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Memorandum of Understanding
ECT/FG/MMM/97.012

ESTEC/Contract N° 12924/98/NL/MV
Contract change notice No 04 of August 2002

TECHNICAL NOTE : 73.2

Release of the Nitrite estimator

Version : 1
Issue' : 0

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June 2003

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Document Change Log

Version	Issue	Date	Observation
0	0	April 2003	Draft
1	0	June 2003	Original version

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Abbreviations or notations:
NH_3 : ammonia (gaseous or solvated)
NO_2 : nitrite ion
NO_3 : nitrate ion
SO4 : sulphate ion
PO4 : phosphate ion
N_s : Nitrosomonas strain
N_b : Nitrobacter strain
solv. : solvated = molecular form (not total form)
PC : Personal Computer
PLC : Programmable Logical Computer
CST : Completely Stirred Tank

1. INTRODUCTION

In a previous study (TN 48.1), the nitrifying column was reduced to its fixed bed alone in order to simplify the internal model of the control. The advantage of this approach was that the state of the internal model was composed of the concentrations in the output flow (O_2, CO_2, NH_3, NO_2, NO_3, SO_4 and PO_4). Except NO_2 that was estimated, all the other concentrations can be measured. So the state was known at each sampling period of the control in a very simple way. But tests on simulator proved this model was too far from the process and cannot be used for the scenario on the forecast horizon of the control.

The approach is now to consider the column with its 3 parts A, B and C as described in the First Principles model built by LGCB. Then the state becomes much bigger (its size is multiplied by factor 3) : concentrations of O_2, CO_2, NH_3, NO_3, SO_4 and PO_4 at column output only (part C) can be measured and the other coefficients of the state corresponding to the part A and B have to be estimated.

Although the fixed bed of the column of the process is better represented with 2 CST's (TN 63.1 p.20 by LGCB), the fixed bed of the model is treated as only one CST (Completely Stirred Tank). The justification of this choice is given in annex 1.

So this study introduces 2 components of the estimator :

1. a component for estimation of NO2 in the part C and of biomass in the fixed bed;
2. another one for estimation of the state system for the control.

2. DESCRIPTION OF THE ESTIMATOR

2.1. Estimation of NO2 and biomass

The column can be represented by a series of 3 tanks ideally stirred where dynamic behaviour is described by a first order transfer (figure 1).

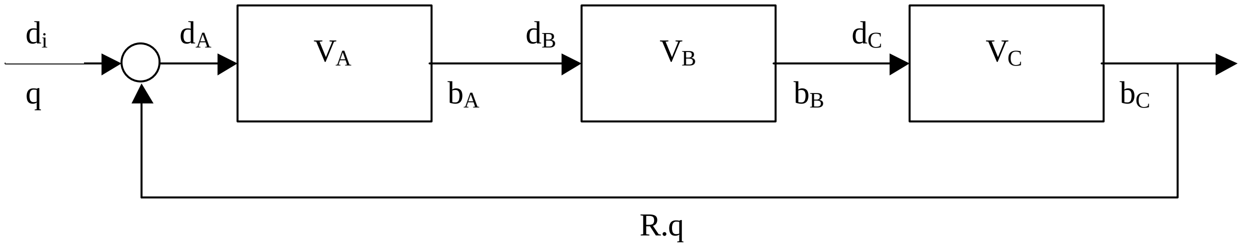

Figure 1 : Scheme of the column
A,B,C : indices of the 3 parts
d : concentration of a compound at input of a tank
d_i : concentration of a compound at input of the column
b : concentration of a compound at output of a tank
q : liquid flow rate
R : re-circulating ratio
V : volume

Given $\tau = \frac{V}{(1+R)\cdot q}$ the time constant of a tank of volume V where the flow is $(1+R)\cdot q$.

Given r the variation rate of a compound produced or consumed in a tank (in fact, only in tank B where the bacteria are fixed).

Using the Laplace transforms (variable p), the behaviour of any compound of the liquid phase is described by the following set of equations :

$$b = \frac{1}{1+\tau\cdot p}\cdot d + \tau\cdot r \qquad \text{(no indices, evolution in a tank A, B or C)}$$

$$\begin{aligned} d_A &= \frac{1}{1+R} d_i + \frac{R}{1+R}\cdot b_C \\ d_B &= b_A \\ d_C &= b_B \end{aligned} \tag{1}$$

Solving the system (1) leads to compute the roots ξ_1 , ξ_2 and ξ_3 of a third order polynomial whose coefficients are :

$$\begin{aligned} p_3 &= 1 \\ p_2 &= -\frac{(1+R)\cdot(\tau_A\cdot\tau_C + \tau_B\cdot\tau_A + \tau_C\cdot\tau_B)}{D} \\ p_1 &= \frac{(1+R)\cdot(\tau_A+\tau_B+\tau_C)}{D} \\ p_0 &= -\frac{1}{D} \\ \text{with}\quad D &= (1+R)\cdot(\tau_A\cdot\tau_B\cdot\tau_C) \end{aligned} \tag{2}$$

Then the output b_C can be expressed from the inputs d_i and r :

$$\begin{aligned} b_C &= \frac{1}{H}\cdot d_i + \frac{1+\tau_A\cdot p}{H}\cdot(1+R)\cdot\tau_B\cdot r \\ \text{with}\quad H &= (1+\xi_1\cdot p)\cdot(1+\xi_2\cdot p)\cdot(1+\xi_3\cdot p) \end{aligned} \tag{3}$$

As shown in annex 2, the transfer $\frac{1+\tau_A\cdot p}{H}$ can be approximated to a first order with time constant θ whose value has been identified such that $\theta\cdot q = 3.56$ l, which is slightly lower than the total volume of liquid of the column.

So, expression (3) becomes :

$$b_C = \frac{1}{H}\cdot d_i + \frac{1}{1+\theta\cdot p}\cdot(1+R)\cdot\tau_B\cdot r \tag{4}$$

This expression (4) is applied successively to NH_3 and NO_3 in order to estimate their variation rate from the measurements of their concentration at input and output of the column :

$$r = (1+\theta\cdot p)\cdot\frac{1}{(1+R)\cdot\tau_B}\cdot\left(b_C - \frac{1}{H}\cdot d_i\right) \tag{5}$$

In the case of NH_3, a corrective term is added to the measurement at column output, b_C, to take into account the gaseous NH_3 outgoing in the air flux and that is not measured. This corrective term comes from the First Principles model of the column.

Given r_1 and r_2, the variation rates of NH_3 and NO_3 respectively estimated by (5), the variation rate of NO_2 is given by the following relation previously established ((A.13) in TN 48.1) :

$$r_3 = \beta_1 \cdot r_1 + \beta_2 \cdot r_2 \qquad (6)$$

where β_1 and β_2 are function of the stoechiometry and limiting conc.

Then NO_2 concentration at column output, b_{C3}, can be estimated by 2 equivalent ways :

- with relation (4) where the input concentration d_i is zero (no NO_2 assumed at column input) :

$$b_{C3} = \frac{1}{1+\theta \cdot p} \cdot (1+R) \cdot \tau_B \cdot r_3 \qquad (7)$$

- or from relation (6) :

$$b_{C3} = \beta_1 \cdot b_{C1} + \beta_2 \cdot b_{C2} - \frac{1}{H} \cdot (\beta_1 \cdot d_{i1} + \beta_2 \cdot d_{i2}) \qquad (7bis)$$

where indices 1,2 and 3 are affected to NH_3, NO_3 and NO_2

For each strain k (k=1,2 for Nitrosomonas and Nitrobacter respectively), the biomass concentration c_{Xk} in the fixed bed is given by the following relation already established ((A.14) in TN 48.1) :

$$c_{Xk} = \delta_{k1} \cdot r_1 + \delta_{k2} \cdot r_2 \qquad (8)$$

where δ_{k1} and δ_{k2} are function of the stoechiometry and limiting factors

2.2. Estimation of the complete state of the internal model of the control

The estimation of the state of the internal model is based on the hypothesis that the concentration of all the compounds (except NO_2) in the incoming gas and liquid and in the outgoing liquid can be measured. However concerning compounds (such as SO4 and PO4) that are not limiting substrates and whose measurement could be difficult, it could be possible to replace their measure by a constant.

The estimation in part A is obtained by means of the measurements at input and output of the column and by means of the dilution model in this part A considered as a ideally stirred tank.

Two ways are possible for part B :

1. Starting from measurements at column output and using dilution model of part C to rebuilt the signals at input of C (which are the same as inside B);
2. Starting from estimations of part A and using dilution and chemical models of part B.

The first is the simplest and most robust.

So from system (1), the concentrations of a mono-phasis compound (NO_2, NO_3, SO_4, and PO_4) in the parts A and B are given by :

$$b_A = \frac{1}{1+\tau_A \cdot p} \cdot \left(\frac{1}{1+R} \cdot d_i + \frac{R}{1+R} \cdot b_C \right) \qquad (9)$$

$$b_B = (1+\tau_C \cdot p) \cdot b_C \qquad (9bis)$$

For the bi-phasis compounds (O_2, CO_2 and NH_3) :

- the variable d_i of (9) has to be replaced by the following expression established in TN44.2, (A2.7) :

  $$G_1 \cdot d_{Li} + G_2 \cdot d_{Gi} \qquad (10)$$

  where d_{Gi} and d_{Li} are concentrations in Gas and Liquid input flow

  where G_1 and G_2 are function of dissociation and Gas/Liquid equilibrium
- (9bis) should be replaced by a more complex relation where the concentration in the gas at input of B should be estimated. Now this estimation is not done to minimize the size of the estimated state vector. So the concentration is assumed zero. This assumption will over-estimate the concentration of O_2 mainly because it is the most important compound of the gas. Consequently it will affect the biomass estimation. Considering that O_2 is about 10^{-4} mol/l (instead of 2 10^{-4} mol/l, according to the estimation) and that the half saturation constants are 5.05 10^{-6} and 1.7 10^{-5} mol/l, this assumption implies an underestimation of about 3 and 8 % for the biomasses Ns and Nb respectively.

3. ROBUSTNESS

3.1. Introduction

The stability of the estimator has to be studied according to the noise on main measurements (O_2, NH_3, and NO3) and to the parameters of the model (dissociation constant, limiting concentrations, specific growth and maintenance rates, gas/liquid transfer Kla, gas/liquid equilibrium).

General description of the figures for each simulation :

Each simulation of the robustness study produces a group of 4 figures whose size has been reduced to save room. As some data overlap one another, here is a general description of the figures. All the abscissa represent the variation of the time from 0 to 20 h with an interval of 5 h.

1. The first of the 4 figures contains 5 graphs :
   - 3 graphs for NH3, NO3 and NO2 variation rates whose ranges are generally $[-8\ \ -4]*10^{-3}$, $[4\ \ 8]*10^{-3}$ and $[0\ \ 1]*10^{-3}$ mol/l/h, respectively.
   - 2 graphs for the concentration of Ns and Nb biomass whose ranges are generally [1 2] and [0.4 0.8] g/l, respectively.

   On this figure, from top to bottom :
   - NH_3 and NO_3 rates are deduced from their measurement with (5);
   - estimation rate of NO_2 at column output with (7);
   - estimation of biomass concentration with (8).

2. The 3 following figures are for concentration of some components (O2 solvated, CO2 solvated, NH3 solvated, NO2, NO3 and PO4) of parts A, B and C of the column, respectively. All these concentrations are expressed in mol/l and their general ranges are gathered in the table hereafter :

	O2 solv	**CO2 solv**	**NH3 solv**	**NO2**	**NO3**	**PO4**
part A	1.99 10^{-4}	[1 1.4] 10^{-3}	[2.8 3.2] 10^{-4}	[0 4] 10^{-4}	[1.9 2.1] 10^{-2}	1.56 10^{-3}

part B	$[1 \;\; 2]\ 10^{-4}$	$[1 \;\; 1.4]\ 10^{-3}$	$[0 \;\; 1]\ 10^{-4}$	$[0 \;\; 5]\ 10^{-4}$	$[2.2 \;\; 2.6]\ 10^{-2}$	$1.56\ 10^{-3}$
part C	$[1.85\ 1.95]\ 10^{-4}$	$1.2\ 10^{-3}$	$[0 \;\; 1]\ 10^{-4}$	$[0 \;\; 5]\ 10^{-4}$	$[2.2 \;\; 2.6]\ 10^{-2}$	$1.56\ 10^{-3}$

On these figures, the blue and red lines represent the process and the filtered estimation, respectively. The dephasing is precisely due to the low pass filter.

To illustrate numerically the study, a typical process, close to the pilot one, is chosen for simulation :

- input air flow : G_{in} = 60 l/h;
- input liquid flow F_{in} = 0.4 l/h;
- gas re-circulating ratio R_G = 0;
- liquid re-circulating ratio R_L = 6;
- 2 CST's for the fixed bed of the process . The value of 2 CST's, that comes from TN 63.1, p.20 by LGCB, corresponds in the best way to G_{in} = 60 l/h and $(1+ R_L)* F_{in}$ = 2.8 l/h.
- high load of ammonia (10^{-2} mol/h) to have to most difficult condition for estimation;
- 50 % increase step of flow at time t=0.2 h;
- all the other specifications of the simulation (pH, temperature, concentrations …) are defined in the initializing files 'i_sim.m' and 'i_sim_3.m' of annex 3 of TN 73.1 .

The figure 2 shows that for the reference simulation with no noise and no parameter mismatch, NO_2 is correctly estimated but the biomass is under-estimated : a bias of about 6 % for Ns and 30 % for Nb.

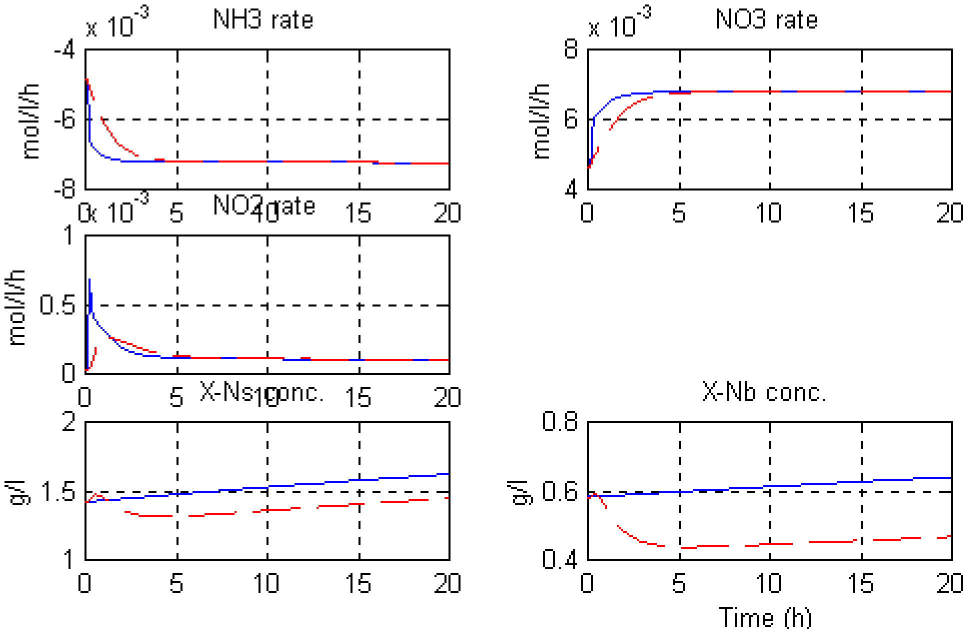

Figure 2 : Comparison estimation versus process
Top graphs : NH3 and NO3 variation rates estimated with relation (5)
Middle graph : NO2 variation rate estimated with relation (7)
Bottom graphs : Nitrosomonas and Nitrobacter biomass with (8)
Process : continuous blue line - Estimation : dotted red line

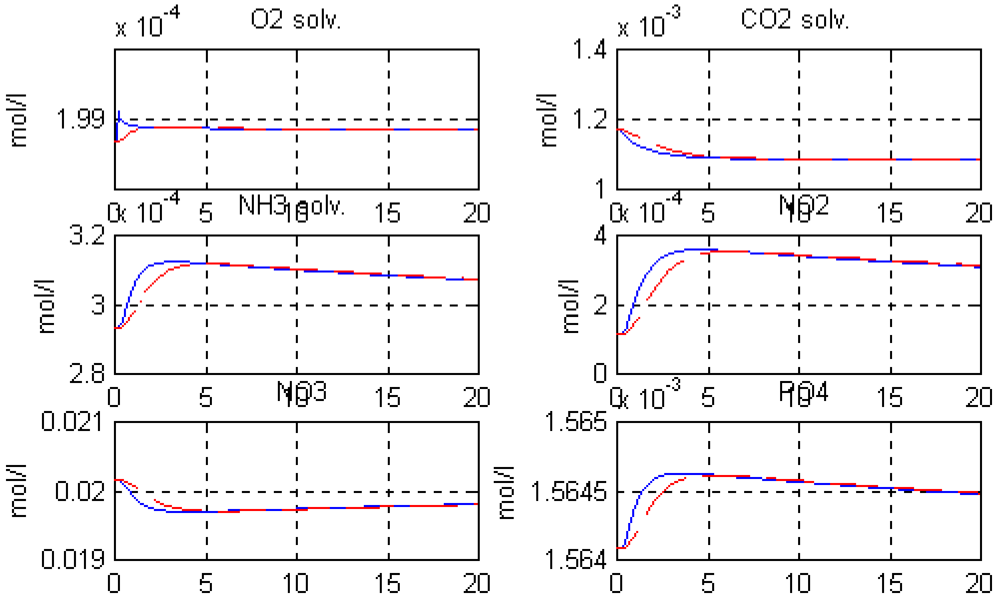

Figure 3 : Comparison of the estimated state versus the process one for part A
Process : continuous blue line. Estimation : dotted red line

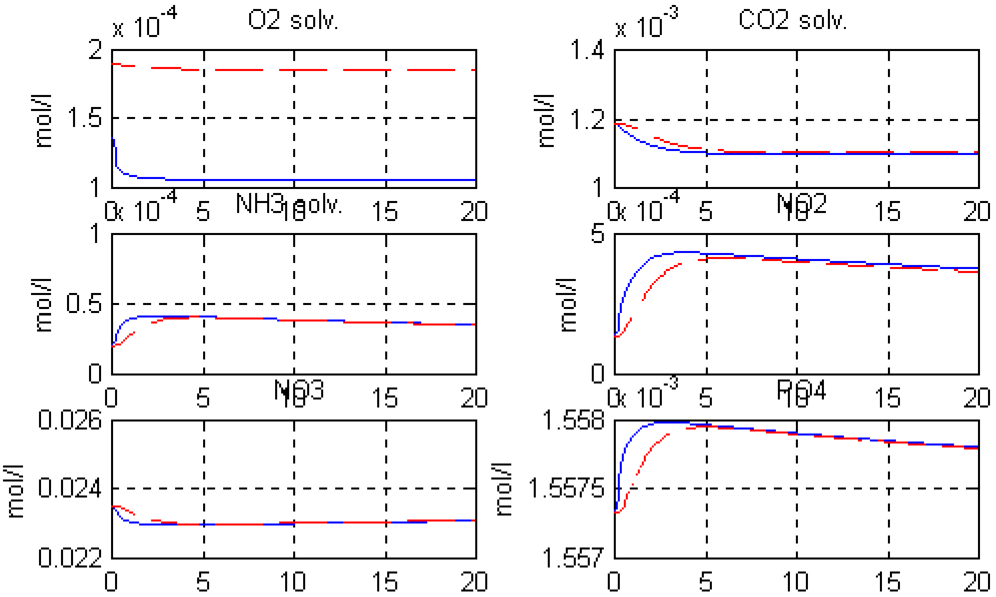

Figure 4 : Comparison of the estimated state versus the process one for part B
Process : continuous blue line. Estimation : dotted red line

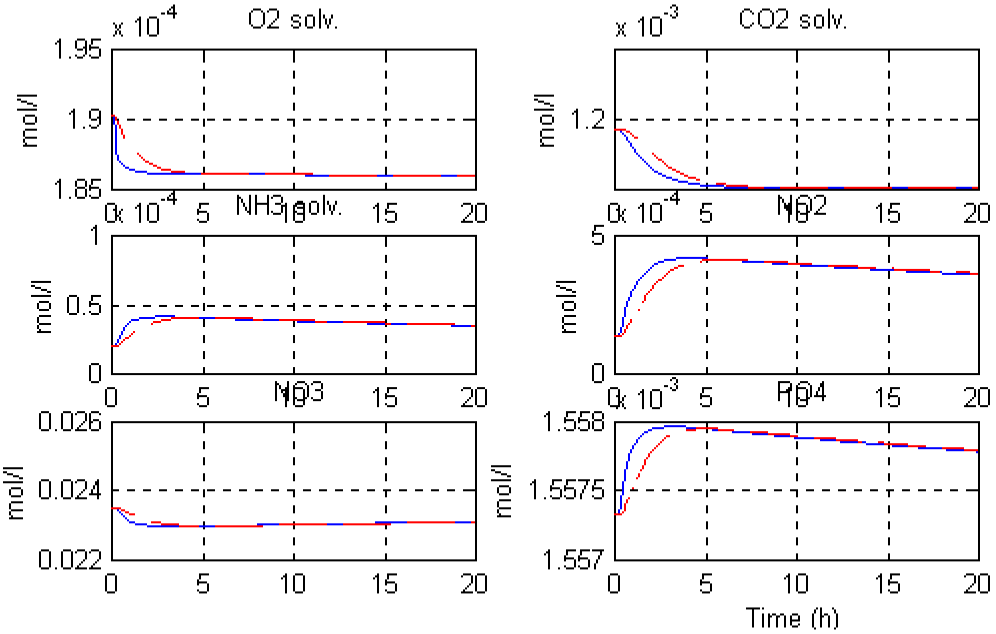

Figure 5 : Comparison of the estimated state versus the process one for part C
Process : continuous blue line. Estimation : dotted red line

3.2. Noise on NH_3 and NO_3 measurements

The measurements are filtered with a low pass filter as it is explained in TN 73.1 .
In the simulation of figure 6 to 9, a white noise has been added on NH_3 and NO_3 measurements at column output with a standard deviation of 10^{-4} mol/l (about 0.5 % of the mean signal). As foreseen by relations (6) and (7bis), the noise on NO_2 estimation is high : on NO_2 concentration at column output it is about 5 10^{-5} mol/l (10 % of the mean value). Simulations show that a noise ten times as high on NH_3 and NO_3 measurements is unacceptable.

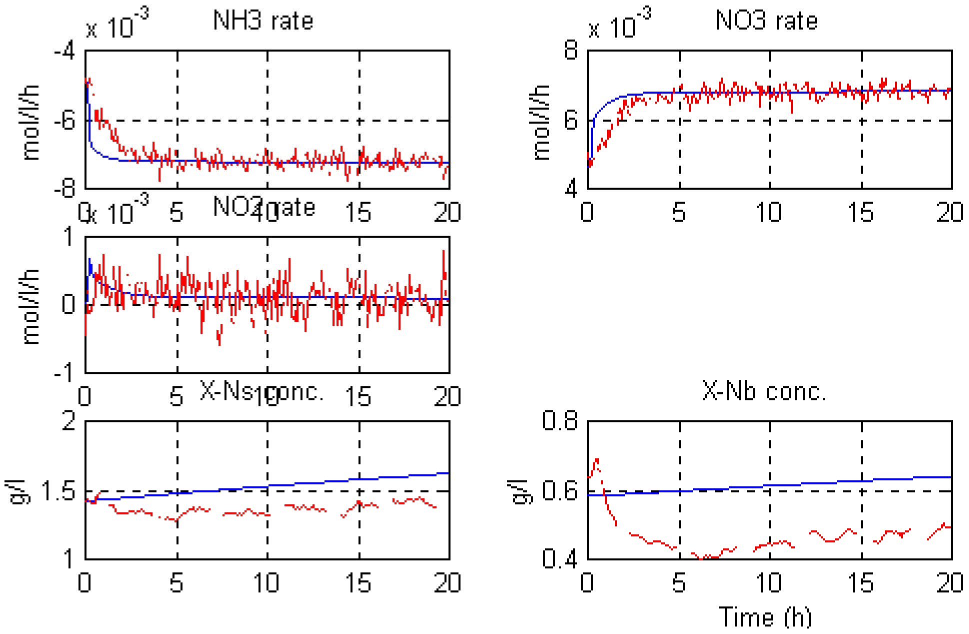

Figure 6 : Comparison estimation versus process (noise on NH3 and NO3)
Top graphs : NH3 and NO3 variation rates estimated with relation (5)
Middle graph : NO2 variation rate estimated with relation (7)
Bottom graphs : Nitrosomonas and Nitrobacter biomass with (8)
Process : continuous blue line - Estimation : dotted red line

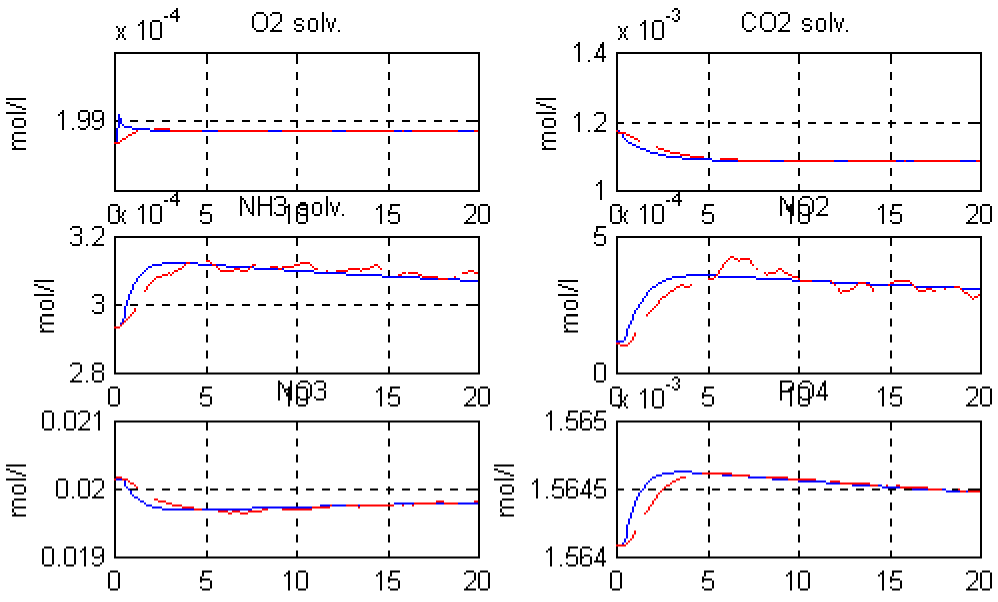

Figure 7 : Comparison estimation versus process (noise on NH3 and NO3) for part A
Process : continuous blue line. Estimation : dotted red line

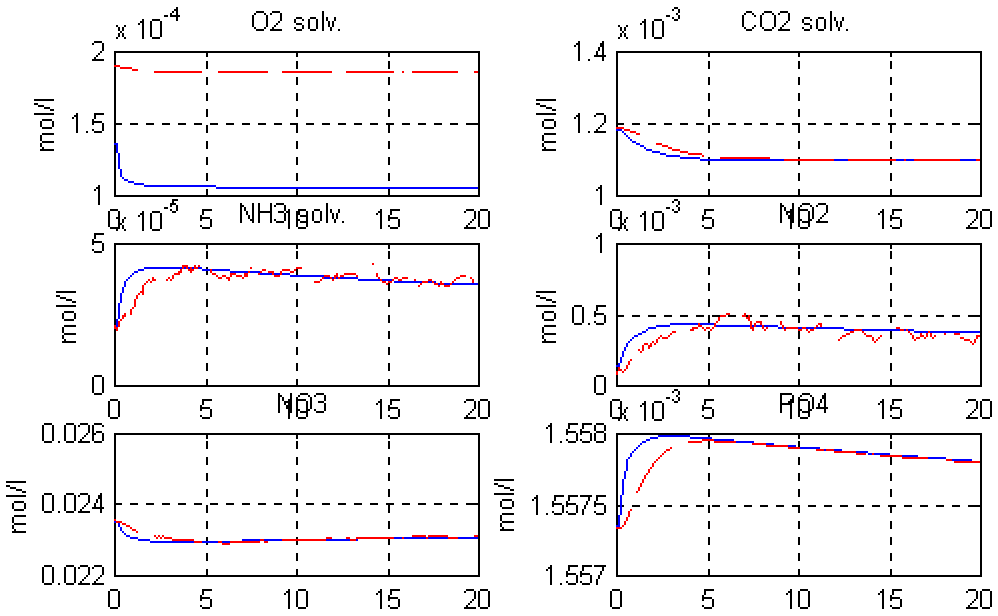

Figure 8 : Comparison estimation versus process (noise on NH3 and NO3) for part B
Process : continuous blue line. Estimation : dotted red line

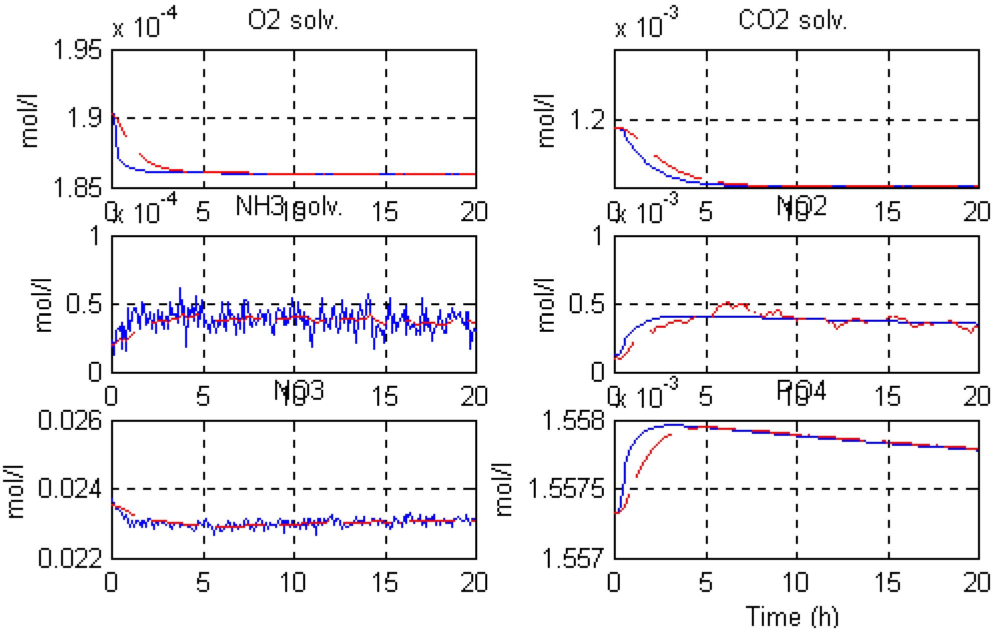

Figure 9 : Comparison estimation versus process (noise on NH3 and NO3) for part C
Process : continuous blue line. Estimation : dotted red line

3.3. Noise on O_2 measurement

The results of figure 10 to 13 show that a noise whose relative standard deviation is about 5 % (% compared to the mean signal) on O_2 in the liquid at column output is quite bearable.

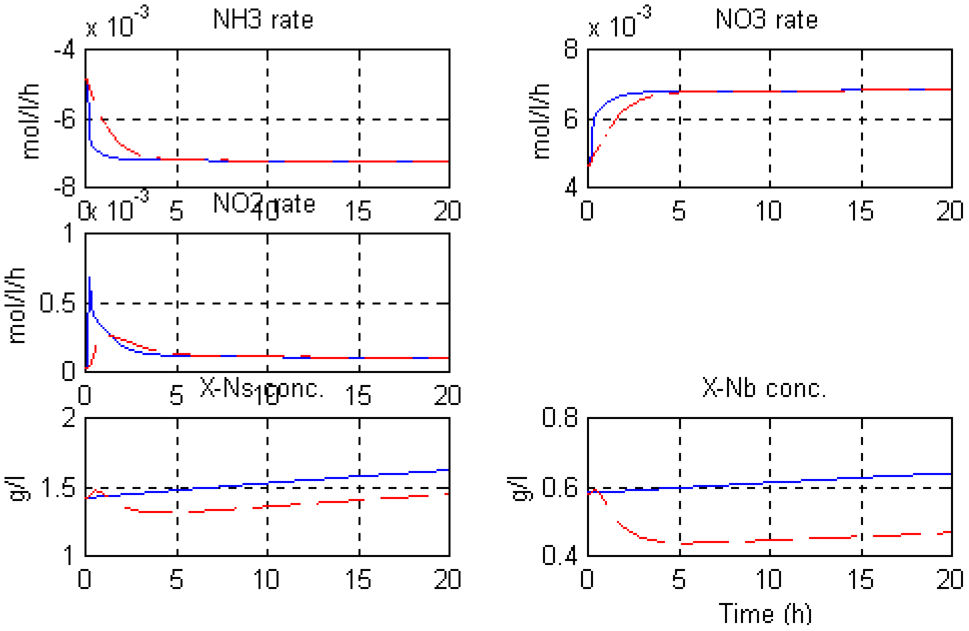

Figure 10 : Comparison estimation versus process (noise on O2)
Top graphs : NH3 and NO3 variation rates estimated with relation (5)
Middle graph : NO2 variation rate estimated with relation (7)
Bottom graphs : Nitrosomonas and Nitrobacter biomass with (8)
Process : continuous blue line - Estimation : dotted red line

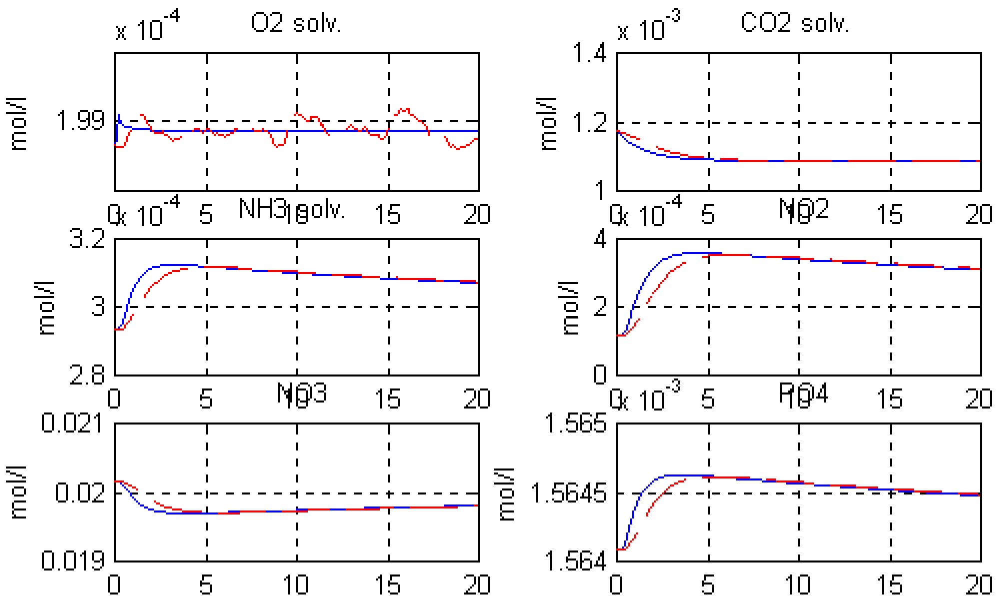

Figure 11 : Comparison estimation versus process (noise on O2) for part A
Process : continuous blue line. Estimation : dotted red line

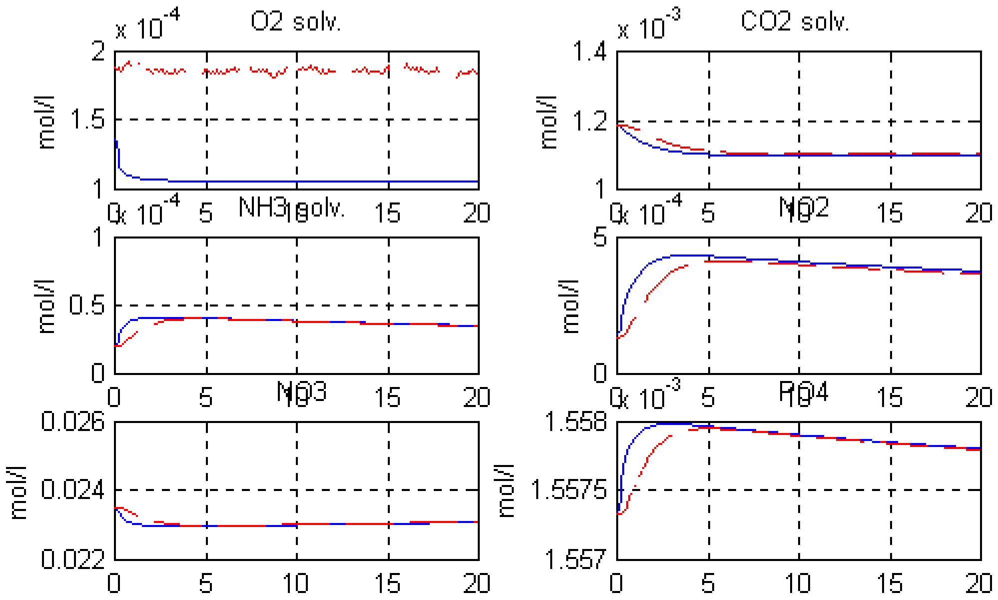

Figure 12 : Comparison estimation versus process (noise on O2) for part B
Process : continuous blue line. Estimation : dotted red line

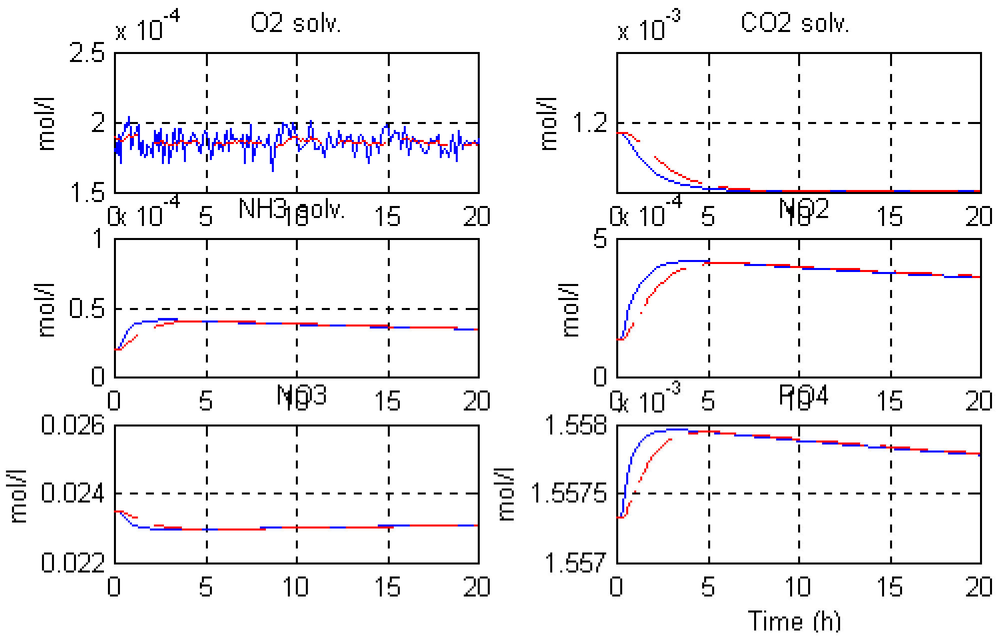

Figure 13 : Comparison estimation versus process (noise on O2) for part C
Process : continuous blue line. Estimation : dotted red line

3.4. Mismatch on dissociation constant of NH_3

As the concentration of NH3 in the output gas flow is low, it is not measured and the quantity of this compound that is extracted from the column by this way is simply approximated by the formula (relation (A2.10) in TN 44.2) :

$$db_C = b_C \cdot \frac{\alpha \cdot K}{K + \alpha \cdot \frac{G_{in}}{V_C}} \cdot \frac{G_{in}}{F_{in}} \cdot \frac{1}{1+k} \qquad (11)$$

with db_C : quantity of NH3 extracted in the gas expressed in mol/l in the liquid
b_C : conc. in the liquid output stream
α : liquid/gas thermodynamical equilibrium constant of NH3
K : liquid/gas transfer parameter (KLa)
G_{in} : input gas flow rate
F_{in} : input liquid flow rate
k : dissociation constant

The sensitivity of the NO_2 and biomass estimations versus the dissociation constant k are given by (A3.18) and (A3.20) recalled hereafter :

$$\frac{\delta b_{C3}}{b_{C3}} = 0.1 \cdot \frac{\delta k}{k} \qquad (12)$$

and

$$\frac{\delta c_{Xk}}{c_{Xk}} = a_k \cdot \frac{\delta k}{k} \qquad (13)$$

$$\begin{aligned} a_k &\leq 0.04 \quad \text{for } k = 1 \text{ (Nitrosomonas)} \\ &= 0 \quad \text{for } k = 2 \text{ (Nitrobacter)} : \delta_{k1} = 0 \end{aligned}$$

These relations show that the estimations are very little sensitive to the dissociation constant k. This is illustrated on the figure 14 to 17 where the dissociation constant of the estimator is 10 % higher than the dissociation constant of the process.

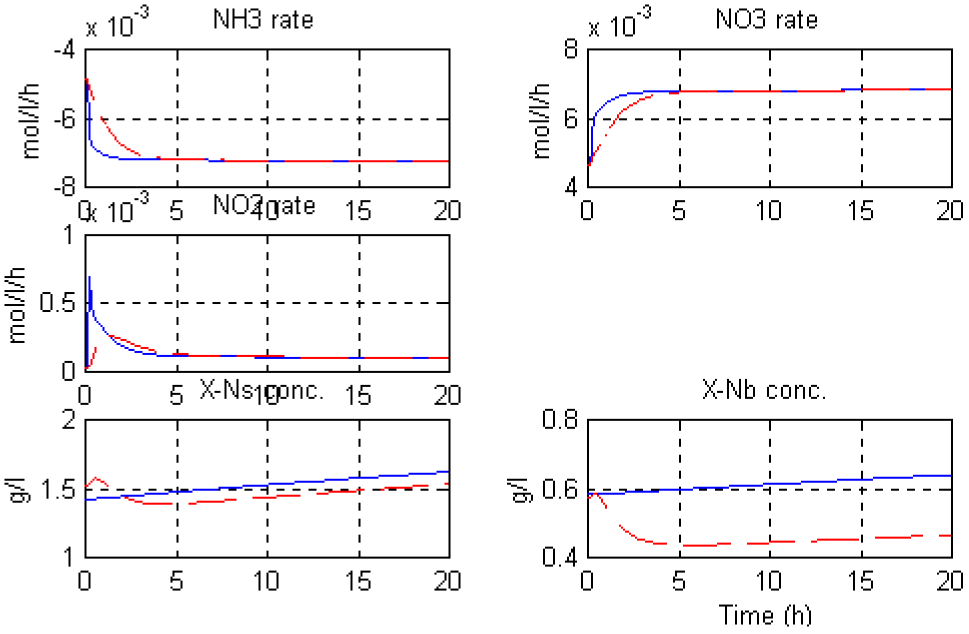

Figure 14 : Comparison estimation versus process (mismatch on dissociation)
Top graphs : NH3 and NO3 variation rates estimated with relation (5)
Middle graph : NO2 variation rate estimated with relation (7)
Bottom graphs : Nitrosomonas and Nitrobacter biomass with (8)
Process : continuous blue line - Estimation : dotted red line

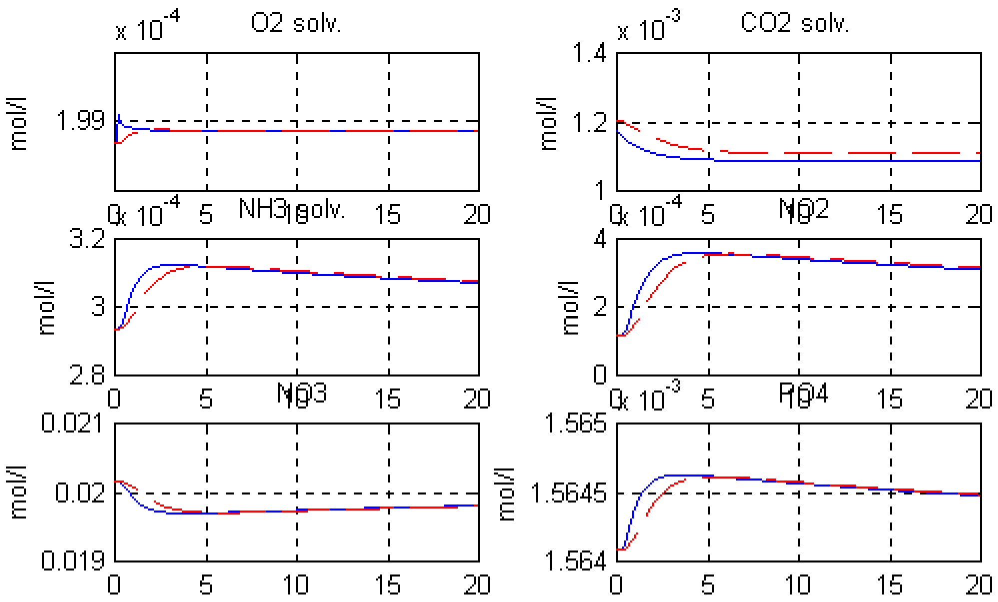

Figure 15 : Comparison estimation versus process (mismatch on dissociation) for part A
Process : continuous blue line. Estimation : dotted red line

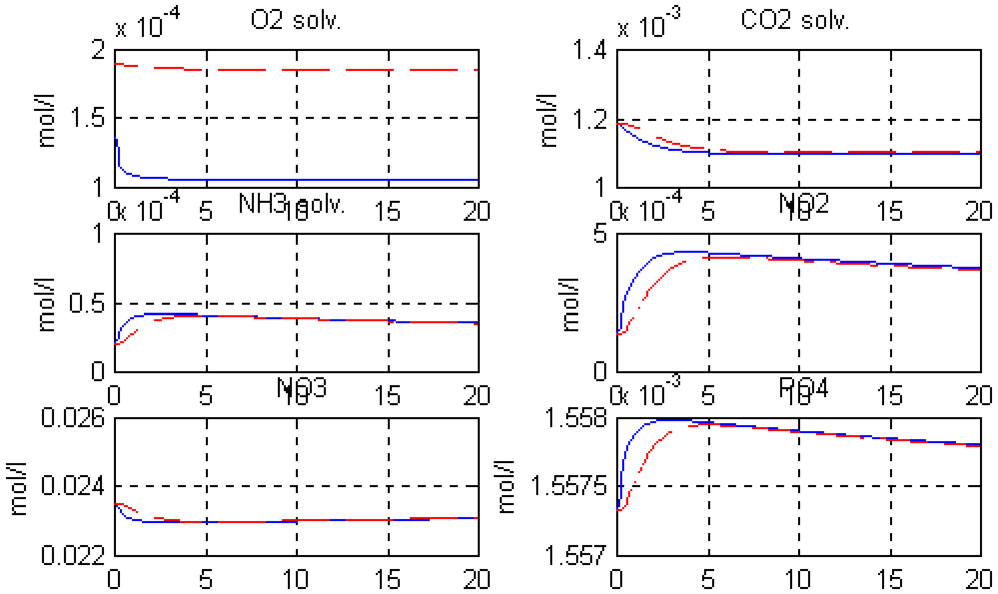

Figure 16 : Comparison estimation versus process (mismatch on dissociation) for part B
Process : continuous blue line. Estimation : dotted red line

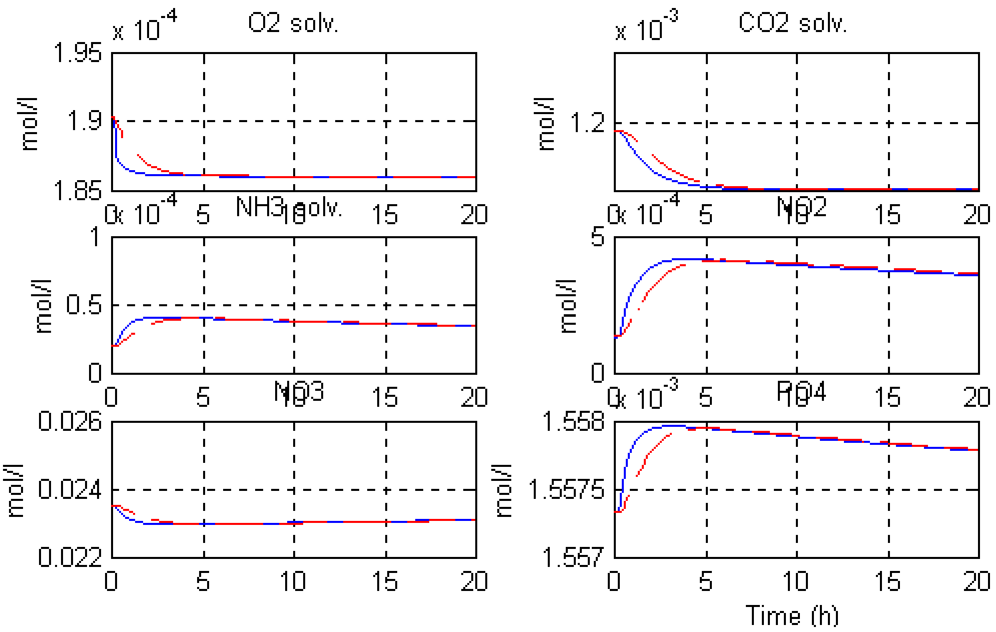

Figure 17 : Comparison estimation versus process (mismatch on dissociation) for part C Process : continuous blue line. Estimation : dotted red line

3.5. Mismatch on limiting concentrations

The sensitivity of the active biomass regarding the limiting concentrations is given by (A3.28) recalled hereafter :

$$\frac{\delta C_{Xk}}{C_{Xk}} = \sum_i \frac{K_{Ski}}{K_{Ski} + S_i} \cdot \frac{\delta K_{Ski}}{K_{Ski}} \qquad (14)$$

In the following simulation, the Nitrosomonas limiting concentrations of the internal model are 50 % higher than those of the process.

The numerical values of the terms $\frac{K_{Ski}}{K_{Ski} + S_i}$ for the limiting substrates O_2 and NH_3 are 0.02 and 0.67

$\Rightarrow \frac{\delta C_{Xk}}{C_{Xk}} = 0.34$, which means that the Ns biomass estimation is increased of 34 %. This can be observed in fig.18 compared to fig.2.

It can be noted that the limiting concentrations have no influence on the estimation of NO_2 (fig. 21).

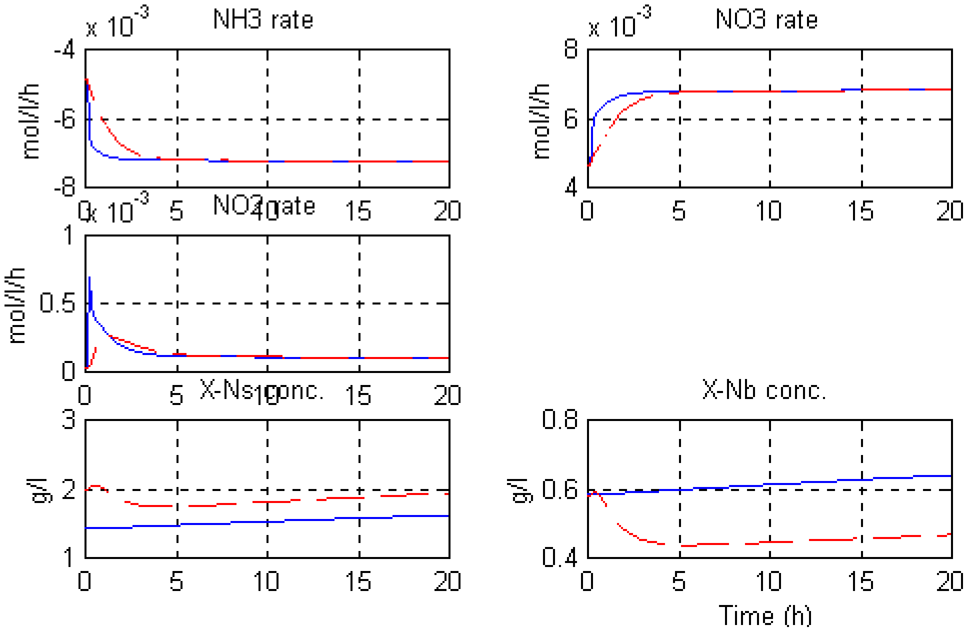

Figure 18 : Comparison estimation versus process (mismatch on limiting conc.)
Top graphs : NH3 and NO3 variation rates estimated with relation (5)
Middle graph : NO2 variation rate estimated with relation (7)
Bottom graphs : Nitrosomonas and Nitrobacter biomass with (8)
Process : continuous blue line - Estimation : dotted red line

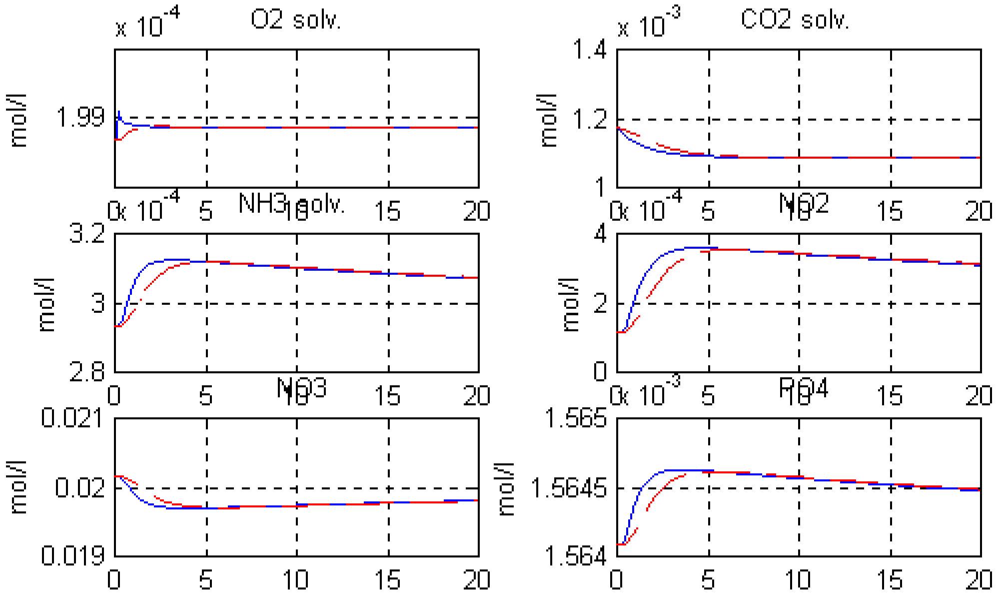

Figure 19 : Comparison estimation versus process (mismatch on limiting conc.) part A
Process : continuous blue line. Estimation : dotted red line

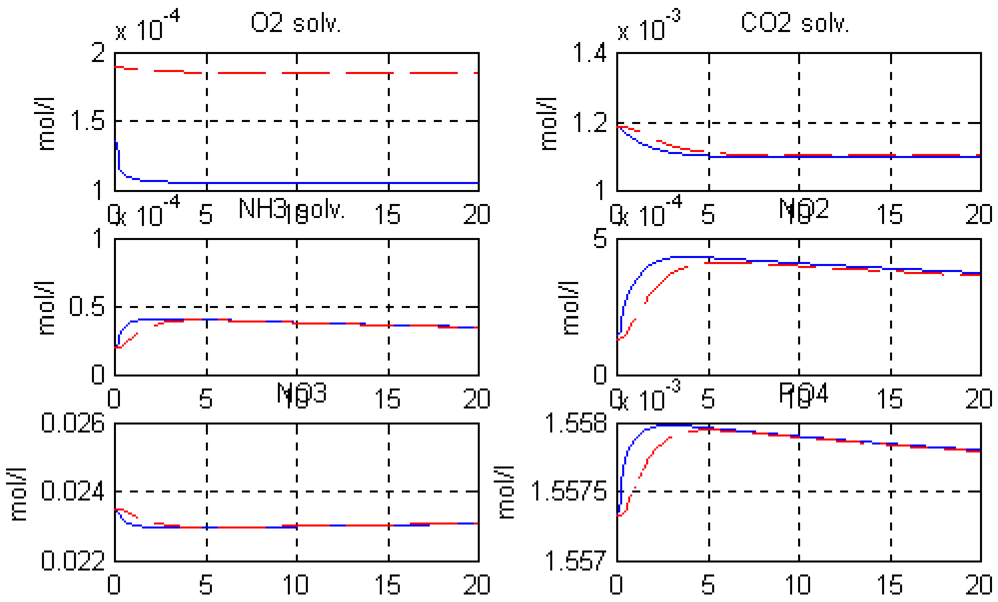

Figure 20 : Comparison estimation versus process (mismatch on limiting conc.) part B
Process : continuous blue line. Estimation : dotted red line

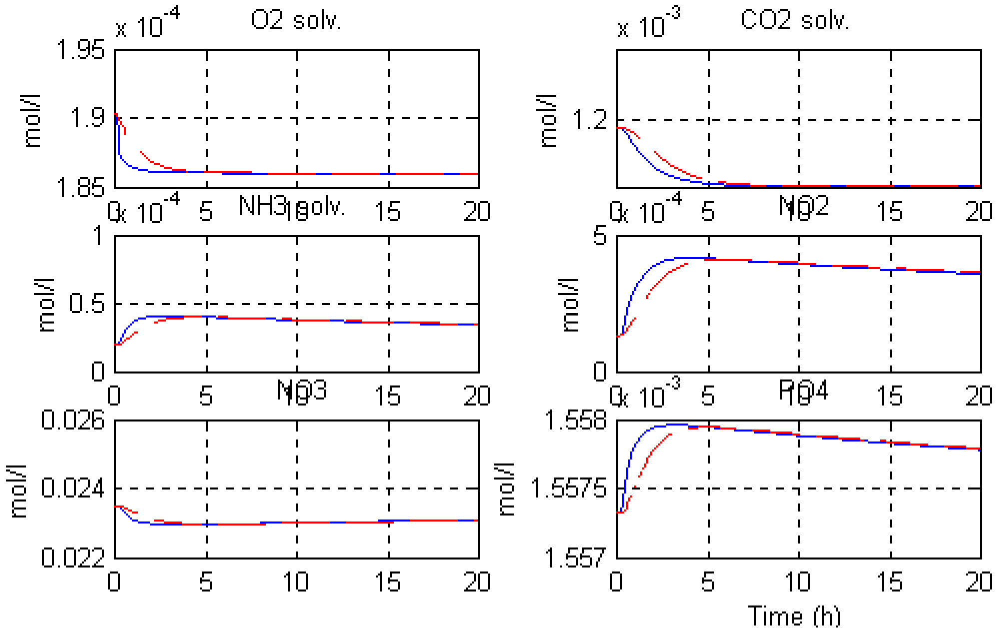

Figure 21 : Comparison estimation versus process (mismatch on limiting conc.) part C
Process : continuous blue line. Estimation : dotted red line

3.5. Mismatch on specific growth and maintenance rates

At steady state, the sensitivity of NO_2 estimation, δb_3 (otherwise δb_C) , versus the specific growth and maintenance rates is expressed in (A3.11) of annex 3 and recalled hereafter :

$$\delta b_3 = d_{i1} \cdot \left(s_1 \cdot \left(-\frac{\delta\mu_1}{\mu_1} + \frac{\delta m_1}{m_1} \right) + s_2 \cdot \left(\frac{\delta\mu_2}{\mu_2} - \frac{\delta m_2}{m_2} \right) \right)$$

with :

$$s_1 = \varepsilon_1 \cdot \left(1 - \frac{Y_{x1(3,1)} \cdot \mu_1}{\sigma_{11}} \right) = \varepsilon_1 \cdot \frac{Y_{m1(3,1)} \cdot m_1}{\sigma_{11}}$$

$$\varepsilon_1 = \frac{\left(Y_{x1(3,1)} + Y_{x1(4,1)} \right) \cdot \mu_1}{\sigma_{11}} \qquad (15)$$

$$s_2 = \varepsilon_2 \cdot \left(\frac{Y_{x1(3,2)}}{\sigma_{12}} - \frac{Y_{x1(5,2)}}{\sigma_{22}} \right) \cdot \mu_2 = -\varepsilon_2 \cdot \left(\frac{Y_{m1(3,2)}}{\sigma_{12}} - \frac{Y_{m1(5,2)}}{\sigma_{22}} \right) \cdot m_2$$

$$\varepsilon_2 = \frac{\sigma_{12}}{\sigma_{22}}$$

where : μ_1 is the specific growth rate of Ns

μ_2 is the specific growth rate of Nb

m_1 is the specific maintenance rate of Ns

m_2 is the specific maintenance rate of Nb

d_{i1} : NH_3 concentration at column input

$\sigma_{11}, \sigma_{12}, \sigma_{22}$ expressed in (A.11) of TN 48.1

Y_{x1}, Y_{m1} : stoechiometric ratios

In the present example where di1=0.025 mol/l of total ammonia and according to this relation (15), a 10 % increase on specific growth rates μ_1 and μ_2 implies an underestimation of NO_2 of $0.2\ 10^{-4}$ mol/l . This is confirmed in fig. 25 compared to fig.5 .
It could be checked by simulation that a 10 % increase on specific growth and maintenance rates μ_1 and m_1 simultaneously has no effect on NO_2 estimation as given by (15).

The sensitivity of c_s and c_b can is expressed in (A3.15) and is recalled hereafter :

$$\frac{\delta c_s}{c_s} = -0.8 \cdot \frac{\delta\mu_1}{\mu_1} - 0.2 \cdot \frac{\delta m_1}{m_1}$$

$$\frac{\delta c_b}{c_b} = -0.7 \cdot \frac{\delta\mu_2}{\mu_2} - 0.3 \cdot \frac{\delta m_2}{m_2} \qquad (16)$$

It can be checked in fig.22 (compared to fig.2) that a 10 % increase on specific growth rates μ_1 and μ_2 implies an underestimation of c_s and c_b of about 8 %.

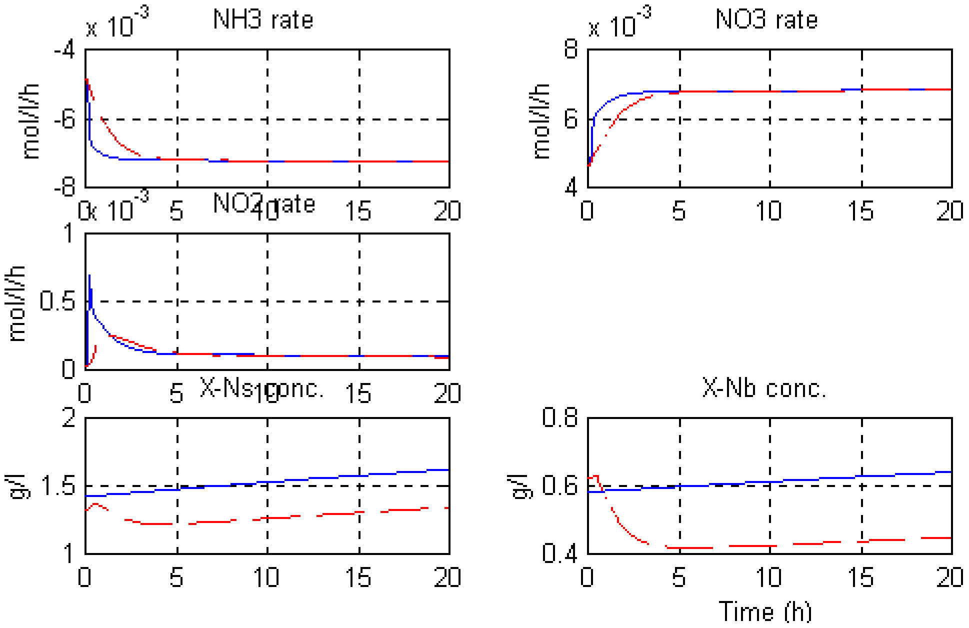

Figure 22 : Comparison estimation versus process (mismatch on growth)
Top graphs : NH3 and NO3 variation rates estimated with relation (5)
Middle graph : NO2 variation rate estimated with relation (7)
Bottom graphs : Nitrosomonas and Nitrobacter biomass with (8)
Process : continuous blue line - Estimation : dotted red line

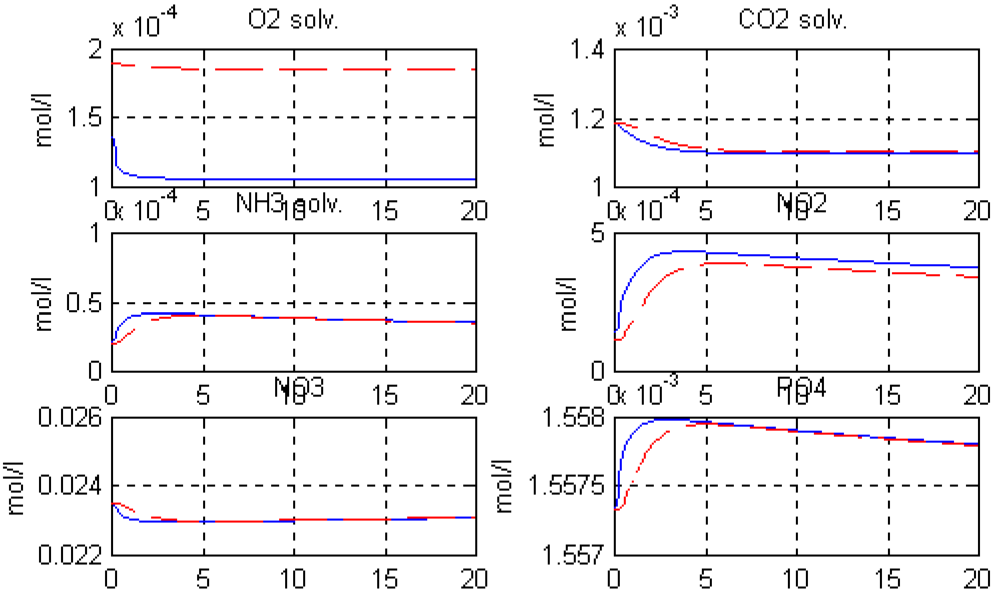

Figure 23 : Comparison estimation versus process (mismatch on growth) part A
Process : continuous blue line. Estimation : dotted red line

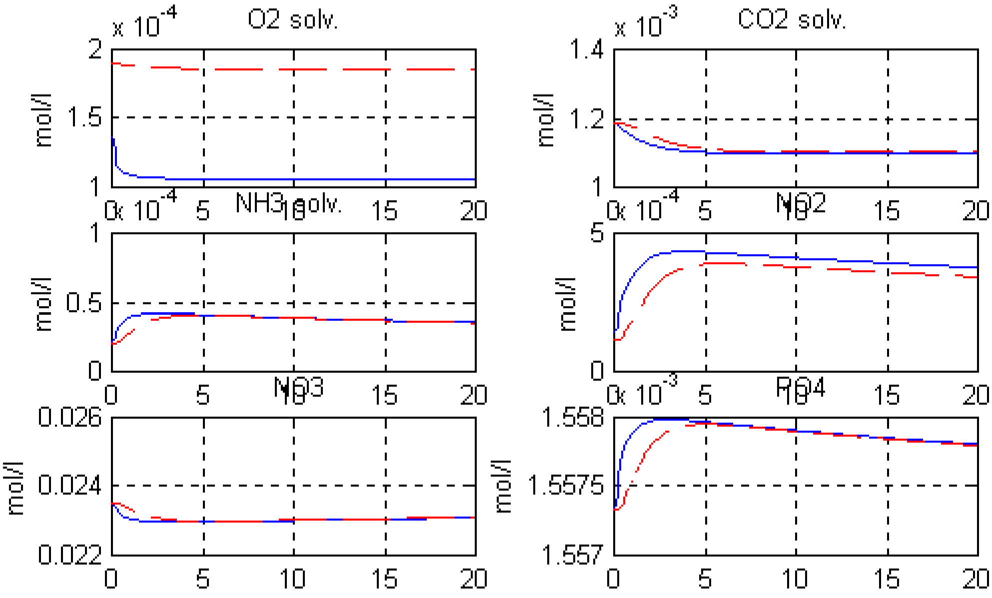

Figure 24 : Comparison estimation versus process (mismatch on growth) part B
Process : continuous blue line. Estimation : dotted red line

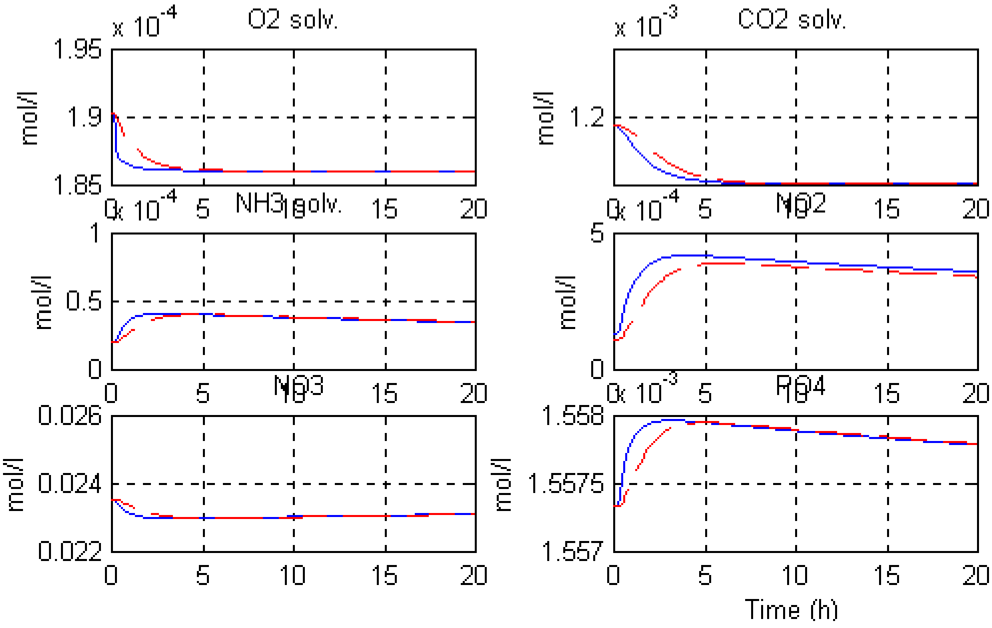

Figure 25 : Comparison estimation versus process (mismatch on growth) part C
Process : continuous blue line. Estimation : dotted red line

3.5. Mismatch on the gas/liquid transfer Kla

The sensitivity of the NO_2 and biomass estimations versus K are given by (A3.22) and (A3.23) recalled hereafter :

$$\frac{\delta b_{C3}}{b_{C3}} = -10^{-3} \cdot \frac{\delta K}{K} \qquad (17)$$

and

$$\frac{\delta c_{Xk}}{c_{Xk}} = a_k \cdot \frac{\delta K}{K} \tag{18}$$

$$-3\cdot 10^{-4} \le a_k \le 0 \quad \text{for } k = 1 \text{ (Nitrosomonas)}$$

$$a_k = 0 \quad \text{for } k = 2 \text{ (Nitrobacter)} : \delta_{k1} = 0$$

These relations show that the estimations are very little sensitive to the gas/liquid transfer K. This is illustrated on the figure 26 to 29 where a reduction by half of the value of KLa in the estimator has a small consequence on the NO_2 and biomass estimations.

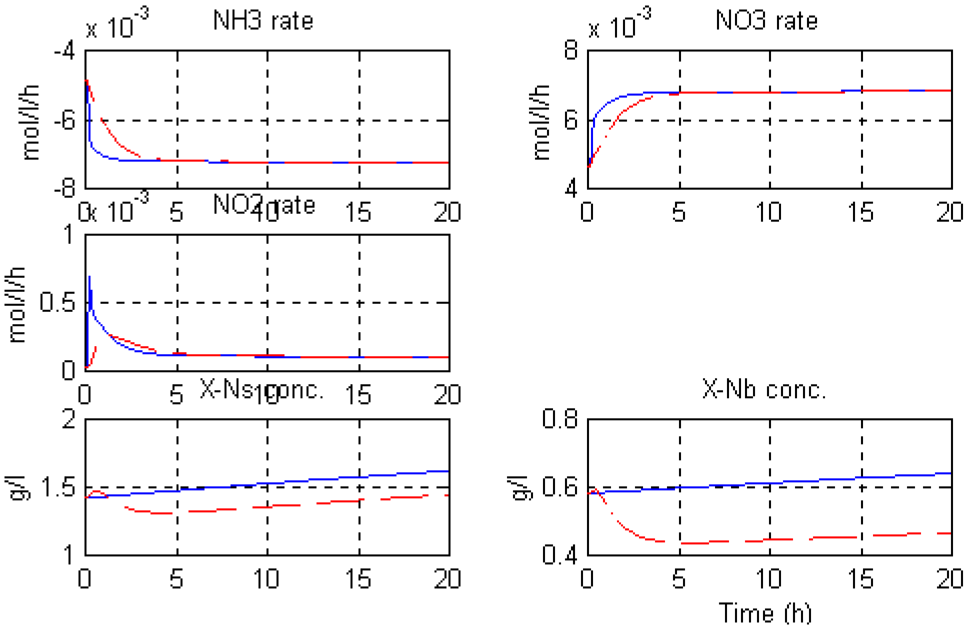

Figure 26 : Comparison estimation versus process (mismatch on KLa)
Top graphs : NH3 and NO3 variation rates estimated with relation (5)
Middle graph : NO2 variation rate estimated with relation (7)
Bottom graphs : Nitrosomonas and Nitrobacter biomass with (8)
Process : continuous blue line - Estimation : dotted red line

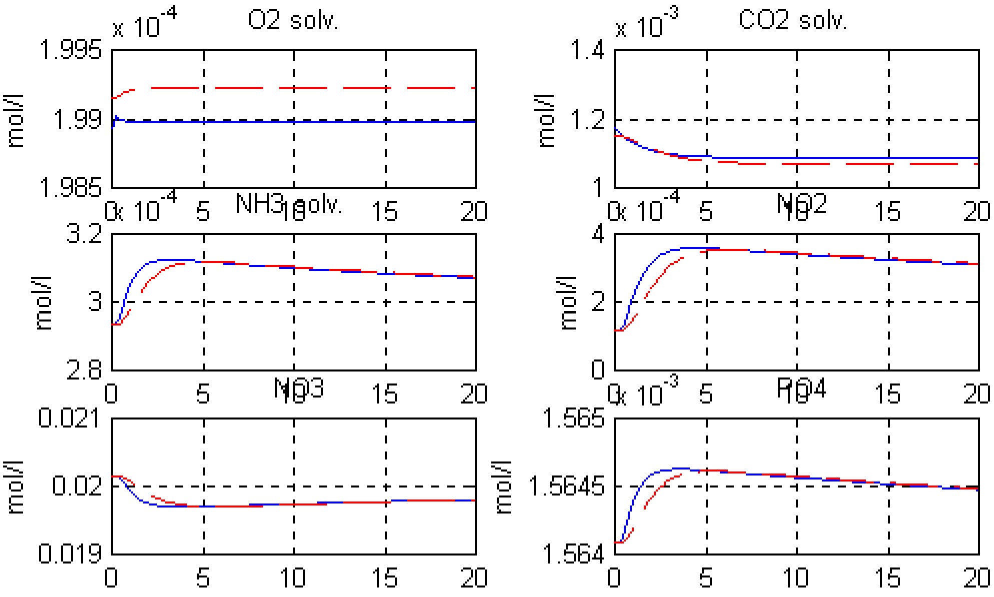

Figure 27 : Comparison estimation versus process (mismatch on KLa) part A
Process : continuous blue line. Estimation : dotted red line

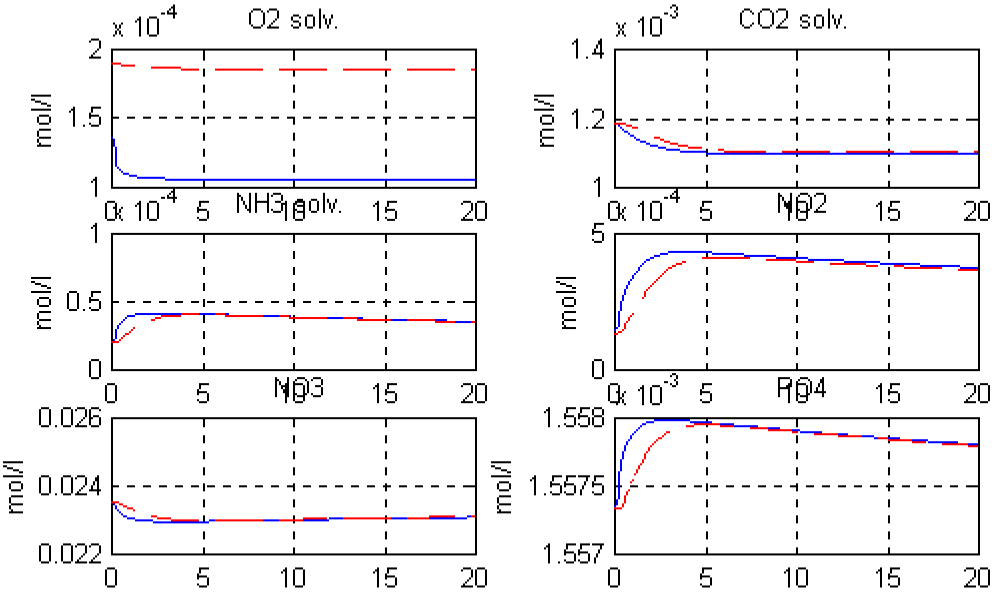

Figure 28 : Comparison estimation versus process (mismatch on KLa) part B
Process : continuous blue line. Estimation : dotted red line

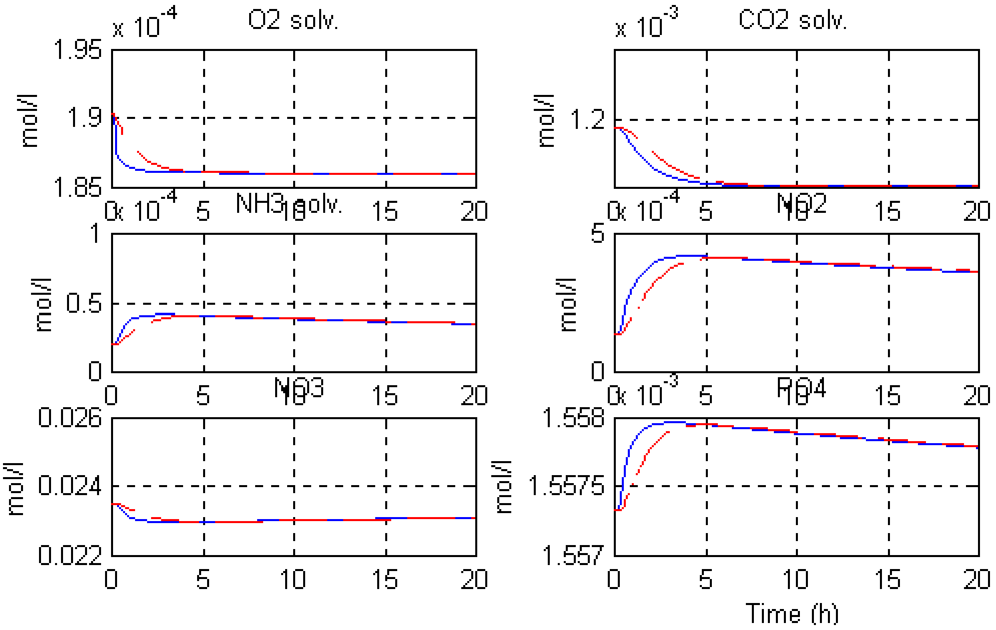

Figure 29 : Comparison estimation versus process (mismatch on KLa) part C
Process : continuous blue line. Estimation : dotted red line

3.6. Growth and maintenance limiting concentrations of the process

Maintenance limiting concentrations have been introduced in TN 48.1 in the same way as growth limiting concentrations have been defined in TN 27.1 by LGCB.

As no values are known for these maintenance limiting concentration, an hypothesis (named H1 in TN 48.1 p.14) was made that maintenance and growth are identical. This hypothesis is not necessary for the estimator. But if it is not made, then the maintenance limiting concentrations have to be determined by experimentation.

The following simulation tries to define the validity range of maintenance limiting concentrations such that the hypothesis may be kept while ignoring their values.

Figures 30 to 33 show the case where maintenance limiting concentrations are double the growth ones. Figures 34 to 37 show the inverse case where the maintenance ones are the half of the growth ones.

So it seems that estimations of NO_2 and biomass are acceptable (fig 30, 33, 34 and 37) when the maintenance ones are between the half and the double of the growth ones.

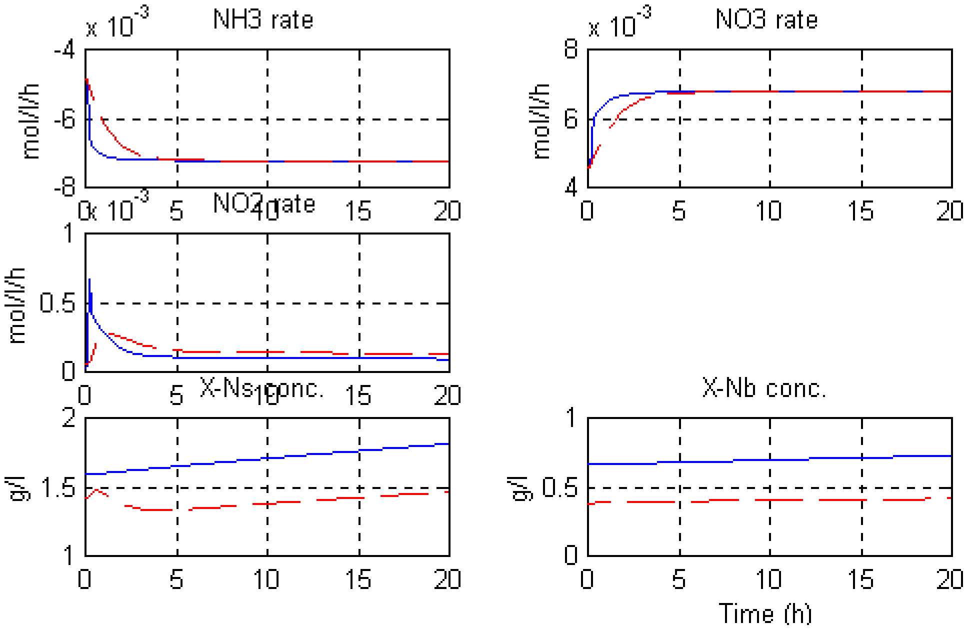

Figure 30 : Comparison estimation versus process (double)
Top graphs : NH3 and NO3 variation rates estimated with relation (5)
Middle graph : NO2 variation rate estimated with relation (7)
Bottom graphs : Nitrosomonas and Nitrobacter biomass with (8)
Process : continuous blue line - Estimation : dotted red line

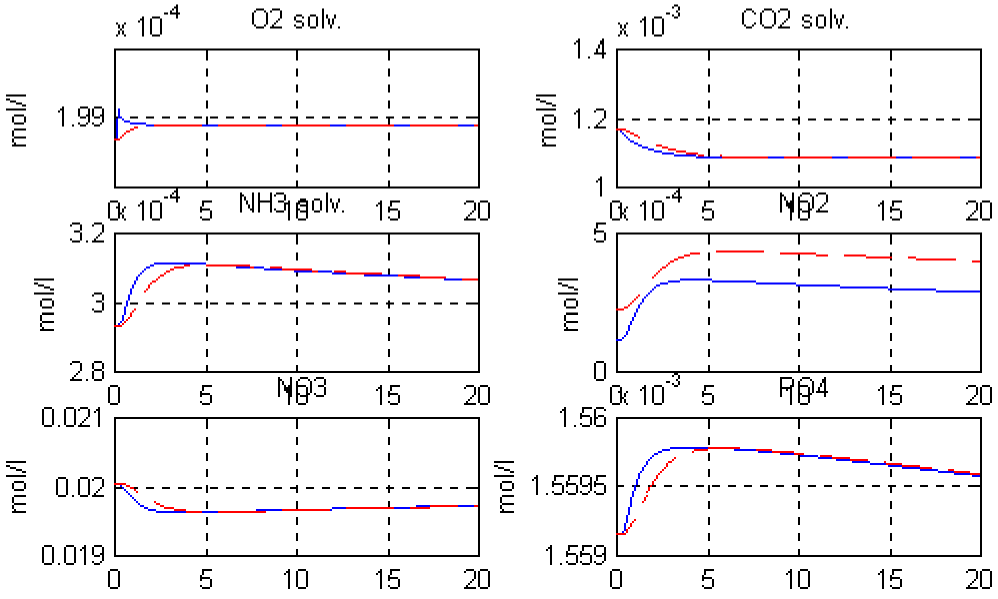

Figure 31 : Comparison estimation versus process (double) part A
Process : continuous blue line. Estimation : dotted red line

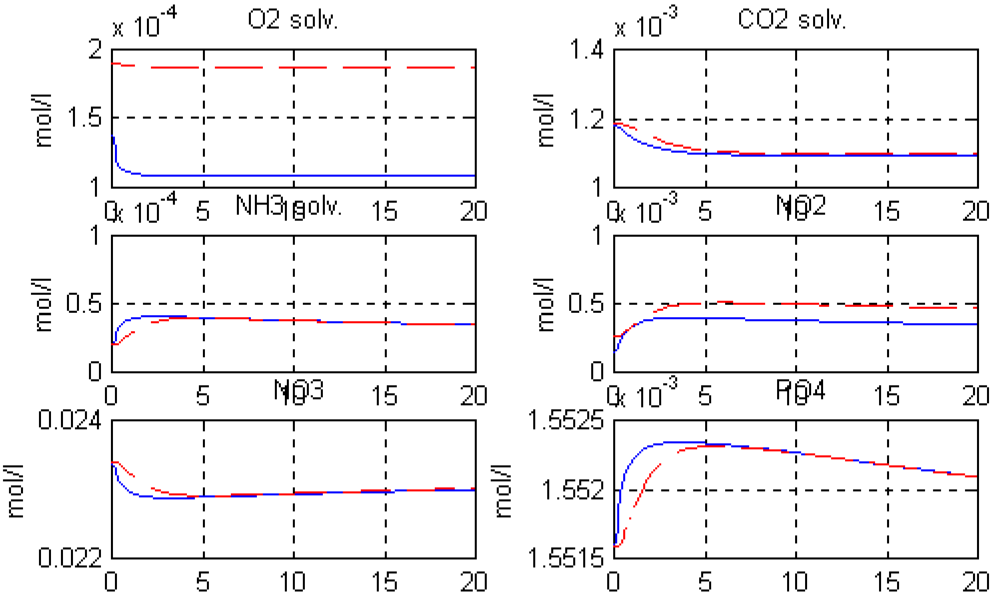

Figure 32 : Comparison estimation versus process (double) part B
Process : continuous blue line. Estimation : dotted red line

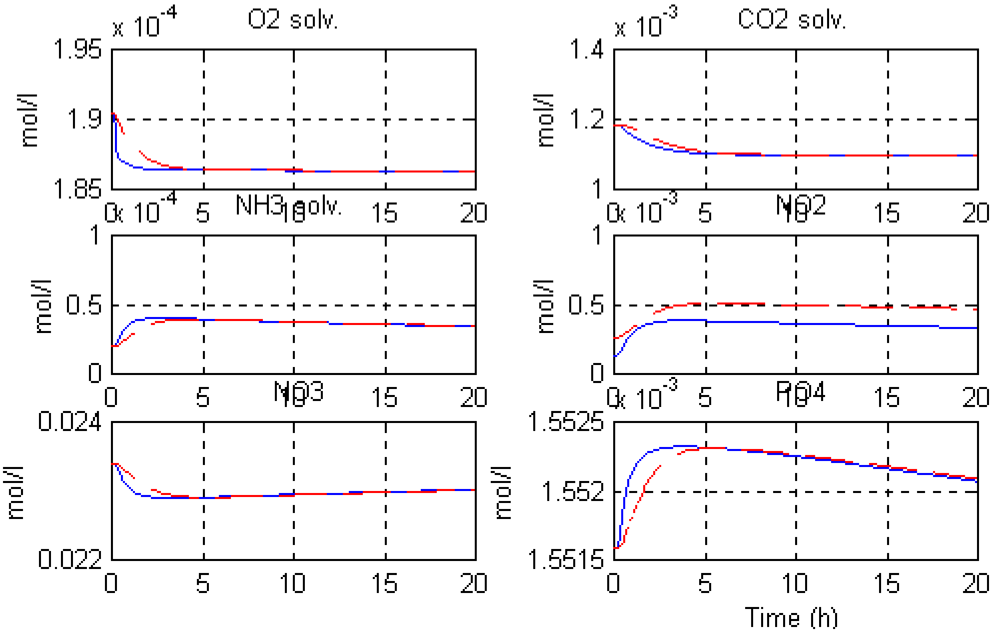

Figure 33 : Comparison estimation versus process (double) part C
Process : continuous blue line. Estimation : dotted red line

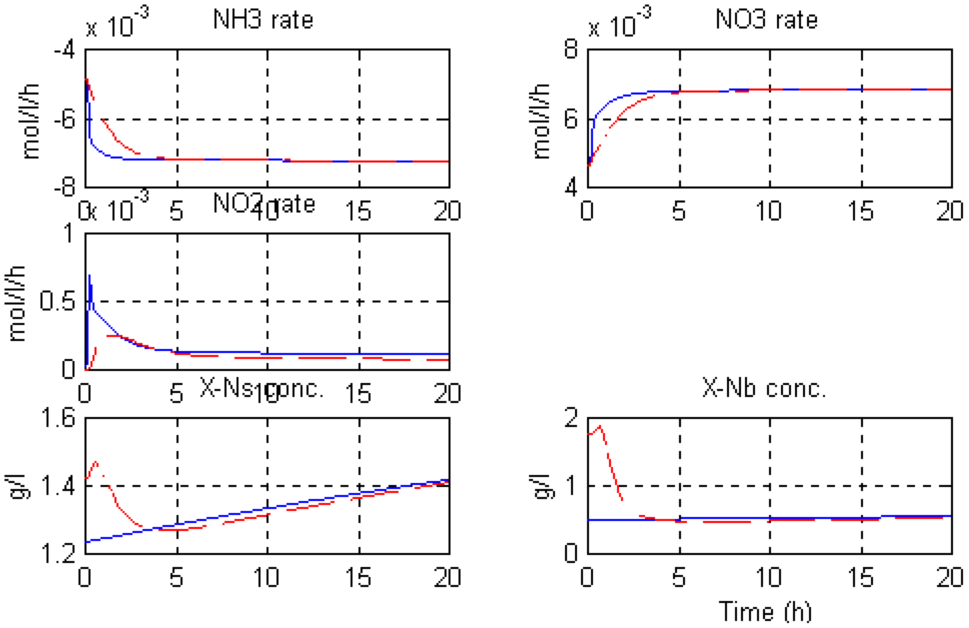

Figure 34 : Comparison estimation versus process (half)
Top graphs : NH3 and NO3 variation rates estimated with relation (5)
Middle graph : NO2 variation rate estimated with relation (7)
Bottom graphs : Nitrosomonas and Nitrobacter biomass with (8)
Process : continuous blue line - Estimation : dotted red line

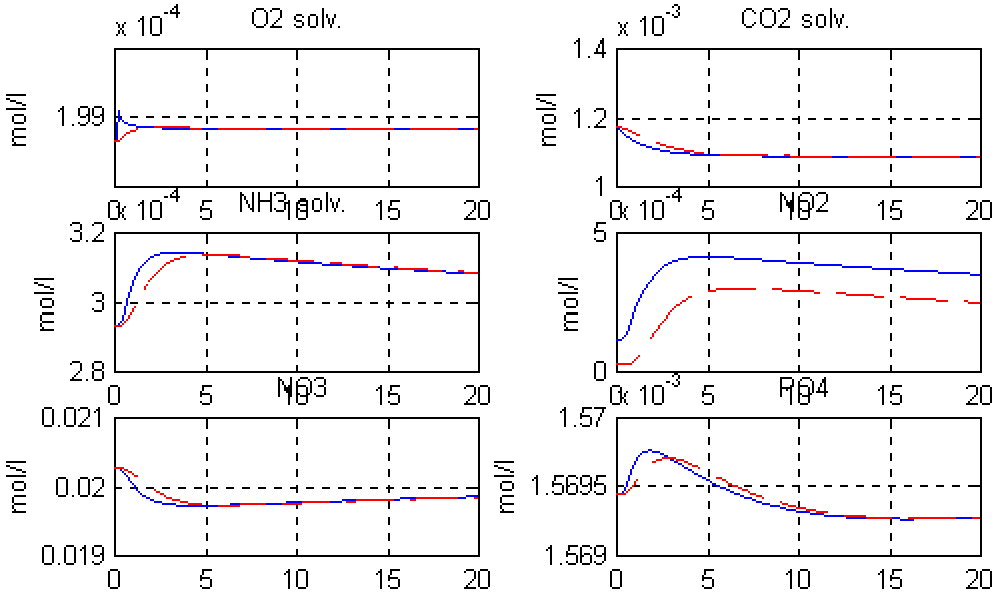

Figure 35 : Comparison estimation versus process (half) part A
Process : continuous blue line. Estimation : dotted red line

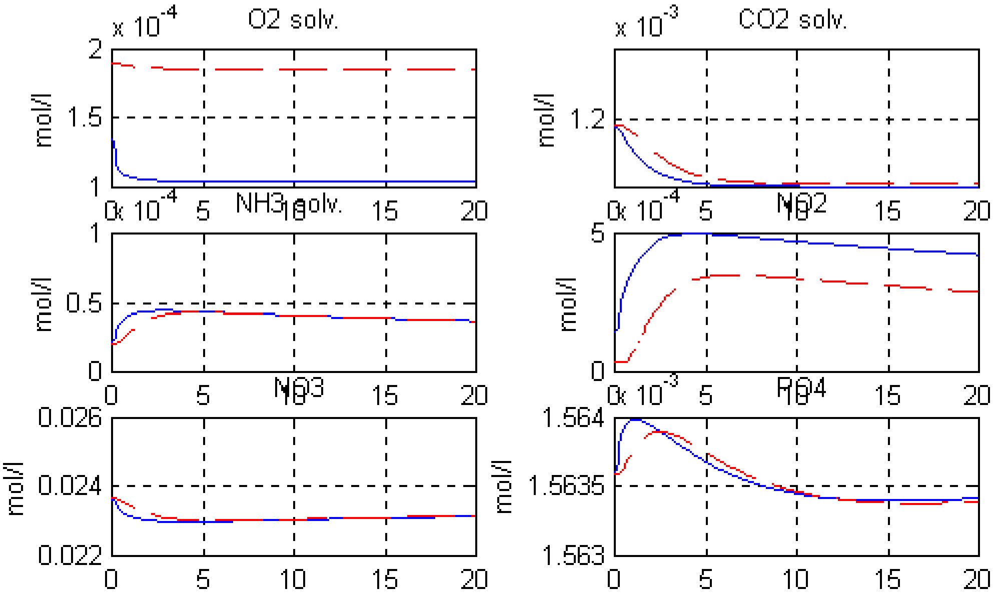

Figure 36 : Comparison estimation versus process (half) part B
Process : continuous blue line. Estimation : dotted red line

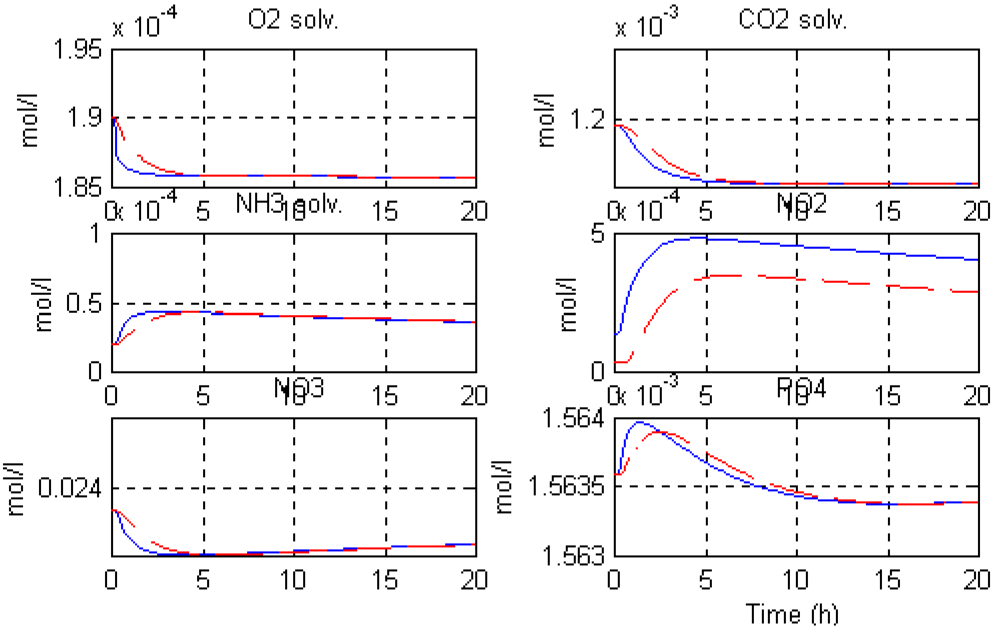

Figure 37 : Comparison estimation versus process (half) part C
Process : continuous blue line. Estimation : dotted red line

3.7. Bias of sensors

Relation (7bis) above shows immediately that a bias of a sensor can be corrected with a compensation term added to the estimation of NO2. This compensation term is an input of the software and has to be set by the operator.

4. CONCLUSION

The study of sensitivity shows that the parameters µ and m are the most influent. Nevertheless no parameter has such high an influence that it should be identified with a high accuracy.
On the contrary, the estimator is very sensitive to the noise on the NH_3 and NO_3 measurements that has to be very low : 0.5 % of the mean value of the input concentration of ammonia.
The estimator has now to be validated on the pilot plant at UAB.

5. REFERENCE

LECLERCQ J.-J. : "Nitrite and Biomass predictors of the nitrifying compartment – Phase I : Mathematical inferred variable". Contract ESTEC n° 12924/98/NL/MV, Contract change notice n° 1 of May 1999, TN 48.1.

PEREZ,J.; MONTESINOS,J.L.; GODIA,F. : "Operation of the packed bed pilot scale bioreactor". Contract ESTEC n° 11549/95/NL/FG, TN 43.3.

POUGHON L.; DUCHEZ D.; CORNET J.F.; DUSSAP C.G. : "RTD analysis of fixed bed columns". ESTEC contract, April 2002, TN 63.1.

6. ANNEX 1 : JUSTIFICATION OF THE MODEL

The TN 63.1 p.20 by LGCB has identified the number of CST's equal to 2 for a gas flow of 60 l/h and a liquid flow of 2.5 l/h, which is the functioning domain of the column of the pilot at UAB.
In order to minimize the size of the state vector to be estimated, the fixed bed of the model is treated as only one CST.
To justify this choice, the process is compared to the model in 2 cases : low and high ammonia load, 10^{-3} and 10^{-2} mol/h of NH_3.
The conditions of the simulations are close to the ones of the pilot :

- input air flow : G_{in} = 60 l/h
- input liqiid flow F_{in} = 0.4 l/h
- gas re-circulating ratio R_G = 0
- liquid re-circulating ratio R_L = 6
- 50 % increase step of flow at time t=0.2 h
- 2 CST's for the fixed bed of the process
- 1 CST for the fixed bed of the model

The comparison is done for each compounds in liquid phase (O_2, CO_2, NH_3, NO_2, NO_3 and PO_4) and for each part A, B and C of the column. For the fixed bed of the process, the plotted value is the mean of the 2 tanks. The biomasses are compared too.

The first group of figures (A1.1 to A1.3) is for the low load and the second one (fig A1.4 to A1.6) is for high load.

It can be seen that for low load, process and model are identical.
For high load, the concentration of NO2 particularly is a third lower with the model.
Despite this discrepancy, the fixed bed of the model is considered as only one CST in order to minimize the size of the state to be estimated.

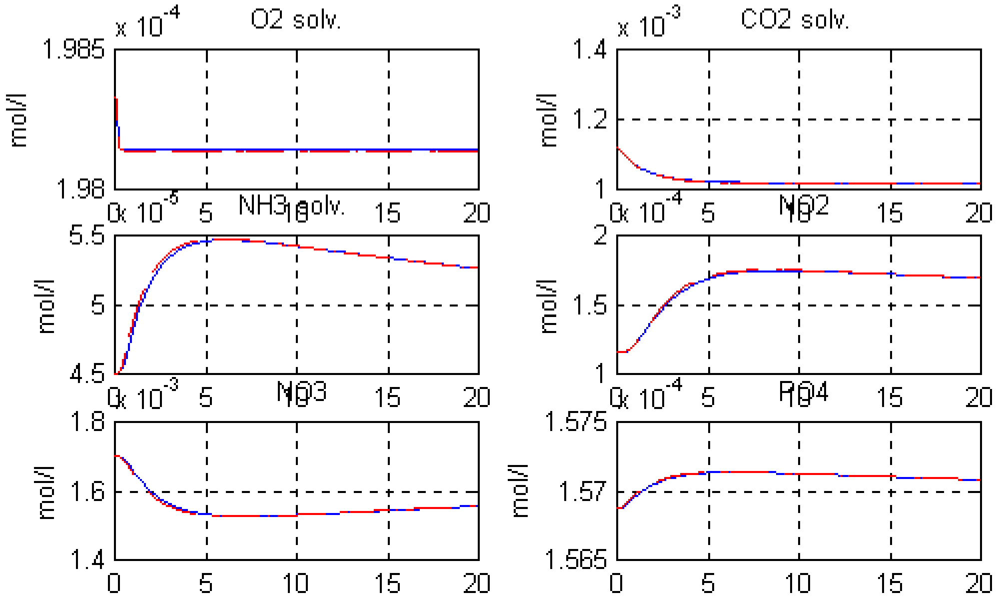

Figure A1.1 : Low load. Comparison estimation versus process : part A of column Process : continuous blue line - Estimation : dotted red line

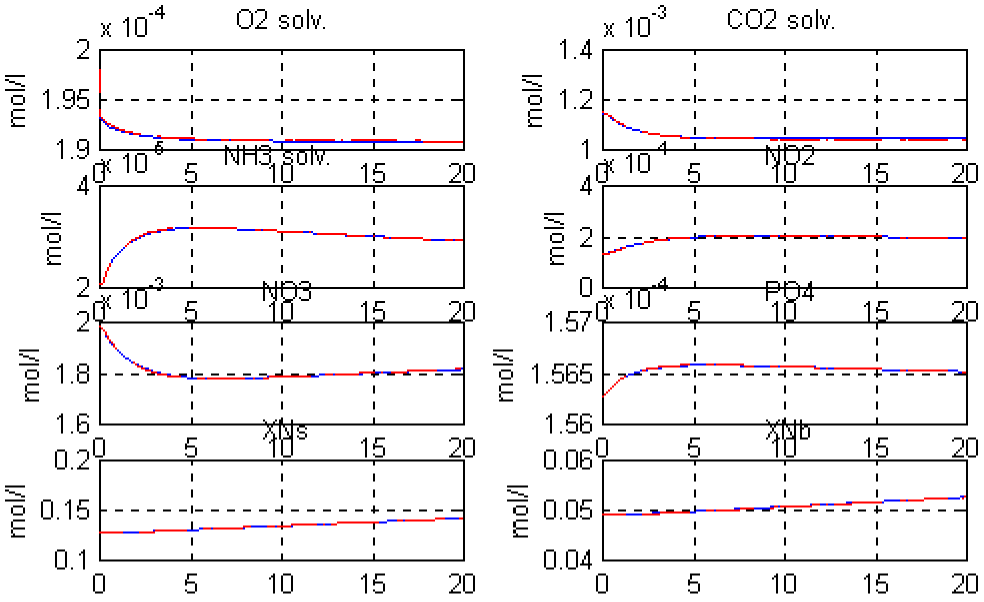

Figure A1.2 : Low load. Comparison estimation versus process : part B of column
Process : continuous blue line - Estimation : dotted red line

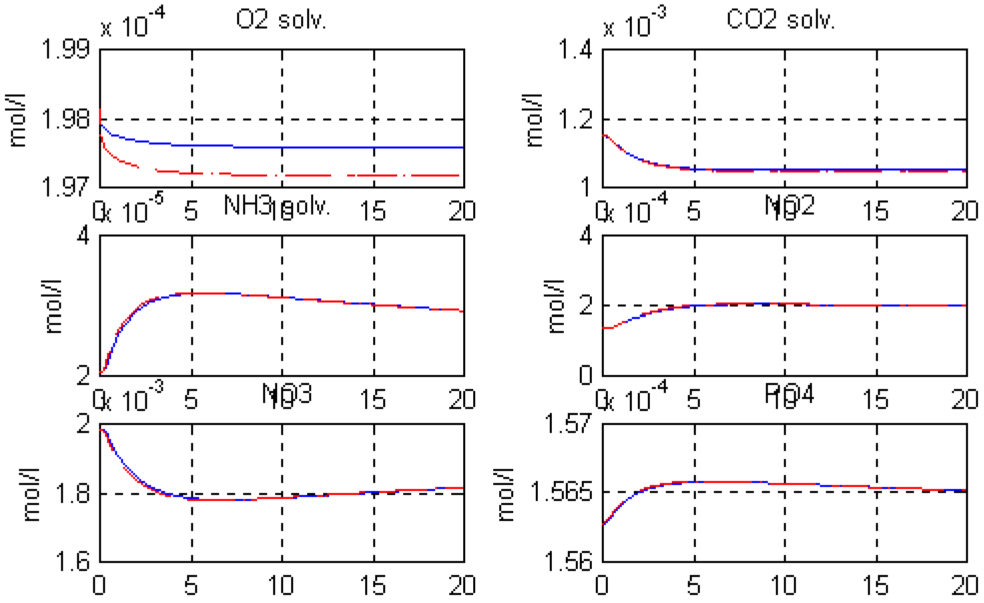

Figure A1.3 : Low load. Comparison estimation versus process : part C of column
Process : continuous blue line - Estimation : dotted red line

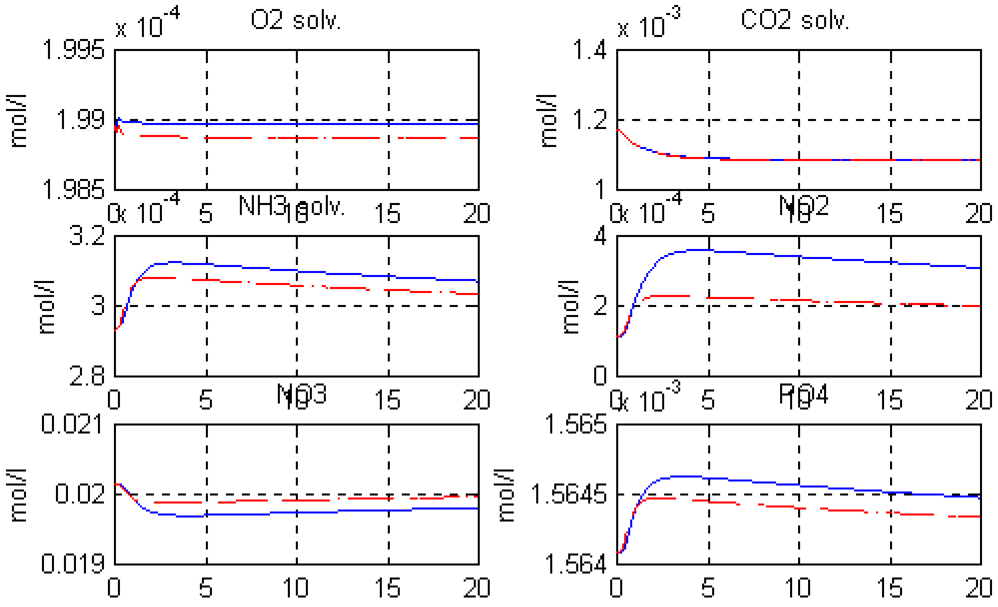

Figure A1.4 : High load. Comparison estimation versus process : part A of column
Process : continuous blue line - Estimation : dotted red line

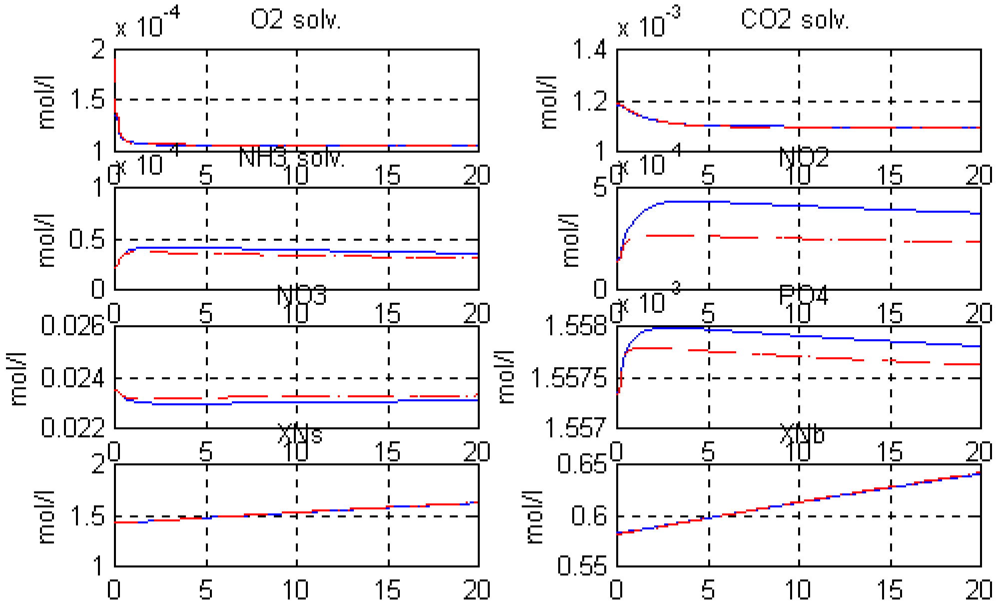

Figure A1.5 : High load. Comparison estimation versus process : part B of column
Process : continuous blue line - Estimation : dotted red line

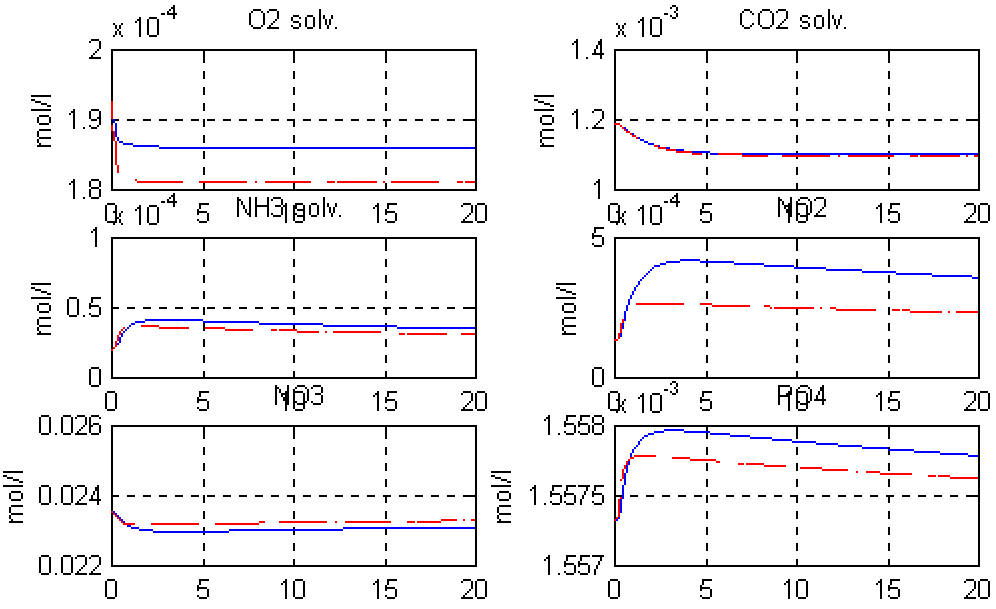

Figure A1.6 : High load. Comparison estimation versus process : part C of column
Process : continuous blue line - Estimation : dotted red line

7. ANNEX 2 : SIMPLIFICATION OF TRANSFER

As said in section 2 above, the column can be represented by a series of 3 tanks ideally stirred (CST) for which dynamic behaviour is described by a first order transfer (figure A2.1).

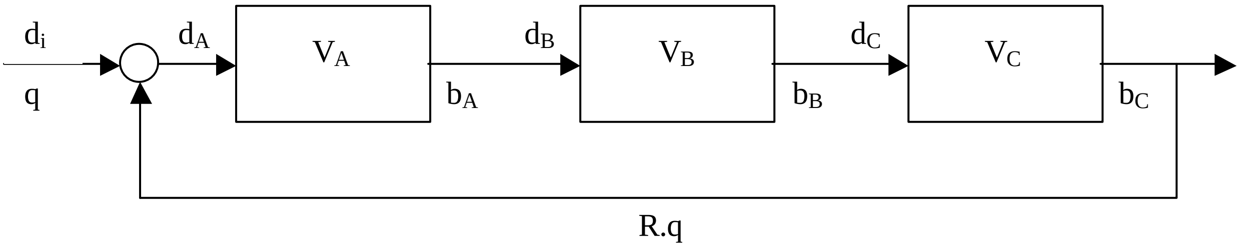

Figure A2.1 : Scheme of the column
A,B,C : indices of the 3 parts
d : concentration of a compound at input of a tank
d_i : concentration of a compound at input of the column
b : concentration of a compound at output of a tank
q : liquid flow rate (any value non zero)
R : re-circulating ratio
V : volume

As shown by relation (3) above, the output b_C can be expressed from the inputs d_i and r :

$$b_C = \frac{1}{H} \cdot d_i + \frac{1 + \tau_A \cdot p}{H} \cdot (1 + R) \cdot \tau_B \cdot r \qquad \text{(A2.1)}$$

$$\text{with} \quad H = (1 + \xi_1 \cdot p) \cdot (1 + \xi_2 \cdot p) \cdot (1 + \xi_3 \cdot p)$$

Thanks to simulator of the hydraulic behaviour of the column (fig. A2.2), it has been checked that the transfer $\frac{1 + \tau_A \cdot p}{H}$ can be approximated to a first order with time constant θ whose value has been identified such that $\theta \cdot q = 3.56 \ \mathrm{l}$. It is equivalent to say that for this transfer the column is equal to only one CST with a volume of 3.56 l. This volume is invariant, independent of q non zero.

The top graphs of figures A2.3 to A2.5 show the step response of the equivalent transfer $\frac{1 + \tau_A \cdot p}{H}$ (blue line) and of the first order (red dotted line) used for simplification, for 3 values of q (0.2, 0.4 and 0.6 l/h). The bottom graphs show the absolute gap (independent of q non zero) between the 2 curves : its maximum value is ± 6 10^{-3}, which justifies the approximation.

So the expression of the output b_C versus the inputs d_i and r becomes:

$$b_C = \frac{1}{H} \cdot d_i + \frac{1}{1 + \theta \cdot p} \cdot (1 + R) \cdot \tau_B \cdot r \qquad \text{(A2.2)}$$

with $H = (1+\xi_1 \cdot p)\cdot(1+\xi_2 \cdot p)\cdot(1+\xi_3 \cdot p)$

$$\theta = \frac{3.56}{q} \quad q = \text{flow rate expressed in l/h}$$

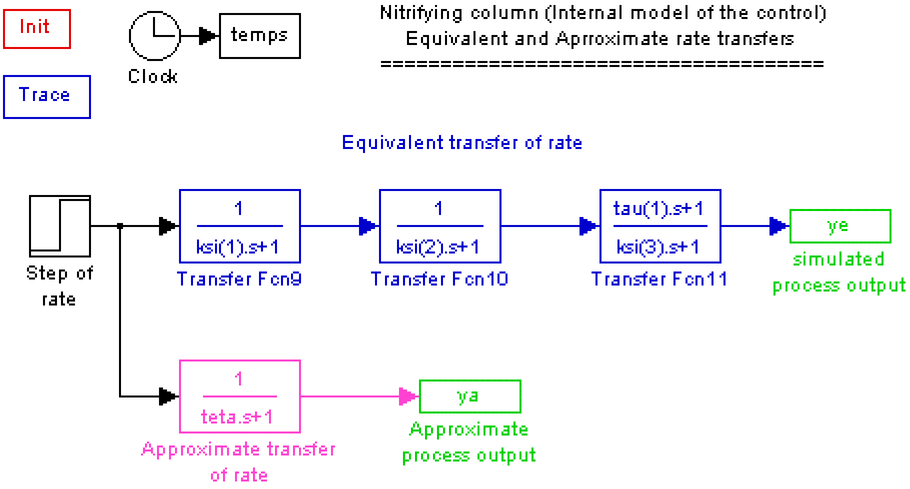

Figure A2.2 : Simulink® simulator of the hydraulic behaviour of the column

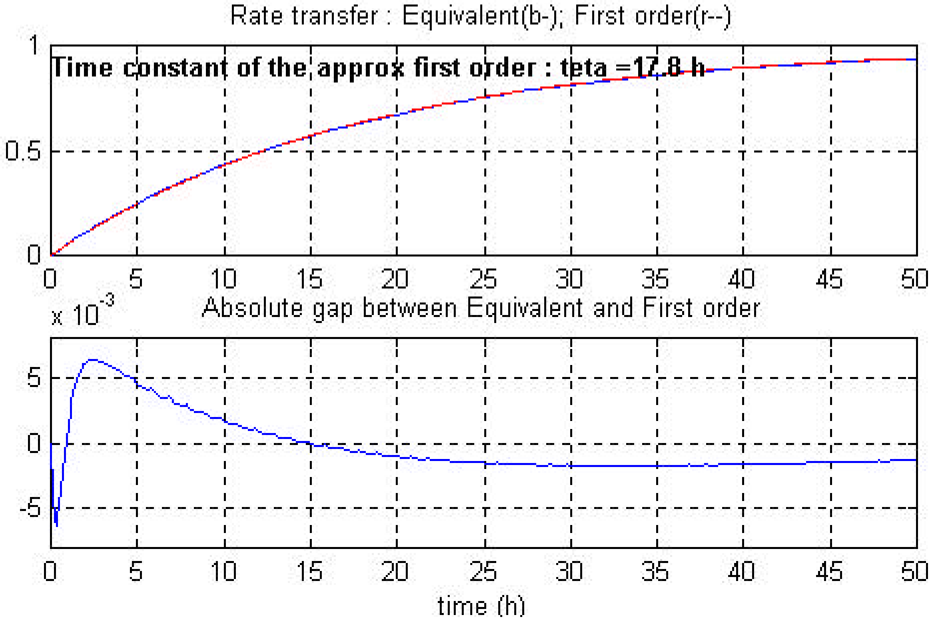

Figure A2.3 : Comparison Equivalent / First Order transfer for q=0.2 l/h

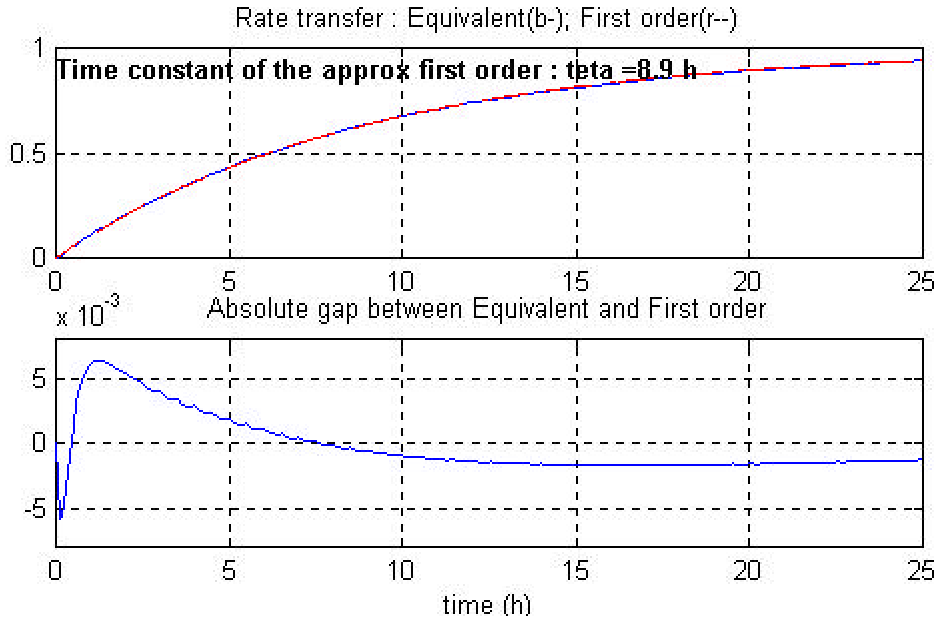

Figure A2.4 : Comparison Equivalent / First Order transfer for q=0.4 l/h

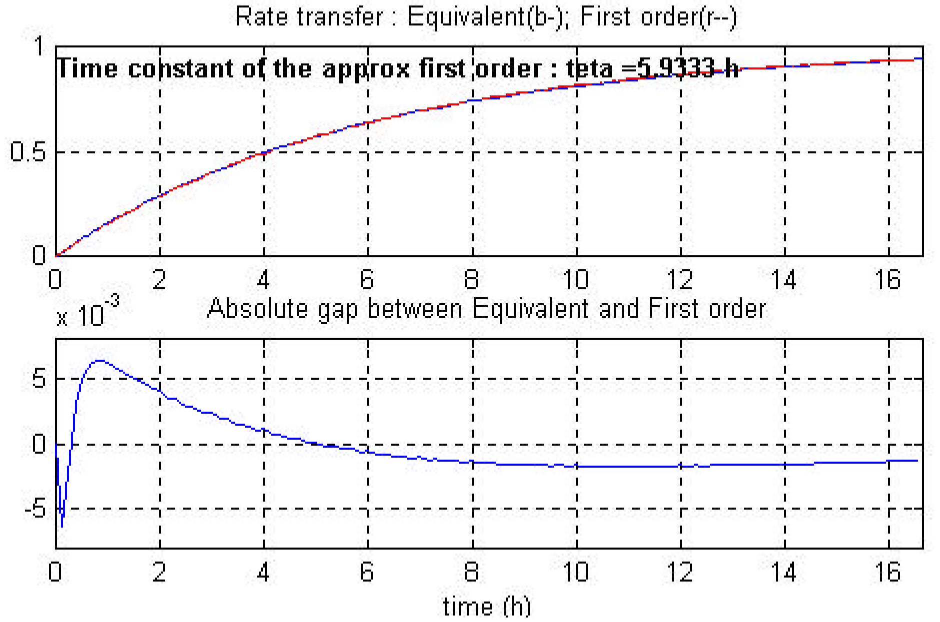

Figure A2.5 : Comparison Equivalent / First Order transfer for q=0.6 l/h

8. ANNEX 3 : SENSITIVITY OF ESTIMATIONS TO THE PARAMETERS

8.1. Sensitivity to specific growth and maintenance rates

8.1.1. Sensitivity of nitrite estimation

The relation (7bis) of section 2 that gives the expression of NO_2 concentration at column output is re-written hereafter (with obvious new names of variables) :

$$b_3 = \beta_1 \cdot b_1 + \beta_2 \cdot b_2 - (\beta_1 \cdot d_{i1} + \beta_2 \cdot d_{i2}) \cdot \frac{1}{H} \tag{A3.1}$$

with $b_1, b_2, b_3 : NH_3, NO_3$ and NO_2 concentrations at column output

d_{i1}, d_{i2} : NH_3, NO_3 concentrations at column input

In order to simplify the expression of sensitivity, it is considered at steady state only. So (A3.1) becomes :

$$b_3 = \beta_1 \cdot b_1 + \beta_2 \cdot b_2 - (\beta_1 \cdot d_{i1} + \beta_2 \cdot d_{i2}) \tag{A3.2}$$

and the sensitivity of b_3 is :

$$\delta b_3 = (b_1 - d_{i1}) \cdot \delta\beta_1 + (b_2 - d_{i2}) \cdot \delta\beta_2 \tag{A3.3}$$

Now with the following simplifications (only in this paragraph) :

b_1 negligible versus d_{i1}

d_{i2} negligible versus b_2

$b_2 \approx d_{i1}$

then

$$\delta b_3 = d_{i1} \cdot (\delta\beta_2 - \delta\beta_1) \tag{A3.4}$$

Expression of $\delta\beta_1$:

From (A.13) in TN 48.1 and taking into account that $\sigma_{21} = 0$:

$$\beta_1 = \frac{\sigma_{31}}{\sigma_{11}} = -1 + \varepsilon_1$$

$$\text{with} \quad \varepsilon_1 = \frac{(Y_{x1(3,1)} + Y_{x1(4,1)}) \cdot \mu_1}{\sigma_{11}} \tag{A3.5}$$

where μ_1 is the specific growth rate of Ns

So the sensitivity of β_1 is :

$$\delta\beta_1 = \delta\varepsilon_1$$

$$\text{with} \quad \frac{\delta\varepsilon_1}{\varepsilon_1} = \frac{\delta\mu_1}{\mu_1} - \frac{\delta\sigma_{11}}{\sigma_{11}}$$

$$\Rightarrow \frac{\delta\varepsilon_1}{\varepsilon_1} = a_1 \cdot \frac{\delta\mu_1}{\mu_1} - a_2 \cdot \frac{\delta m_1}{m_1}$$

$$\text{with} \quad a_1 = 1 - \frac{Y_{x1(3,1)} \cdot \mu_1}{\sigma_{11}} \quad \text{and} \quad a_2 = \frac{Y_{m1(3,1)} \cdot m_1}{\sigma_{11}}$$

Now

$$a_1 = \frac{Y_{x1(3,1)} \cdot \mu_1 + Y_{m1(3,1)} \cdot m_1 - Y_{x1(3,1)} \cdot \mu_1}{\sigma_{11}} = a_2$$

Then

$$\delta\beta_1 = s_1 \cdot \left(\frac{\delta\mu_1}{\mu_1} - \frac{\delta m_1}{m_1} \right)$$

$$\text{with } s_1 = \varepsilon_1 \cdot \left(1 - \frac{Y_{x1(3,1)} \cdot \mu_1}{\sigma_{11}} \right) = \varepsilon_1 \cdot \frac{Y_{m1(3,1)} \cdot m_1}{\sigma_{11}} \qquad \text{(A3.6)}$$

Remark 1 : as the stoechiometric ratios $Yx1(3,1)$ and $Yx1(4,1)$ are nearly opposite, so the term $\varepsilon_1 = \frac{(Yx1(3,1) + Yx1(4,1)) \cdot \mu_1}{\sigma_{11}} = 0.035$, which is small versus 1.

Expression of $\delta\beta_2$:

From (A.13) in TN 48.1 and taking into account that $\sigma_{21} = 0$:

$$\beta_2 = \frac{\sigma_{11} \cdot \sigma_{32} - \sigma_{12} \cdot \sigma_{31}}{\sigma_{11} \cdot \sigma_{22}} = \frac{\sigma_{32}}{\sigma_{22}} - \frac{\sigma_{12}}{\sigma_{22}} \cdot \frac{\sigma_{31}}{\sigma_{11}} \qquad \text{(A3.7)}$$

Considering the term $\frac{\sigma_{32}}{\sigma_{22}} = \frac{Y_{x1(4,2)} \cdot \mu_2 + Y_{m1(4,2)} \cdot m_2}{Y_{x1(5,2)} \cdot \mu_2 + Y_{m1(5,2)} \cdot m_2}$

it can be noted that these stoechiometric ratios represent the transformation of NO_2 into NO_3:

$$Y_{x1(4,2)} = -Y_{x1(5,2)}$$

$$Y_{m1(4,2)} = -Y_{m1(5,2)}$$

$$\Rightarrow \frac{\sigma_{32}}{\sigma_{22}} = -1$$

Considering now the term $\frac{\sigma_{12}}{\sigma_{22}} \cdot \frac{\sigma_{31}}{\sigma_{11}}$ where $\frac{\sigma_{31}}{\sigma_{11}} \approx -1$ (from remark 1) and $\frac{\sigma_{12}}{\sigma_{22}} \approx 10^{-2}$

its value is small (but not neglected) versus 1.

Then

$$\beta_2 = -1 + \varepsilon_2$$

$$\text{with } \varepsilon_2 = \frac{\sigma_{12}}{\sigma_{22}} \qquad \text{(A3.8)}$$

So the sensitivity of β_2 is :

$$\delta\beta_2 = \delta\varepsilon_2 \qquad \text{(A3.9)}$$

$$\text{with } \frac{\delta\varepsilon_2}{\varepsilon_2} = \frac{\delta\sigma_{12}}{\sigma_{12}} - \frac{\delta\sigma_{22}}{\sigma_{22}}$$

$$\Rightarrow \frac{\delta\varepsilon_2}{\varepsilon_2} = a_1 \cdot \frac{\delta\mu_2}{\mu_2} + a_2 \cdot \frac{\delta m_2}{m_2}$$

$$\text{with } a_1 = \left(\frac{Y_{x1(3,2)}}{\sigma_{12}} - \frac{Y_{x1(5,2)}}{\sigma_{22}} \right) \cdot \mu_2 \quad \text{and} \quad a_2 = \left(\frac{Y_{m1(3,2)}}{\sigma_{12}} - \frac{Y_{m1(5,2)}}{\sigma_{22}} \right) \cdot m_2$$

Now

$$a_1 + a_2 = \frac{Y_{x1(3,2)} \cdot \mu_2 + Y_{m1(3,2)} \cdot m_2}{\sigma_{12}} - \frac{Y_{x1(5,2)} \cdot \mu_2 + Y_{m1(5,2)} \cdot m_2}{\sigma_{22}} = 1 - 1 = 0$$

Then

$$\delta\beta_2 = s_2 \cdot \left(\frac{\delta\mu_2}{\mu_2} - \frac{\delta m_2}{m_2} \right) \tag{A3.10}$$

$$\text{with } s_2 = \varepsilon_2 \cdot \left(\frac{Y_{x1(3,2)}}{\sigma_{12}} - \frac{Y_{x1(5,2)}}{\sigma_{22}} \right) \cdot \mu_2 = -\varepsilon_2 \cdot \left(\frac{Y_{m1(3,2)}}{\sigma_{12}} - \frac{Y_{m1(5,2)}}{\sigma_{22}} \right) \cdot m_2$$

Recapitulation :

At steady state, the sensitivity of b_3 is :

$$\delta b_3 = d_{i1} \cdot \left(s_1 \cdot \left(-\frac{\delta\mu_1}{\mu_1} + \frac{\delta m_1}{m_1} \right) + s_2 \cdot \left(\frac{\delta\mu_2}{\mu_2} - \frac{\delta m_2}{m_2} \right) \right)$$

with :

$$s_1 = \varepsilon_1 \cdot \left(1 - \frac{Y_{x1(3,1)} \cdot \mu_1}{\sigma_{11}} \right) = \varepsilon_1 \cdot \frac{Y_{m1(3,1)} \cdot m_1}{\sigma_{11}}$$

$$\varepsilon_1 = \frac{\left(Y_{x1(3,1)} + Y_{x1(4,1)} \right) \cdot \mu_1}{\sigma_{11}} \tag{A3.11}$$

$$s_2 = \varepsilon_2 \cdot \left(\frac{Y_{x1(3,2)}}{\sigma_{12}} - \frac{Y_{x1(5,2)}}{\sigma_{22}} \right) \cdot \mu_2 = -\varepsilon_2 \cdot \left(\frac{Y_{m1(3,2)}}{\sigma_{12}} - \frac{Y_{m1(5,2)}}{\sigma_{22}} \right) \cdot m_2$$

$$\varepsilon_2 = \frac{\sigma_{12}}{\sigma_{22}}$$

where : μ_1 is the specific growth rate of Ns

μ_2 is the specific growth rate of Nb

m_1 is the specific maintenance rate of Ns

m_2 is the specific maintenance rate of Nb

d_{i1} : NH_3 concentration at column input

$\sigma_{11}, \sigma_{12}, \sigma_{22}$ expressed in (A.11) of TN 48.1

Y_{x1}, Y_{m1} : stoechiometric ratios

In normal condition of functioning and at steady state, b_3 is independent of d_{i1} and depends quasi only on the half saturation constant of NO_2 (3.6 10^{-4} mol/l) : $b_3 \approx 1.4\ 10^{-4}$ mol/l .

Assuming that the maximum concentration of input ammonia is 4 10^{-2} mol/l, the range of the terms $\frac{d_{i1} \cdot s_1}{b_3}$ and $\frac{d_{i1} \cdot s_2}{b_3}$ can be approached numerically :

$$0 \le \frac{d_{i1} \cdot s_1}{b_3} \le 2 \qquad \text{and} \qquad -0.8 \le \frac{d_{i1} \cdot s_2}{b_3} \le 0$$

which gives the range of $\frac{\delta b_3}{b_3}$ function of $\frac{\delta\mu_1}{\mu_1}, \frac{\delta m_1}{m_1}, \frac{\delta\mu_2}{\mu_2}, \frac{\delta m_2}{m_2}$

8.1.2. Sensitivity of biomass estimation

The relation (8) of section 2 that gives the expressions of Ns and Nb biomass concentration is re-written hereafter (with obvious new names of variables) :

$$\begin{aligned} c_s &= d_{11} \cdot r_1 + d_{12} \cdot r_2 \quad \text{(Ns)} \\ c_b &= d_{21} \cdot r_1 + d_{22} \cdot r_2 \quad \text{(Nb)} \end{aligned} \tag{A3.12}$$

$$\text{with } r_1 \text{ and } r_2 : \text{variation rates of } NH_3 \text{ and } NO_3$$

From (A.14) in TN 48.1 and taking into account that $\sigma_{21} = 0$:

$$\begin{aligned} d_{11} &= \frac{\sigma_{22}}{\sigma_{11} \cdot \sigma_{22}} = \frac{1}{\sigma_{11}} \\ d_{12} &= -\frac{\sigma_{12}}{\sigma_{11} \cdot \sigma_{22}} = -\frac{1}{\sigma_{11}} \cdot \frac{\sigma_{12}}{\sigma_{22}} \\ d_{21} &= 0 \\ d_{22} &= \frac{\sigma_{11}}{\sigma_{11} \cdot \sigma_{22}} = \frac{1}{\sigma_{22}} \end{aligned}$$

Now $\frac{\sigma_{12}}{\sigma_{22}} \approx 10^{-2}$ can be neglected versus 1

and $r_2 \approx -r_1$ (simplification and assumption for this section only).

Then

$$\begin{aligned} c_s &= \frac{1}{\sigma_{11}} \cdot r_1 \\ c_b &= \frac{1}{\sigma_{22}} \cdot r_2 \end{aligned} \tag{A3.13}$$

The sensitivity of c_s and c_b can be deduced :

$$\begin{aligned} \frac{\delta c_s}{c_s} &= -\frac{\delta\sigma_{11}}{\sigma_{11}} = -\frac{Yx1(3,1) \cdot \mu_1}{\sigma_{11}} \cdot \frac{\delta\mu_1}{\mu_1} - \frac{Ym1(3,1) \cdot m_1}{\sigma_{11}} \cdot \frac{\delta m_1}{m_1} \\ \frac{\delta c_b}{c_b} &= -\frac{\delta\sigma_{22}}{\sigma_{22}} = -\frac{Yx1(5,2) \cdot \mu_2}{\sigma_{11}} \cdot \frac{\delta\mu_2}{\mu_2} - \frac{Ym1(3,1) \cdot m_2}{\sigma_{11}} \cdot \frac{\delta m_2}{m_2} \end{aligned} \tag{A3.14}$$

$$\text{where} \quad Yx1 \text{ and } Ym1 \text{ are stoechiometric ratios}$$

With the numerical values of the parameters, the sensitivity of c_s and c_b is given by :

$$\begin{aligned} \frac{\delta c_s}{c_s} &= -0.8 \cdot \frac{\delta \mu_1}{\mu_1} - 0.2 \cdot \frac{\delta m_1}{m_1} \\ \frac{\delta c_b}{c_b} &= -0.7 \cdot \frac{\delta \mu_2}{\mu_2} - 0.3 \cdot \frac{\delta m_2}{m_2} \end{aligned} \qquad \text{(A3.15)}$$

Remark 2 : according to the above approximate expression (in the case of c_s only), the concentration of Ns is connected to the consumption rate of ammonia only and that the concentration of Nb is connected to the production rate of nitrate only (i.e. the matrix of correlation is diagonal).

8.2. Sensitivity to the dissociation constant

As the concentration of NH3 in the output gas flow is low, it is not measured and the quantity of this compound that is extracted from the column by this way is simply approximated by the formula (relation (A2.10) in TN 44.2) :

$$db_C = b_C \cdot \frac{\alpha \cdot K}{K + \alpha \cdot \frac{G_{in}}{V_C}} \cdot \frac{G_{in}}{F_{in}} \cdot \frac{1}{1+k} \qquad \text{(A3.16)}$$

with :

db_C : quantity of NH3 extracted in the gas expressed in mol/l in the liquid

b_C : conc. in the liquid output stream

α : liquid/gas thermodynamical equilibrium constant of NH3

K : liquid/gas transfer parameter (KLa)

G_{in} : input gas flow rate

F_{in} : input liquid flow rate

k : dissociation constant

8.2.1. Sensitivity of nitrite estimation

With the numerical values of the problem, relation (A3.16) becomes

$$db_C = 0.1 \cdot b_C \qquad \text{(A3.16bis)}$$

Now k is about 10.

Then the relative variation of db_C versus the relative variation on the dissociation constant k is

$$\frac{\delta(db_C)}{b_C} \approx -0.1 \cdot \frac{\delta k}{k}$$

Moreover :

$$\delta b_{C3} = \beta_1 \cdot \delta b_{C1} \qquad \text{(from (7bis))}$$

$$\delta b_{C1} = \delta(db_C) \tag{A3.17}$$

$$\frac{b_{C1}}{b_{C3}} \approx 1 \quad \text{and} \quad \beta_1 \approx -1$$

Then

$$\frac{\delta b_{C3}}{b_{C3}} = 0.1 \cdot \frac{\delta k}{k} \tag{A3.18}$$

8.2.2. Sensitivity of biomass

Concerning biomass, the following relations can be written :

$$\delta c_{Xk} = \delta_{k1} \cdot \delta r_1 \qquad \text{(from (8))}$$

$$\frac{\delta r_1}{r_1} = \frac{\delta b_C}{b_C} = \frac{\delta(db_C)}{b_C} \tag{A3.19}$$

$$r_1 \approx \frac{q \cdot d_{i1}}{V_B}$$

Then

$$\frac{\delta c_{Xk}}{c_{Xk}} = a_k \cdot \frac{\delta k}{k}$$

$$\text{with} \quad a_k = -0.1 \cdot \delta_{k1} \cdot \frac{q \cdot d_{i1}}{c_{Xk} \cdot V_B} \tag{A3.20}$$

$$\begin{aligned} a_k &\le 0.04 \quad \text{for } k = 1 \text{ (Nitrosomonas)} \\ &= 0 \qquad\; \text{for } k = 2 \text{ (Nitrobacter)} : \delta_{k1} = 0 \end{aligned}$$

8.3. Sensitivity to the gas/liquid transfer Kla

8.3.1. Sensitivity of nitrite estimation

Starting from (A3.16) and taking into account (A3.16bis) and (A3.17) the following relation can be established :

$$\frac{\delta b_{C3}}{b_{C3}} = 0.1 \cdot \frac{\beta_1}{1 + \dfrac{K \cdot V_C}{\alpha \cdot G_{in}}} \cdot \frac{\delta K}{K} \tag{A3.21}$$

Now with the numerical data of the problem

$$\frac{K \cdot V_C}{\alpha \cdot G_{in}} \approx 140$$

then

$$\frac{\delta b_{C3}}{b_{C3}} = -10^{-3} \cdot \frac{\delta K}{K} \tag{A3.22}$$

8.3.2. Sensitivity of biomass

Starting from (A3.19) and taking into account (A3.21) the following relation can be established :

$$\frac{\delta c_{Xk}}{c_{Xk}} = a_k \cdot \frac{\delta K}{K} \qquad \text{(A3.23)}$$

$$\text{with } a_k = 0.1 \cdot \delta_{k1} \cdot \frac{q \cdot d_{i1}}{c_{Xk} \cdot V_B} \cdot \frac{1}{1 + \frac{K \cdot V_C}{\alpha \cdot G_{in}}}$$

$$-3 \cdot 10^{-4} \le a_k \le 0 \quad \text{for } k = 1 \text{ (Nitrosomonas)}$$

$$a_k = 0 \quad \text{for } k = 2 \text{ (Nitrobacter)} : \delta_{k1} = 0$$

8.4. Sensitivity to the gas/liquid equilibrium

8.4.1. Sensitivity of nitrite estimation

Relation (A3.16) implies

$$\frac{\delta(db_C)}{db_C} = \frac{\delta\alpha}{\alpha} \qquad \text{(A3.24)}$$

as $\frac{\alpha \cdot G_{in}}{K \cdot V_C}$ is negligible compared to 1.

So, taking into account (A3.17), it comes :

$$\frac{\delta b_{C3}}{b_{C3}} = -0.1 \cdot \frac{\delta\alpha}{\alpha} \qquad \text{(A3.25)}$$

8.4.2. Sensitivity of biomass

In the same way as previously :

$$\frac{\delta c_{Xk}}{c_{Xk}} = a_k \cdot \frac{\delta\alpha}{\alpha} \qquad \text{(A3.26)}$$

$$\text{with } a_k = 0.1 \cdot \delta_{k1} \cdot \frac{q \cdot d_{i1}}{c_{Xk} \cdot V_B}$$

$$-0.04 \le a_k \le 0 \quad \text{for } k = 1 \text{ (Nitrosomonas)}$$

$$a_k = 0 \quad \text{for } k = 2 \text{ (Nitrobacter)} : \delta_{k1} = 0$$

8.5. Sensitivity to the half saturation constant

The half saturation constants appear in the calculation of the active biomass C_{Xk} from the ‘productive’ biomass c_{Xk}, according to the relation (A.11) of TN 48.1 recalled hereafter :

$$C_{Xk} = \frac{1}{\nu_k} \cdot c_{Xk} \qquad \text{(A3.27)}$$

$$\text{with } \nu_k = \prod_i \frac{S_i}{K_{Ski} + S_i}$$

$k = 1$ and 2 for Nitrosomonas and Nitrobacter

K_{Ski} : saturation constant for strain k and substrate S_i

So, for all the substrates S_i of a strain k,

$$\frac{\delta C_{Xk}}{C_{Xk}} = \sum_i \frac{K_{Ski}}{K_{Ski} + S_i} \cdot \frac{\delta K_{Ski}}{K_{Ski}} \qquad \text{(A3.28)}$$

Now the term $\frac{K_{Ski}}{K_{Ski} + S_i}$ is lower than 1.

Then for a given substrate S_i

$$\frac{\delta C_{Xk}}{C_{Xk}} < \frac{\delta K_{Ski}}{K_{Ski}} \qquad \text{(A3.29)}$$

8.6. Recapitulation

The sensitivity of an estimation e (NO_2 or biomass) to a parameter P of the model (dissociation constant, limiting concentrations, specific growth and maintenance rates, gas/liquid transfer Kla, gas/liquid equilibrium, half saturation constant) is evaluated by the function s :

$$s = \frac{\frac{\delta e}{e}}{\frac{\delta P}{P}} \qquad \text{(A3.30)}$$

The numerical values of the sensitivity ‘s’ are gathered in the table that follows.

Parameter	**m**	**m**	**k**	**KLa**	**a**	**K_S**
s(NO_2)	< 2	< 2	0.1	10^{-3}	0.1	0
s(biomass)	0.8	0.3	< 0.04	3 10^{-4}	< 0.04	< 1

Table A3.1 : sensitivity of the estimations to the parameters

m : specific growth rate

m : specific maintenance rate

k : dissociation constant

Kla : gas/liquid transfer constant

a : gas/liquid equilibrium constant

K_S : half saturation constant

The parameters μ and m are the most influent : the value of 2 is reached for concentration of input ammonia of 4 10^{-2} mol/l, which is assumed to be the maximum.

Nevertheless no parameter has such high an influence that it should be identified with a high accuracy.