_{L2} = V_L$).
The full expression of θ_1 and θ_2 are :

$$\theta_1 \ , \ \theta_2 = \frac{V_L}{2 \cdot F_{in}} \cdot \left(1 \pm \sqrt{1 - \frac{4 \cdot V_{L1} \cdot V_{L2}}{(1+R_L) \cdot V_L^2}} \right) \qquad \text{(A.39)}$$

If $V_{L1} = V_{L2}$, then

$$\theta_1 \ , \ \theta_2 = \frac{V_L}{2 \cdot F_{in}} \cdot \left(1 \pm \sqrt{\frac{R_L}{(1+R_L)}} \right)$$

2. Expression of H_1

In (A.35), H_1 is defined by :

$$H_1 = \frac{I_1}{1+R_L \cdot (1-I_1)}$$

So, it comes immediately :

$$H_1 = \frac{1}{(1+\theta_1 \cdot p) \cdot (1+\theta_2 \cdot p)} \qquad \text{(A.40)}$$

3. Expression of I_3

In (A.35), I_3 is defined by :

$$I_3 = \frac{I_2}{1+R_L \cdot (1-I_1)}$$

So, it comes immediately :

$$I_3 = \frac{(1+\tau_{11}\cdot p)\cdot(1+\tau_{L2}\cdot p)}{(1+\theta_1\cdot p)\cdot(1+\theta_2\cdot p)}$$

4. Expression of H_2

In (A.35), H_2 is defined by :

$$H_2 = \frac{1}{\xi}\cdot(I_3 - (1-\xi)\cdot H_1) - 1$$

After developing H_2 with the expression of I_3 and H_1, it can be written as :

$$H_2 = \frac{1+S_n\cdot p + P_n\cdot p}{1+S_d\cdot p + P_d\cdot p} - 1$$

$$\text{with} \quad S_n = \frac{\tau_{11}+\tau_{L2}}{\xi} \qquad P_n = \frac{\tau_{11}\cdot\tau_{L2}}{\xi} \qquad (A.41)$$

$$S_d = \theta_1 + \theta_2 \qquad P_d = \theta_1\cdot\theta_2$$

Expression of S_n :

First, considering the definition of ξ in (A.35) and taking into account (A.4) :

$$\xi = \frac{1}{1+\chi}\cdot\left(\frac{1}{1+R_L} + \frac{\chi}{1+R_G}\right)$$

$$\xi = \frac{1+\chi_0}{(1+R_L)\cdot(1+\chi)}$$

$$\text{with} \qquad \chi = \frac{1+R_G}{1+R_L}\cdot\chi_0 \qquad \chi_0 = \frac{\alpha\cdot G_{in}}{(1+k)\cdot F_{in}} \qquad (A.42)$$

Then, considering (A.6), S_n becomes :

$$S_n = \tau_{L1}\cdot(1+R_L) + \tau_{L2}\cdot(1+R_L)\cdot(1+\chi)$$

$$S_n = S_d + \varepsilon_1 \qquad \text{with} \qquad \varepsilon_1 = \chi\cdot(1-\chi_0)\cdot\frac{V_{L2}}{F_{in}} - \chi_0\cdot\frac{V_L}{F_{in}} \qquad (A.43)$$

Expression of P_n :

In the same way,

$$P_n = (1+R_L)\cdot\tau_{L1}\cdot\tau_{L2}\cdot(1-\chi_0)$$

$$P_n = P_d + \varepsilon_2 \qquad \text{with} \qquad \varepsilon_2 = -\chi_0\cdot(1+R_L)\cdot\tau_{L1}\cdot\tau_{L2}$$

So, the expression of H_2 becomes :

$$H_2 = \frac{\varepsilon_1 \cdot p + \varepsilon_2 \cdot p^2}{(1+\theta_1 \cdot p)\cdot(1+\theta_2 \cdot p)}$$

$$\text{with} \quad \varepsilon_1 = \chi \cdot (1-\chi_0)\cdot \frac{V_{L2}}{F_{in}} - \chi_0 \cdot \frac{V_L}{F_{in}} \qquad (A.44)$$

$$\varepsilon_2 = -\chi_0 \cdot \frac{V_{L1} \cdot V_{L2}}{(1+R_L)\cdot F_{in}^2}$$

where V_{L1} and V_{L2} are the volumes of liquid (without beads) of the 2 tanks ($V_{L1} + V_{L2} = V_L$).

So, considering that

$$\frac{\tau_{L1} \cdot \xi \cdot (1+R_L)}{G_{31}} = 1 + k + \alpha \cdot \frac{G_{in}}{F_{in}} \qquad (A.45)$$

the concentration of the nitrite concentration is summed up from (A.36) where the nitrite is assumed to be null in the 'fresh' incoming flow :

$$b_{32} = \beta_1 \cdot \left(1 + k + \alpha \cdot \frac{G_{in}}{F_{in}}\right) \cdot \left((1+H_2)\cdot b_{12} - H_1 \cdot d_{L10}\right) + \beta_2 \cdot \left(b_{22} - H_1 \cdot d_{L20}\right) \qquad (A.46)$$

where :

- d_{L10} and d_{L20} are, respectively, ammonia and nitrate concentrations in the 'fresh' incoming liquid flow of the column whose flow rate is F_{in} ;
- b_{12} and b_{22} are, respectively, ammonia and nitrate concentrations at output of the column;
- H_1 and H_2 are detailed in (A.40) and (A.44).

Remark :
From this relation (A.46), it is immediately deduced that the static behaviour of the nitrite concentration is identical for each of the models of the predictors 1 and 3. This can be checked in the figure 5.

A.4.3 Expression of the biomass concentration

From the point of view of the biomass, the model of the predictor 3 is composed of the 2 following set of equations (A.47) and (A.48) . The relation (A.47) is deduced from (A.31) only applied to the tank i = 1. The relation (A.48) is identical to (A.33) and traduces the dilution phenomenon in a ideally stirred tank for each compound j (j = 1 to 2 for the substrates NH_3 and NO_3^- , respectively).

$$c_{x11} = \delta_{11}.r_{11} + \delta_{12}.r_{21}$$
$$c_{x21} = \delta_{21}.r_{11} + \delta_{22}.r_{21}$$

$$\text{where} \quad r_{11} = \frac{1}{G_{31}} \cdot \left((1+\tau_{11} \cdot p)\cdot b_{11} - G_{11} \cdot d_{L11} - G_{21} \cdot d_{G11}\right) \qquad (A.47)$$

$$r_{21} = \frac{1}{\tau_{L1}} \cdot \left((1+\tau_{L1} \cdot p)\cdot b_{21} - d_{L21}\right)$$

$$b_{j2} = \frac{1}{1+\tau_{L2}\cdot p}\cdot b_{j1} \qquad j = 1 \text{ or } 2 \tag{A.48}$$

The non measured input variables of (A.47) have the same expressions as (A.27) to (A.30).

Using ξ defined in (A.35) , it can be shown easily that :

$$r_{11} = \frac{\xi}{G_{31}}\cdot\left(\left(1+\frac{\tau_{11}+\tau_{L2}}{\xi}\cdot p+\frac{\tau_{11}\cdot\tau_{L2}}{\xi}\cdot p^2\right)\cdot b_{12} - d_{L10}\right)$$

$$r_{11} = \frac{F_{in}}{V_{L1}}\cdot\left(1+k+\alpha\cdot\frac{G_{in}}{F_{in}}\right)\cdot\left(\left(1+\omega_{11}\cdot p+\omega_{12}\cdot p^2\right)\cdot b_{12} - d_{L10}\right)$$

with
$$\omega_{11} = \frac{V_L}{F_{in}}\cdot\left(1+\chi\cdot\frac{V_{L2}}{V_L}\right)\cdot(1-\chi_0)$$
$$\omega_{12} = \frac{V_{L1}\cdot V_{L2}}{(1+R_L)\cdot F_{in}^2}\cdot(1-\chi_0) \tag{A.49}$$
$$\chi = \frac{1+R_G}{1+R_L}\cdot\chi_0 \qquad\qquad \chi_0 = \frac{\alpha\cdot G_{in}}{(1+k)\cdot F_{in}}$$

In the same way :

$$r_{21} = \frac{1}{\tau_{L1}}\cdot\left(\left(\frac{1}{1+R_L}+(\tau_{L1}+\tau_{L2})\cdot p+\tau_{L1}\cdot\tau_{L2}\cdot p^2\right)\cdot b_{22} - \frac{1}{1+R_L}\cdot d_{L20}\right)$$

$$r_{21} = \frac{F_{in}}{V_{L1}}\cdot\left(\left(1+\omega_{21}\cdot p+\omega_{22}\cdot p^2\right)\cdot b_{22} - d_{L20}\right)$$

with
$$\omega_{21} = \frac{V_L}{F_{in}} \tag{A.50}$$
$$\omega_{22} = \frac{V_{L1}\cdot V_{L2}}{(1+R_L)\cdot F_{in}^2}$$

<u>Recapitulation :</u>

The mean ‘productive’ biomass concentrations are given by :

$$c_{x1} = \frac{V_{L1}}{V_L}\cdot c_{x11}$$
$$c_{x2} = \frac{V_{L1}}{V_L}\cdot c_{x21}$$

with (A.51)

$$c_{x11} = \delta_{11}.r_{11} + \delta_{12}.r_{21}$$
$$c_{x21} = \delta_{21}.r_{11} + \delta_{22}.r_{21}$$

where r_{11} and r_{21} are expressed by (A.49) and (A.50).

The relations (A.49) , (A.50) and (A.51) of the predictor 3, when compared to the relation (A.23) of the predictor1, demonstrates that the mean growth rates of the total volume V_L are identical for these 2 predictors, in steady state running. And, as $\chi$and χ_0 are low versus 1, the dynamics of these 2 predictors are nearly identical : this can be checked in the figure 6. So the biomass predictors 1 and 3 are very close to each other.