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TECHNICAL NOTE : 48.2

Nitrite and Biomass Predictors
of the Nitrifying Compartment
Phase II : Robustness study on simulator

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Abbreviations :

N_s : Nitrosomonas

N_b : Nitrobacter

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NOTATION

The notation is the one of TN 44.2 or TN48.1 and is recalled hereafter, for each substrate of the problem and for each tank of the column :

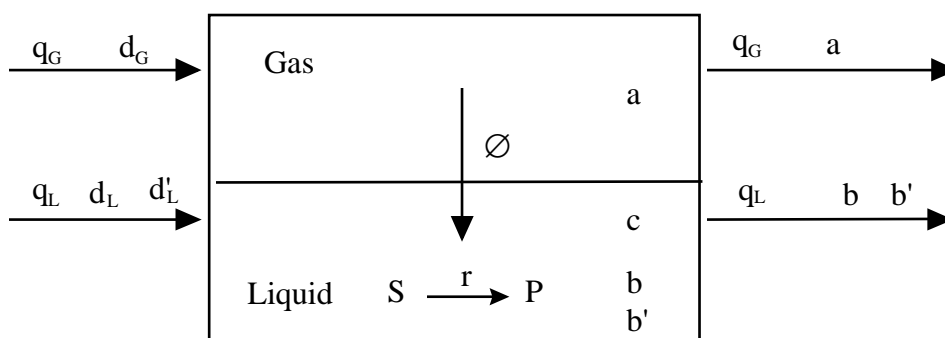
- a : molar concentration in the gas phase
- b : molar concentration in the liquid phase of the molecular form
- c : molar concentration at the thermodynamic equilibrium
- d_G : molar concentration in the incoming gas flow
- d_L : molar concentration in the incoming liquid flow of the molecular form
- 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 $k = \frac{K_b \cdot [H^+]}{K_e}$ for NH_3 solvated

$k = 0$ for the other compounds



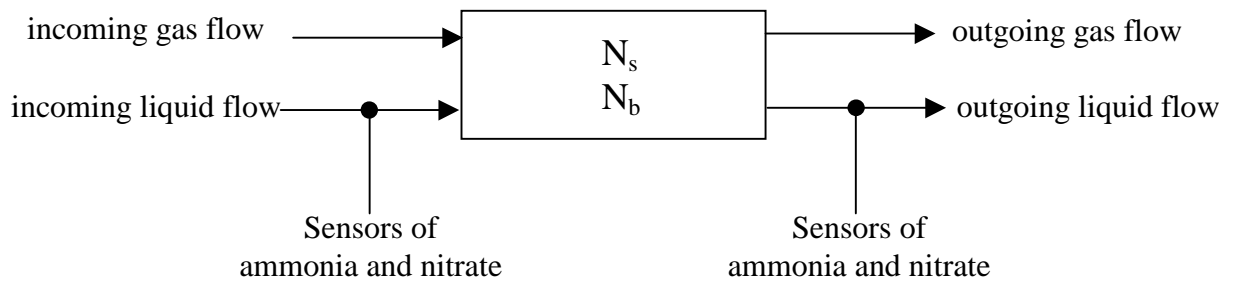
General flow sheet of a tank
(S = substrate , P = product)

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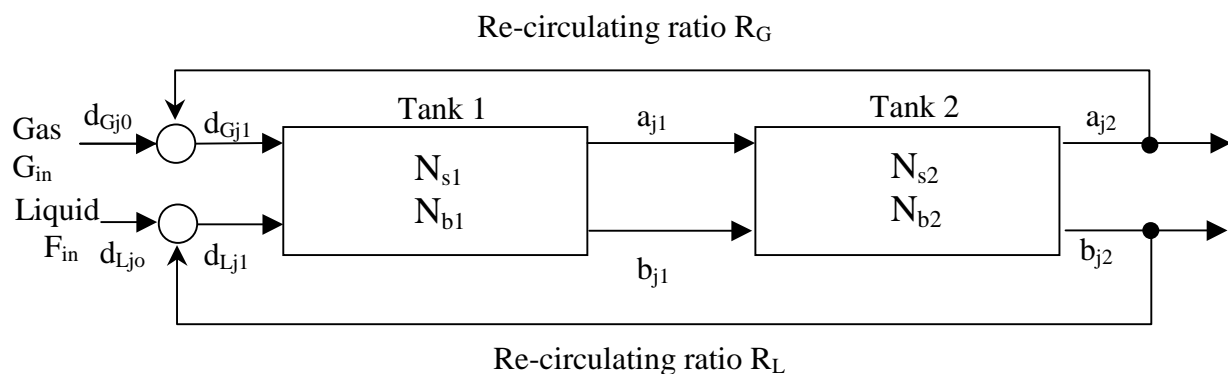
1. INTRODUCTION

In the previous study TN 48.1, three candidates of predictors are proposed. Their models, more or less complex, are recalled hereafter :

- **Predictor1** : the column is considered as only one tank in which the strains are equally distributed throughout the volume of liquid (scheme 1). The corresponding is a mere first order. Only 2 sensors of nitrate and 2 ones of ammonia are needed (1 at each end of the column).
- **Predictor2** : the column is assumed to be composed of 2 tanks (non necessarily equal) in each of which the strains are equally distributed and at different concentrations (scheme 2). 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).
- **Predictor3** : the column is a combination of these 2 previous models. It is still parted into 2 tanks of non necessarily equal volume but the biomass is presumed to be present only in the first one and null in the second one (scheme 3). This hypothesis lies on the fact that the strains migrate towards the input of the column where the concentrations of substrates are 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).



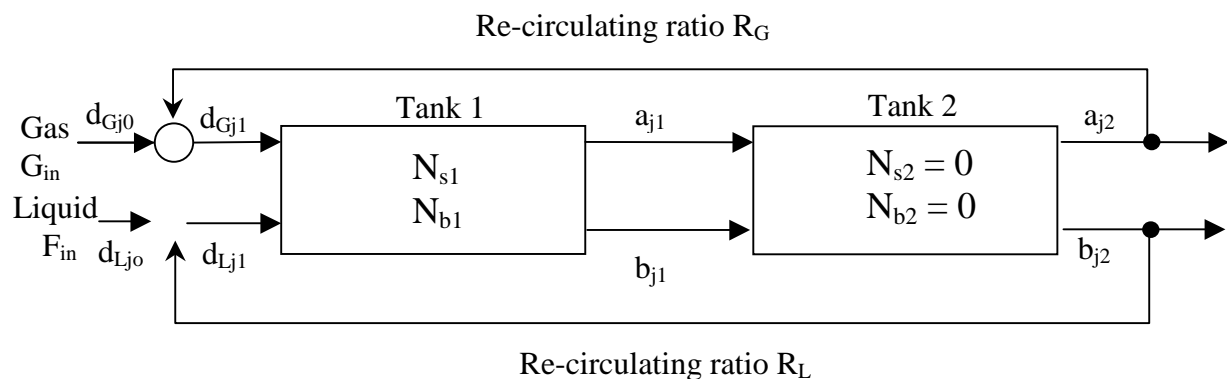
Scheme 1 : Model of the predictor 1



Scheme 2 : Model of the predictor 2

Substrate j : NH_3 , NO_3^- or NO_2^-

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Scheme 3 : Model of the predictor 3

In the present study, the 3 models are compared on their behaviours and robustness versus the noise of measurement and versus their parameters.

The reference behaviour is the one of the nitrite column done in standard conditions defined by the Laboratoire de Genie Chimique et Biologique in TN 27.2 :

- at the beginning, the strains are equally distributed throughout the fixed bed of the column;
- the concentrations of substrates in the incoming flow are standard and constant all along the duration (300 hours) of the simulation, excepted the ammonia concentration which is doubled at time $t=150$ h;
- the number of equivalent tanks of the fixed bed is set to 5.

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.

2. NITRITE PREDICTORS

2.1. Behaviours without mismatch and without noise

As the predictor models are simplified models of the column, none of them have the same behaviour as the column. This is recalled in the figure 1 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 to 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.

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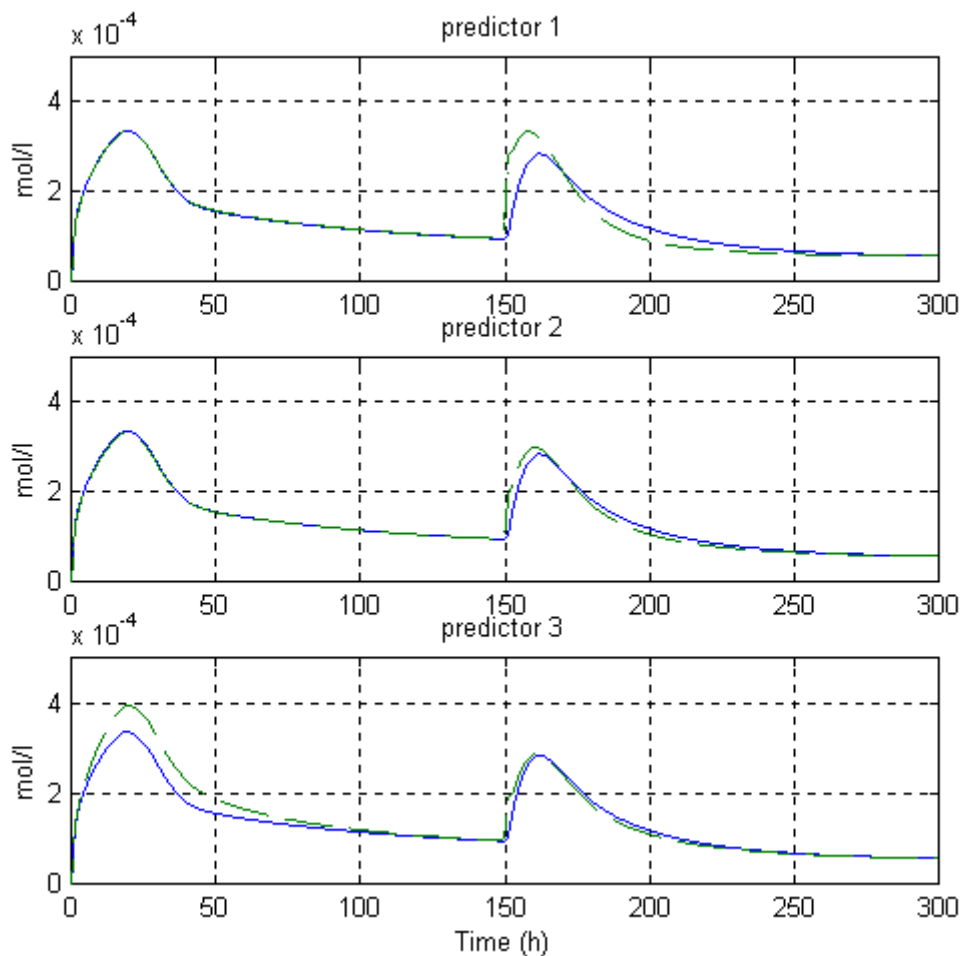


Figure 1 : Behaviour of the nitrite predictors (no noise , no mismatch)

2.2. Sensitivity

From the formulas (A.21) and (A.46) established in TN 48.1, the parameters of the predictors are :

- the dissociation constant k ;
- the stoichiometric factors β_1 and β_2 ;
- the time constant $\tau_L = V_L/F_{in}$;
- the equivalent gas/liquid equilibrium constant α ;
- the 'fresh' incoming gas and liquid flow rates G_{in} and F_{in} ;
- the gas and liquid re-circulating ratios R_G and R_L .

The next figures 2 to 10 illustrate the sensitivity of the nitrite predictors to each of these parameters. The simulated column is represented by the blue continuous lines and the predictors by the green dotted lines.

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1. Dissociation constant of ammonia : k

The figure 2 shows that only a 1 % mismatch on the dissociation constant of ammonia, k, causes a rather big static bias for all the predictors (k interferes in the static gain of the predictors with a big weight, as it will be explained in a following paragraph about static bias on measurement).

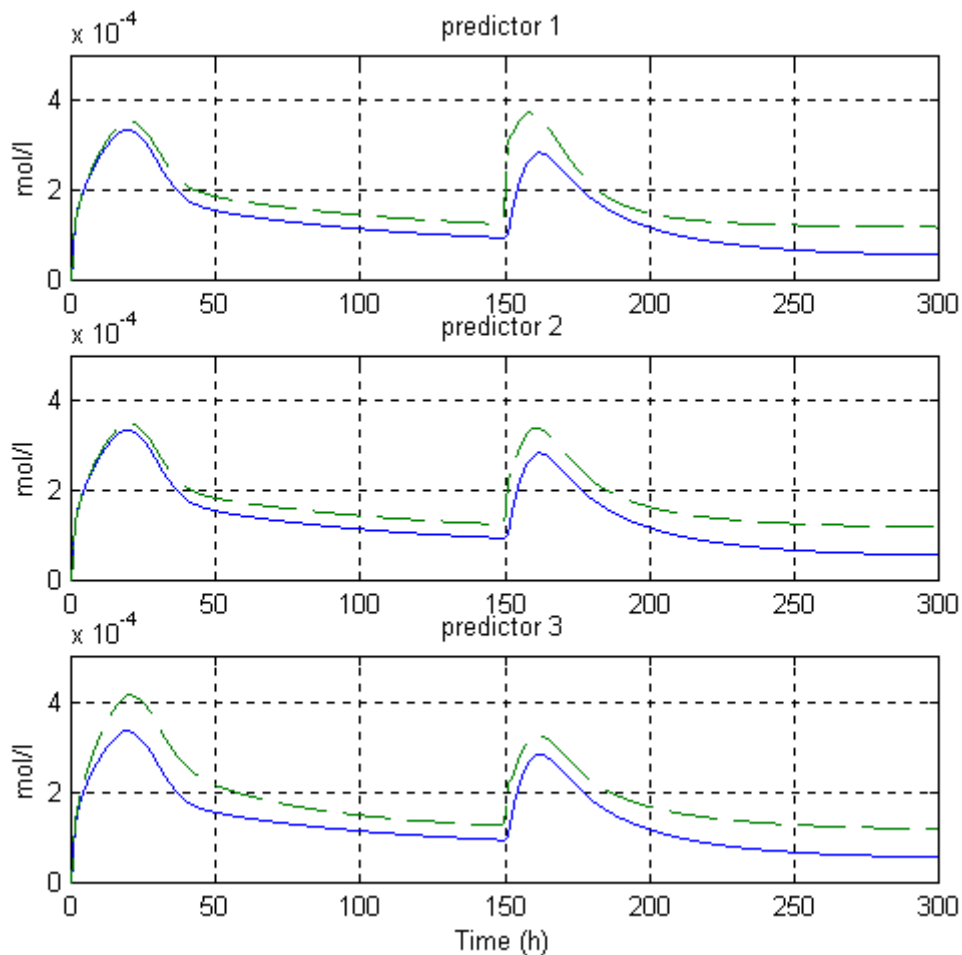


Figure 2 : 1% mismatch on the dissociation constant of ammonia k

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2. Stoichiometric factor β_1

As previously, the figure 3 shows that only a 1 % mismatch on the stoichiometric factor β_1 , causes a rather big static bias for all the predictors (β_1 interferes in the static gain of the predictors with a big weight, as the parameter k does).

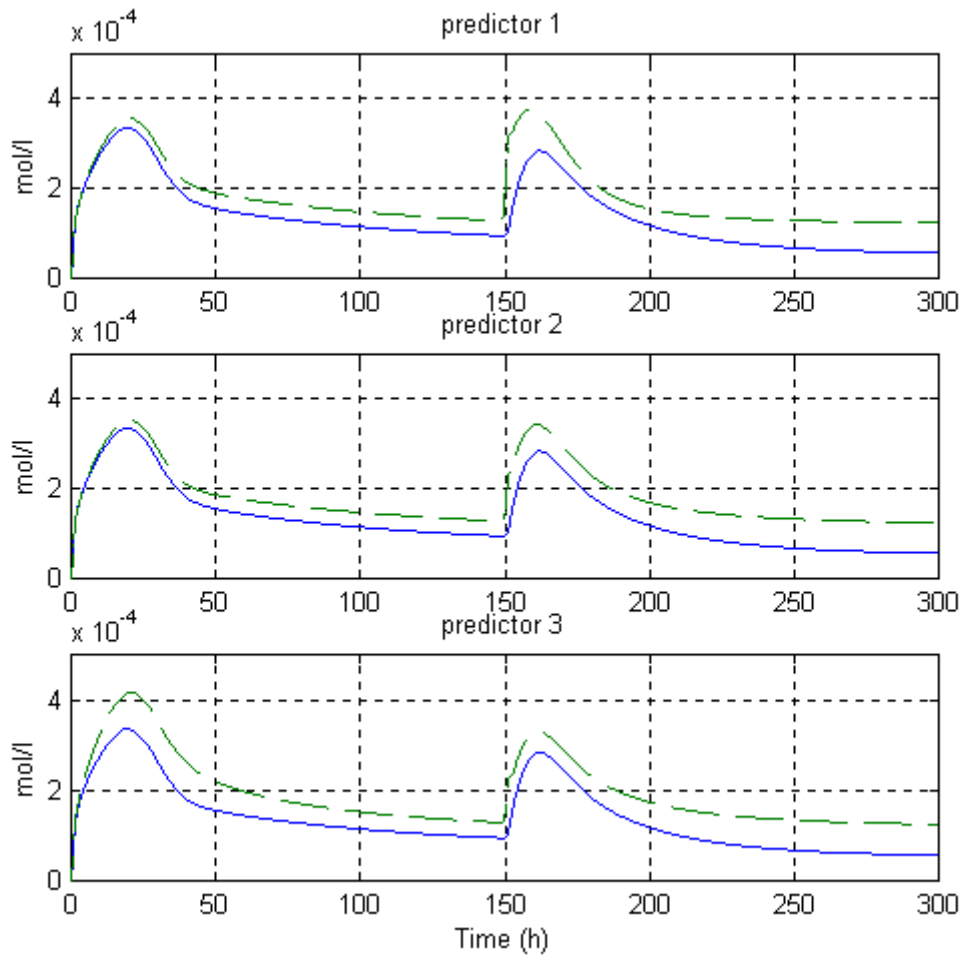


Figure 3 : 1% mismatch on the stoichiometric factor β_1

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3. Stoichiometric factor β_2

As for β_1 , the figure 4 shows that only a 1 % mismatch on the stoichiometric factor β_2 , causes a rather big static bias for all the predictors (β_2 interferes in the static gain of the predictors with a big weight).

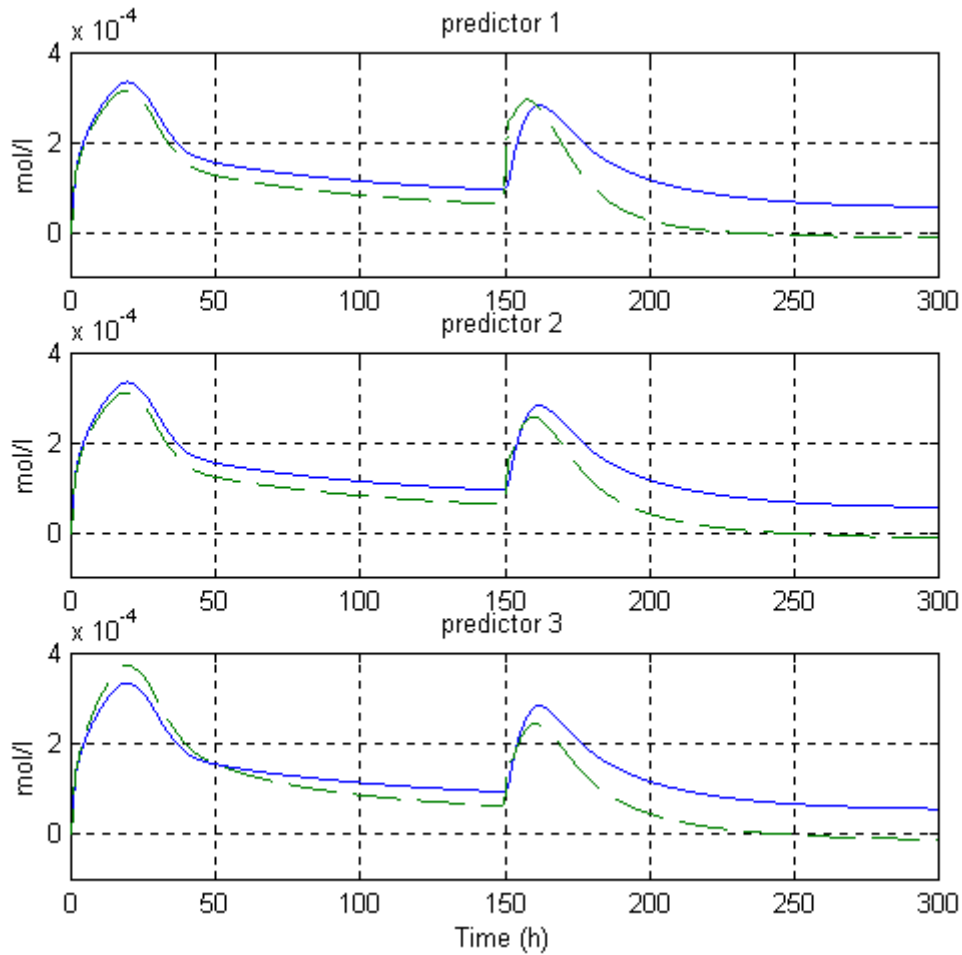


Figure 4 : 1% mismatch on the stoichiometric factor β_2

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4. Time constant $\tau_L = V_L/F_{in}$

The figure 5 shows that a 5 % mismatch on the time constant τ_L affects the dynamic of all the 3 predictors, particularly the one of the predictor 1 during long running of the column (top graph).

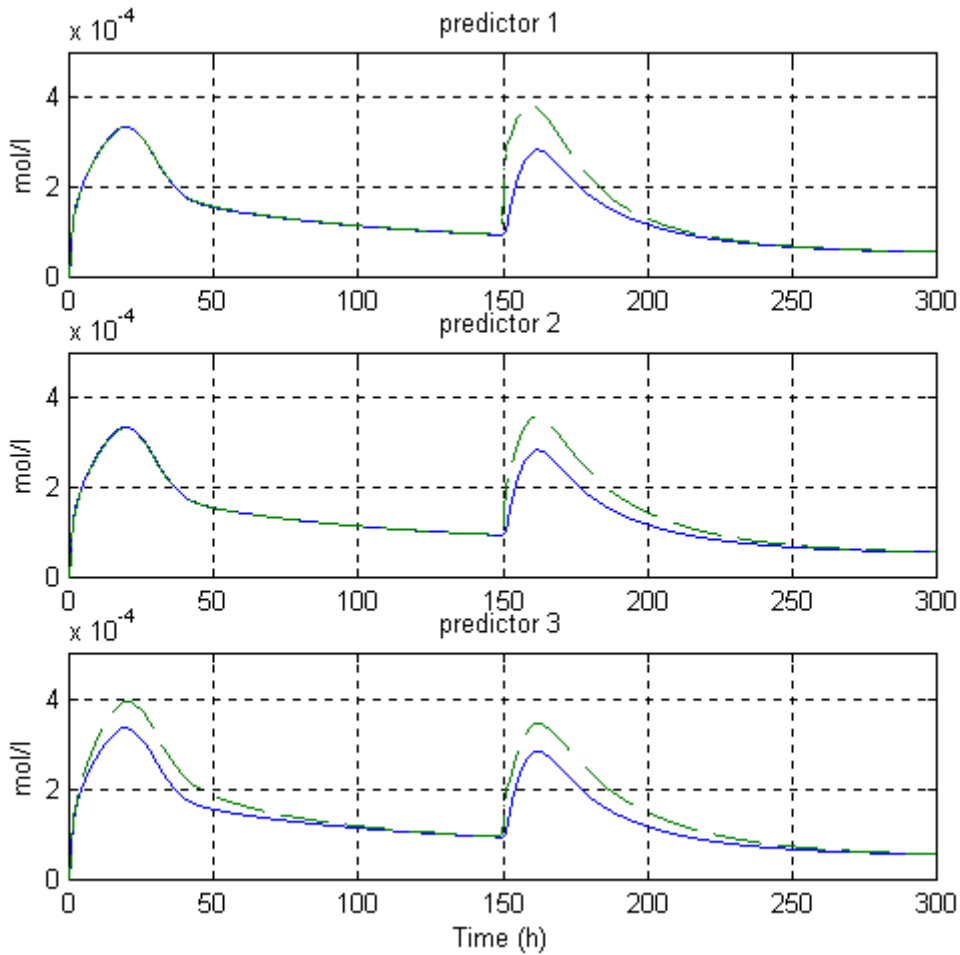


Figure 5 : 5% mismatch on the time constant τ_L

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5. Equivalent gas/liquid equilibrium constant α

The figure 6 shows that the impact of the equivalent gas/liquid equilibrium constant, α , is negligible on each of the predictors.

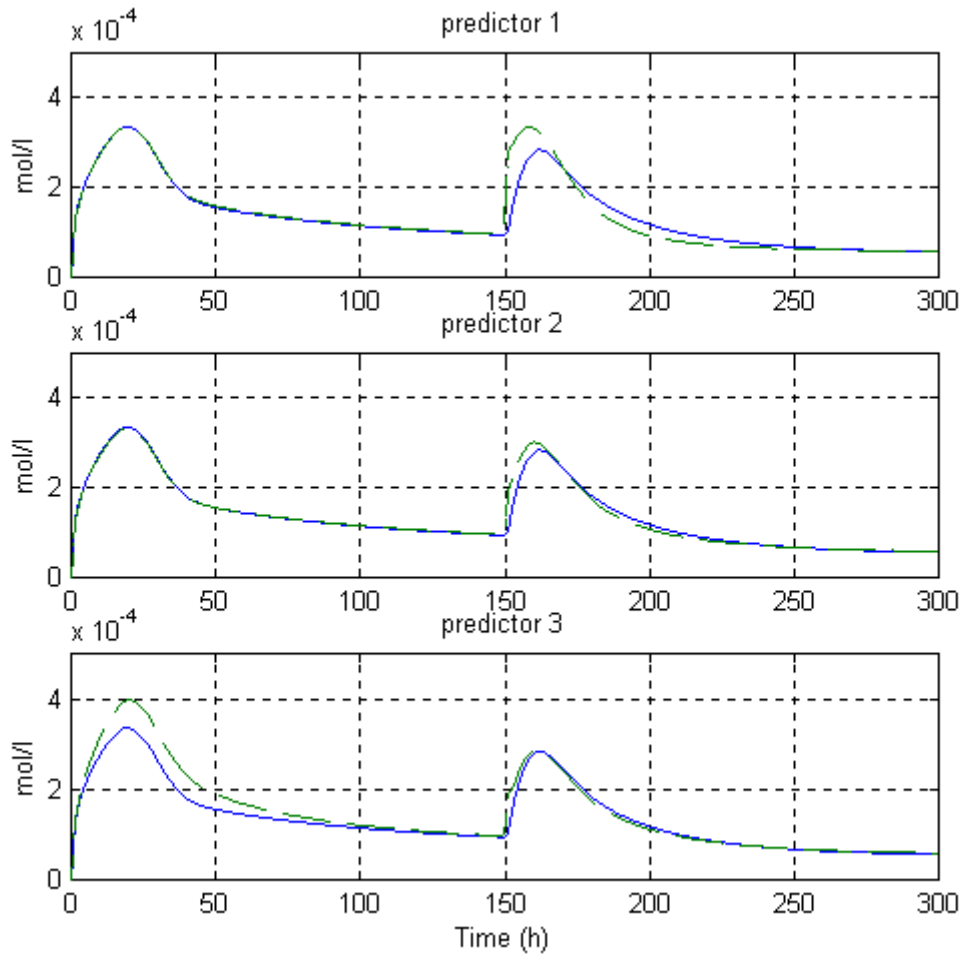


Figure 6 : 5% mismatch on the equivalent gas/liquid equilibrium constant α

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6. 'Fresh' incoming gas flow rate G_{in}

The figure 7 shows that the impact of the 'fresh' incoming gas flow rates, G_{in} , is negligible on each of the predictors.

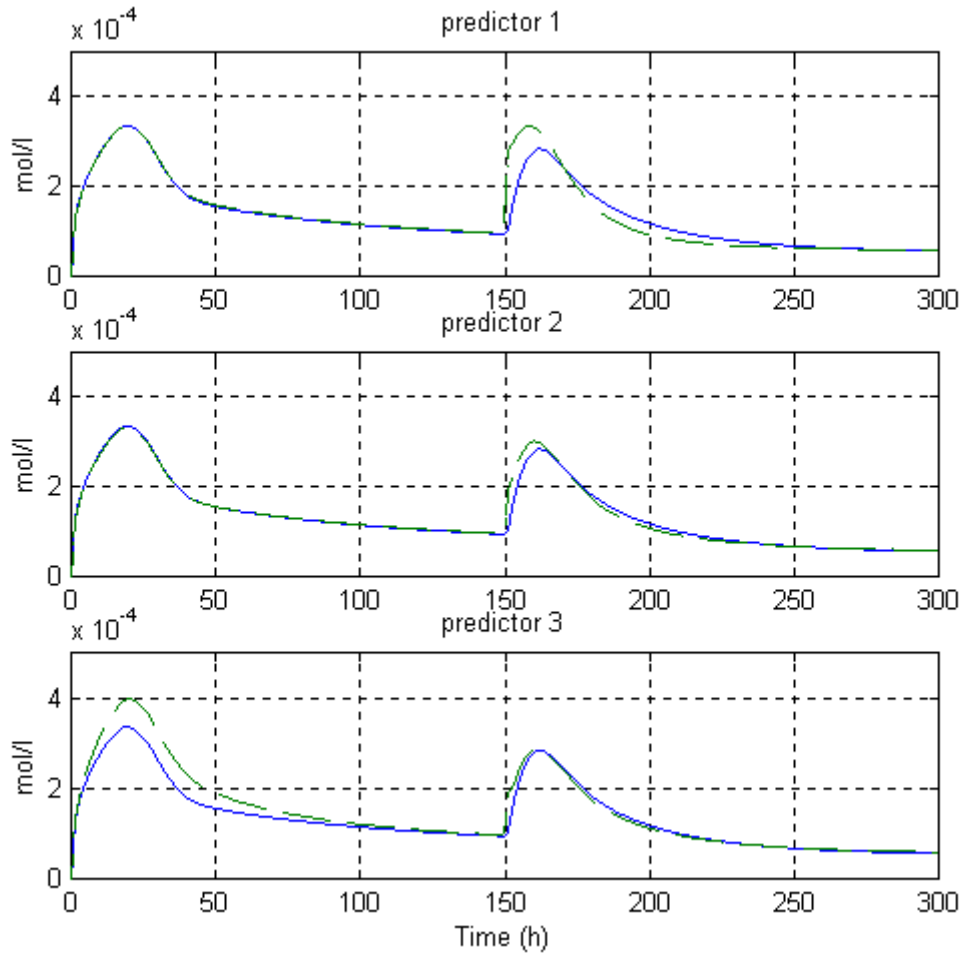


Figure 7 : 5% mismatch on the 'fresh' incoming gas flow rate G_{in}

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7. 'Fresh' incoming liquid flow rate F_{in}

The figure 8 shows that the impact of the 'fresh' incoming gas flow rates too, F_{in} , is negligible on each of the predictors.

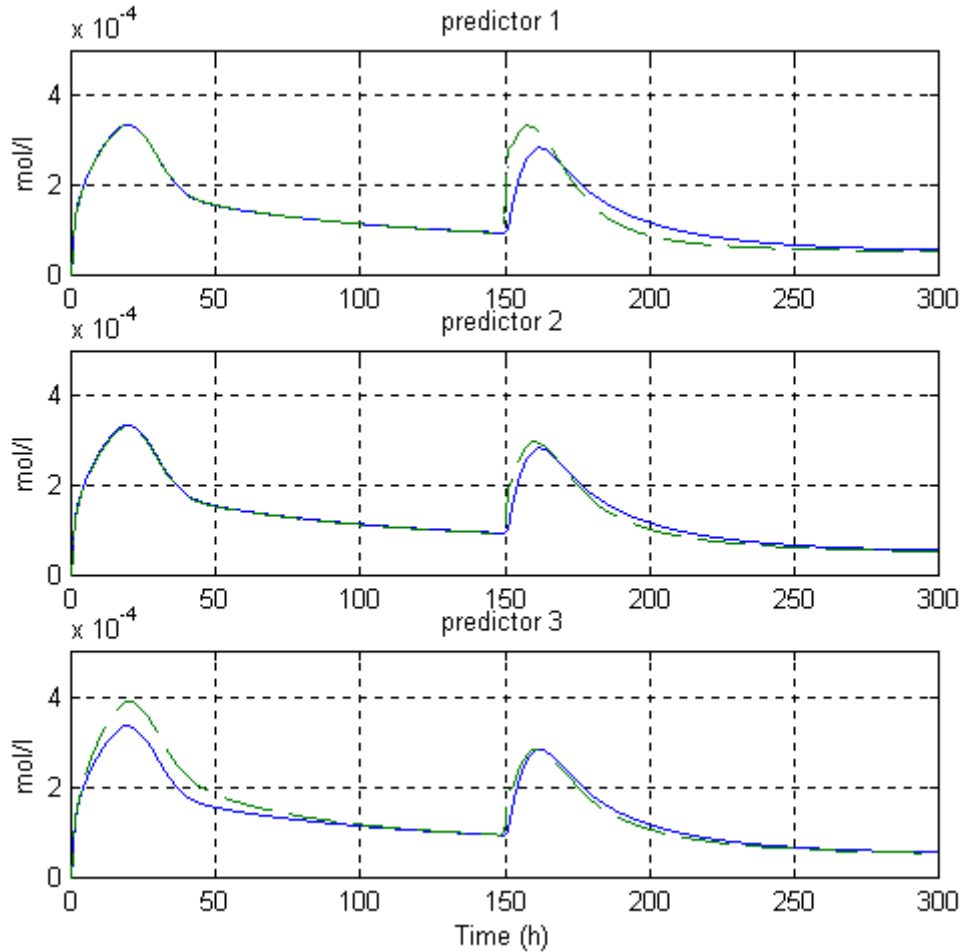


Figure 8 : 5% mismatch on the 'fresh' incoming liquid flow rate F_{in}

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8. Gas re-circulating ratio R_G

The figure 9 shows that the impact of the gas re-circulating ratio too, R_G , is negligible on each of the predictors.

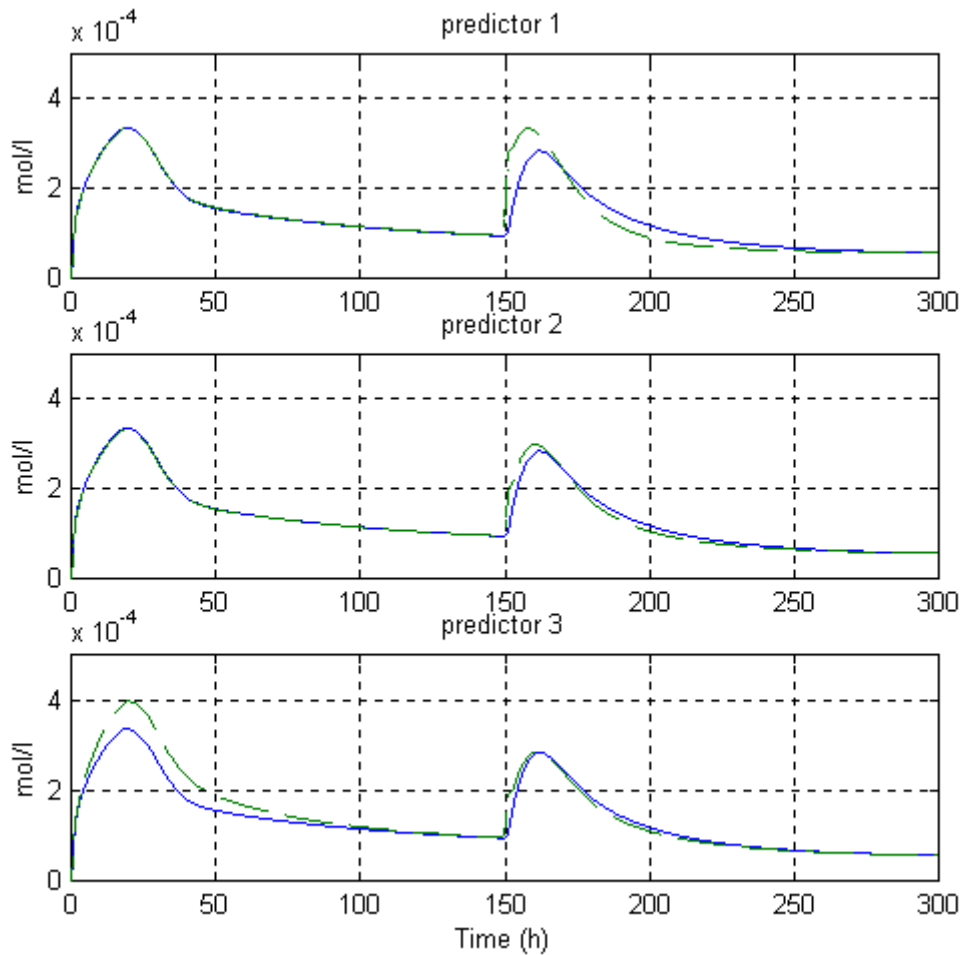


Figure 9 : 5% mismatch on the gas re-circulating ratio R_G

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9. Liquid re-circulating ratio R_L

The figure 10 shows that the impact of the liquid re-circulating ratio too, R_L , is negligible on each of the predictors.

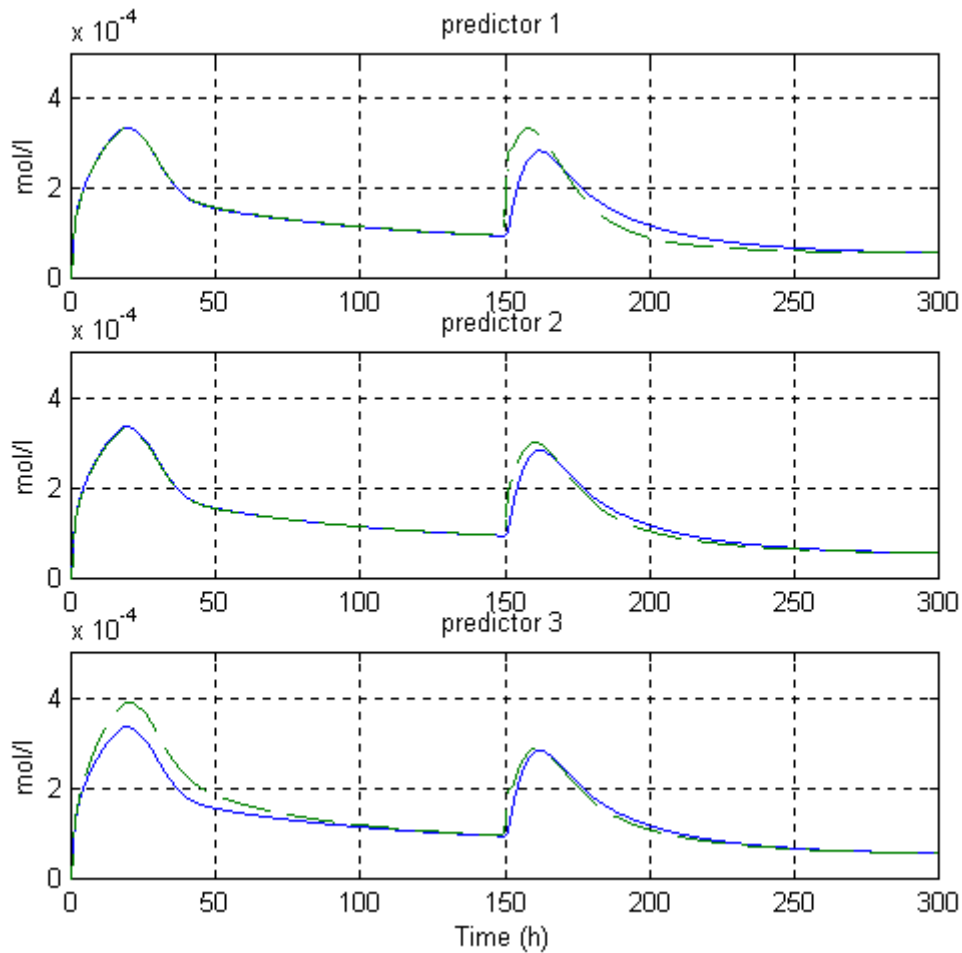


Figure 10 : 5% mismatch on the liquid re-circulating ratio R_L

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2.3. Measurements with white noise

A white noise on the measurements of nitrate and ammonia (equal to $\pm 10^{-4}$ mol/l) does not affect the estimations (figure 11).

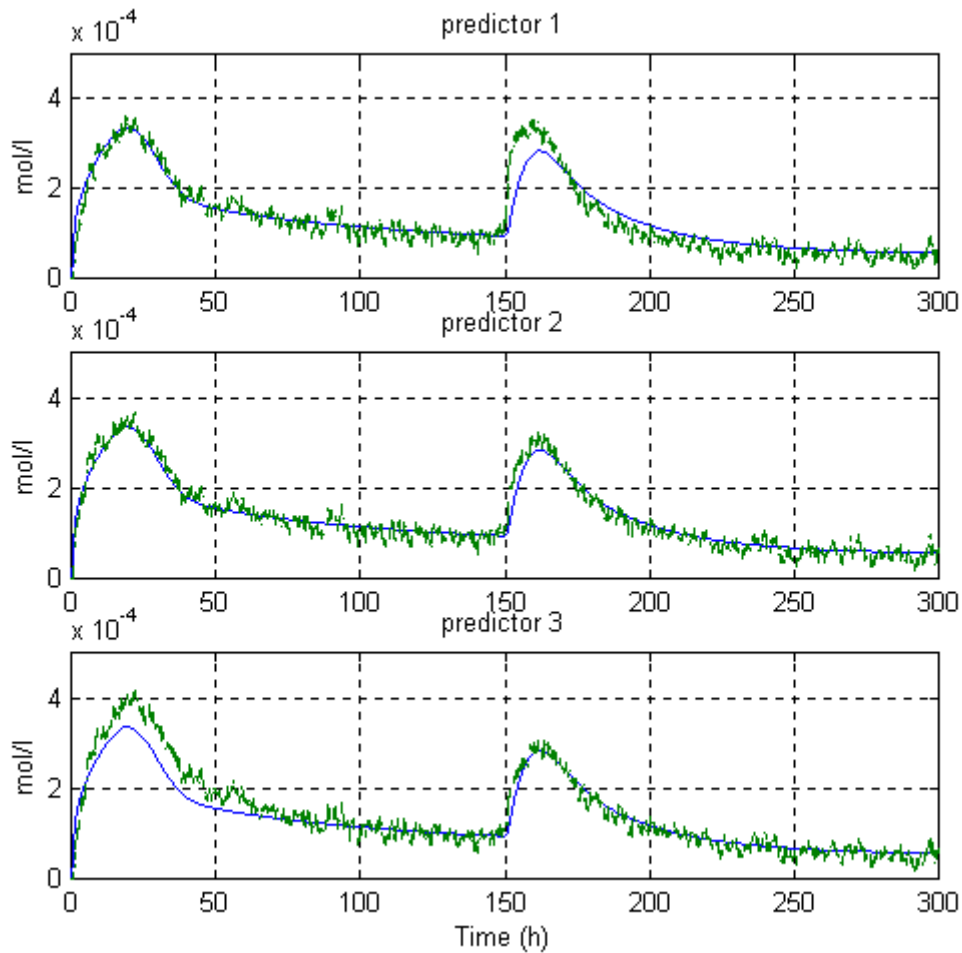


Figure 11 : White noise on nitrate and ammonia measurements : $\pm 10^{-4}$ mol/l

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2.4. Static bias on measurement

The effect of a bias on the measurements of ammonia and nitrate is studied on the model of the predictor 1. The results would be the same for the 2 other predictors.

The expression of the nitrite concentration at column output is recalled hereafter, for the predictor 1 (from (A.20) of TN 48.1) :

$$b_3 = s_2 - s_1$$

$$\text{with } s_2 = \beta_1 \left(1 + k + \alpha \cdot \frac{q_G}{q_L} \right) \cdot b_1 + \beta_2 \cdot b_2$$

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

$$e = \beta_1 \left(1 + k + \alpha \cdot \frac{q_G}{q_L} \right) \cdot d_{L1} + \beta_2 \cdot d_{L2}$$

The factors β_1 and β_2 are scalar (dimension less) and their values are close to -1 ($\beta_1 = -0.966$ and $\beta_2 = -1.02$). The other terms are physical parameters or concentration measurements that are positive.

So the nitrite concentration, b_3 , is the difference between 2 variables s_1 and s_2 that have both the same sign (negative) and whose absolute value are close to each other (about 10^{-2} mol/l) and great versus their difference ($s_1 - s_2$ equals about 10^{-4} mol/l).

Consequently a static bias on the measurements (b_1 , b_2 , d_{L1} and d_{L2}) will induce a static bias on the nitrite prediction. This static bias has to be compensated with a corrective term whose value will be calculated from time to time by comparing the modelled nitrite concentration to the actual one obtained from laboratory analysis.

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Figure 12 illustrates a 1% static bias on the ammonia measurement in the ‘fresh’ incoming liquid flow.

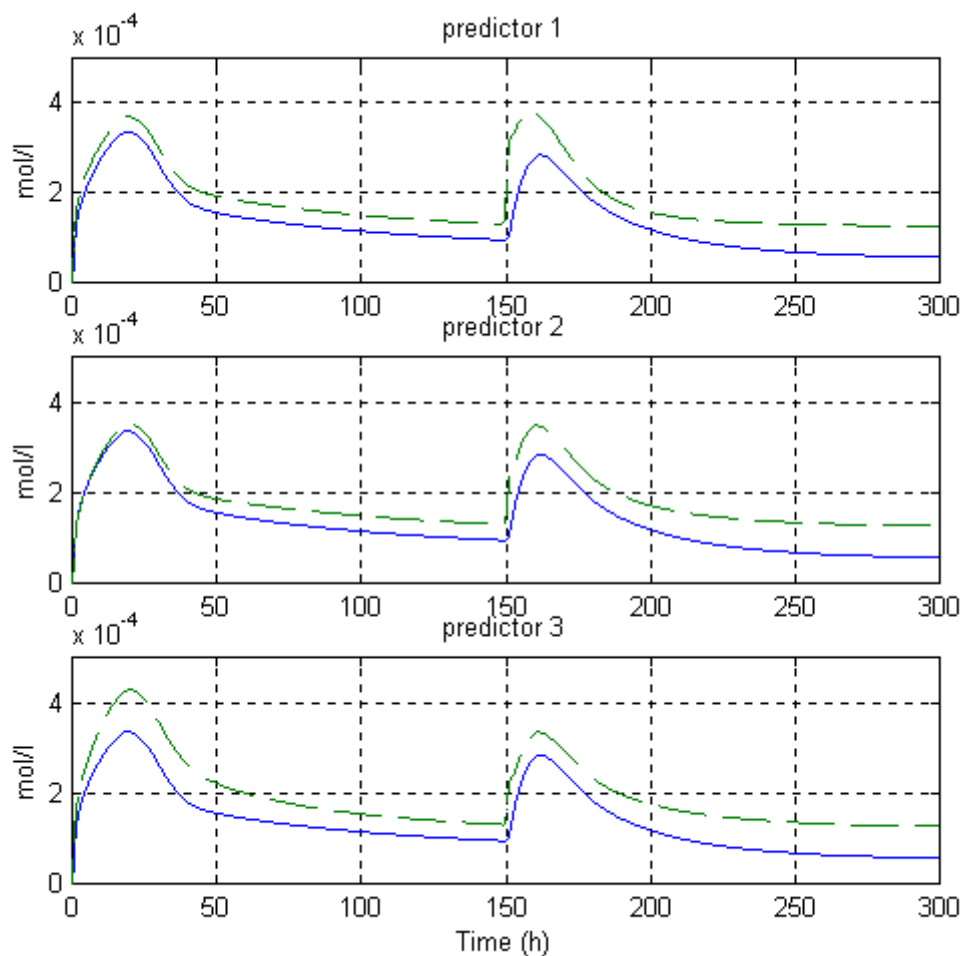


Figure 12 : 1 % static bias on the ammonia measurement in the incoming flow

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2.5. Hypothesis H1

The so called hypothesis *H1* has been introduced in the paragraph A.1.3. of TN 48.1 relative to the expression of the variation rate of the nitrite versus the variation rates of ammonia and nitrate. According to this hypothesis, the growth limiting factor and the maintenance limiting factor are identical for each strain :

$$V_{G1} = V_{M1}$$

(Hypothesis *H1* in TN 48.1)

$$V_{G2} = V_{M2}$$

The figure 13 illustrates the case where *H1* is not true : the half maximum maintenance rate saturation constant of the simulated column is the tenth part of the growth one. It causes a bias on the predicted nitrite concentration. This static bias will also be compensated by a corrective term.

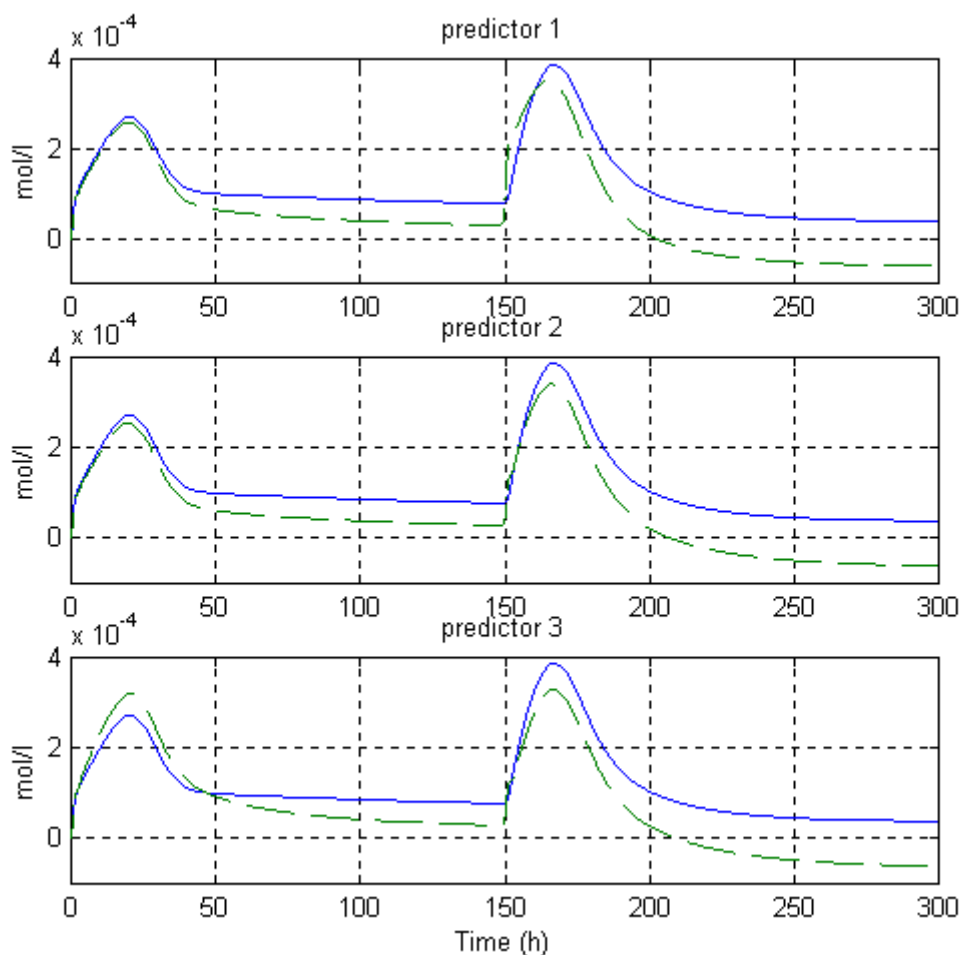


Figure 13 : Case where hypothesis *H1* is not true

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2.6. Choice of the nitrite predictor

From the previously studied points, it results that :

- The predictor 1 is good for a starting column and during steady state running and it is bad during transient behaviour of a long term running column;
- The predictor 2 is satisfactory at any time but requires a supplementary sensor of ammonia and one of nitrate in the middle of the column;
- The predictor 3 is good for transient in long term running column and in steady state and it is bad for a starting column.

So the resulting nitrite predictor will be composed of :

- predictor 1 for a starting column and its output will be taken into account each time a column is restarted (after maintenance operation, for example);
- predictor 3 for a long term running column.

The parameters of these 2 estimators will be identified by means of real tests.

Due to inevitable static bias on the measurements, the modelled nitrite concentration will be corrected, from time to time (twice a week, probably), from laboratory analysis. Thanks to this correction the predicted nitrite will be reliable during transient behaviour, which is the critical period because of possible peak of nitrite.

2.7. Expression of the nitrite predictors

2.6.1. Predictor 1

Starting from the expression (A.21) in TN48.1 of the nitrite concentration b_3

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

the nitrite predictor is :

$$\hat{b}_3 = \gamma_1 \cdot \left(\hat{b}_1 - \frac{1}{1 + \tau \cdot p} \cdot \hat{d}_{L10} \right) + \gamma_2 \cdot \left(\hat{b}_2 - \frac{1}{1 + \tau \cdot p} \cdot \hat{d}_{L20} \right) + \gamma_3 \quad (1)$$

where :

- \hat{d}_{L10} and \hat{d}_{L20} are, respectively, ammonia and nitrate concentrations in the 'fresh' incoming liquid flow of the column (whose flow rate is F_{in});
- \hat{b}_1 and \hat{b}_2 are, respectively, ammonia and nitrate concentrations at output of the column;
- γ_1 , γ_2 and τ are identified through tests on the real nitrifying column;
- γ_3 is a corrective term to compensate the static bias of the measurements and the static bias due to the fact that the Monod constants are different for growth rate and maintenance rate (hypothesis *H1* not true).

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2.6.2. Predictor 3

Starting from the expression of the nitrite concentration (A.46) of TN 48.1,

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

with

$$H_1 = \frac{1}{(1 + \theta_1 \cdot p) \cdot (1 + \theta_2 \cdot p)} \quad \text{from (A.40) of TN 48.1}$$

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

and

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

$$\text{with } \varepsilon_1 = \chi \cdot (1 - \chi_0) \cdot \frac{V_{L2}}{F_{in}} - \chi_0 \cdot \frac{V_L}{F_{in}} \quad \text{from (A.44) of TN 48.1}$$

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

the formula of the nitrite predictor 3 is :

$$\hat{b}_3 = \gamma_1 \cdot (H_2 \cdot \hat{b}_{12} - H_1 \cdot \hat{d}_{L10}) + \gamma_2 \cdot (\hat{b}_{22} - H_1 \cdot \hat{d}_{L20}) + \gamma_3 \quad (2)$$

with :

$$H_1 = \frac{1}{(1 + \theta_1 \cdot p) \cdot (1 + \theta_2 \cdot p)}$$

$$\theta_1, \theta_2 = \frac{\tau}{2} \cdot \left(1 \pm \sqrt{1 - \frac{4 \cdot V_{L1} \cdot V_{L2}}{(1 + R_L) \cdot V_L^2}} \right)$$

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

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

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

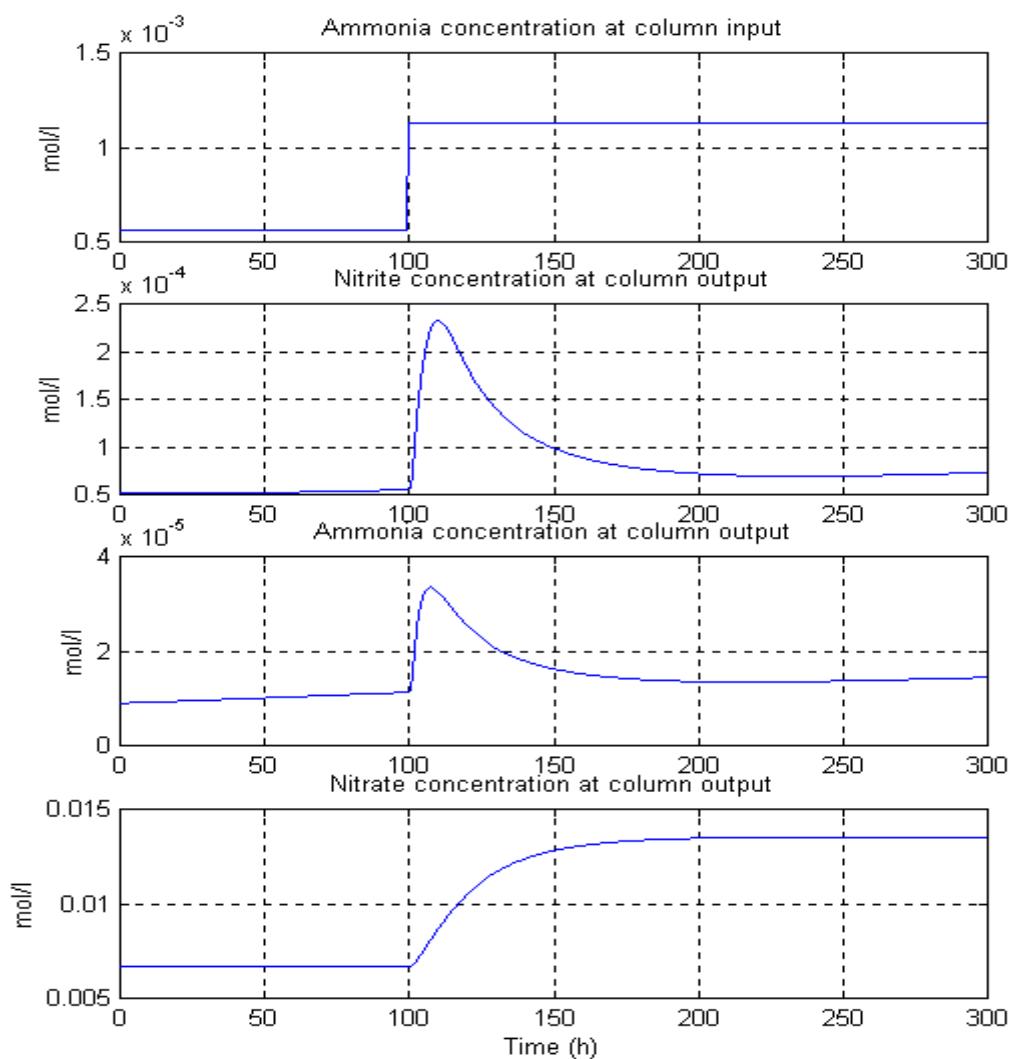
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where \hat{d}_{L10} , \hat{d}_{L20} , \hat{b}_{12} , \hat{b}_{22} , τ , γ_1 , γ_2 and γ_3 have same meaning as in the formula (1) of the predictor 1.

2.7. Identification of the parameters of the nitrite predictors

For identification, the process will be excited by steps on the ammonia concentration in the incoming flow (figure 14). The sampling period of the data acquisition (ammonia and nitrate in the incoming and outgoing flow) will be between 0.1 and 0.25 hour.

The static coefficients (γ_1 , γ_2 and γ_3) and the time constants of the relations (1) and (2) will be tuned so that to minimize the distance process/model.



**Figure 14 : Step of ammonia in the incoming flow
Expected responses of the column**

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Nitrite measurements of the outgoing flow are necessary. As these measurements are not easy, the number of samples will be as low as possible : 1 sample per 10 hours during steady state running and 1 sample per 2 hours during transient behaviour.

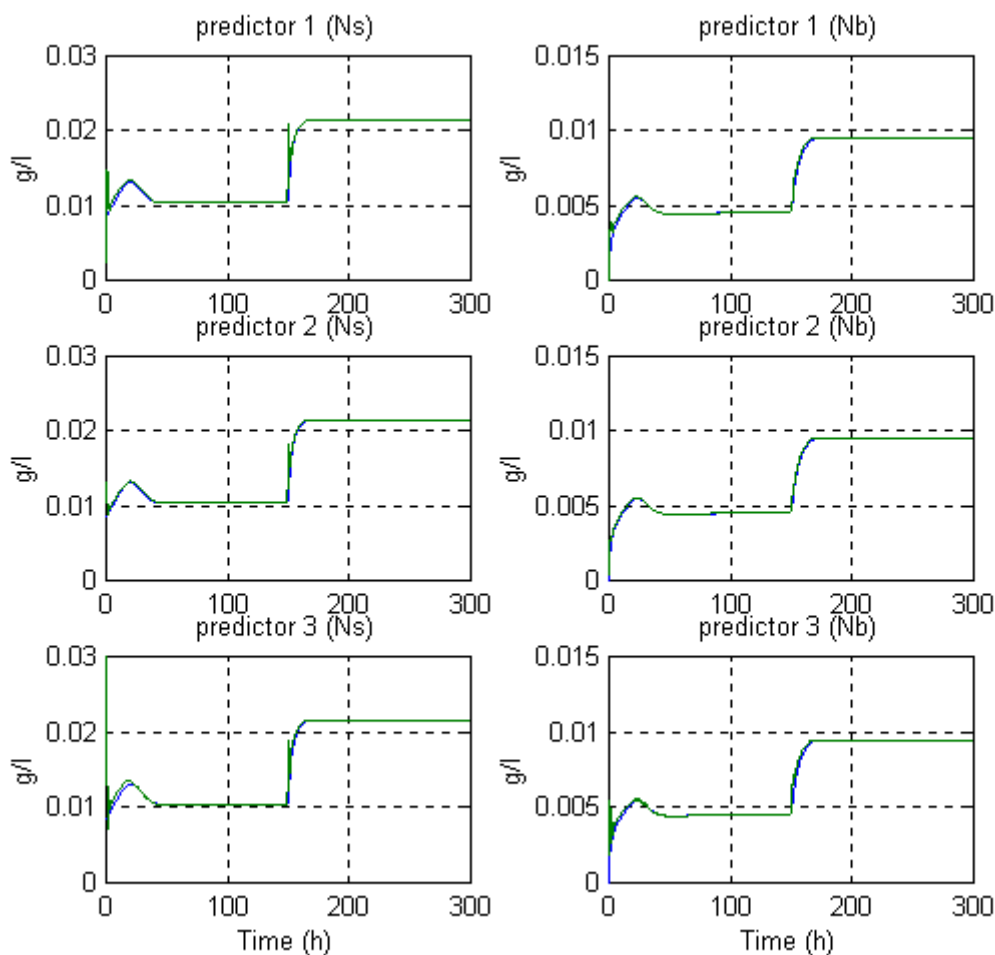
The time constant τ has to be identified versus the liquid flow rate.

3. BIOMASS PREDICTORS

3.1. Behaviours without mismatch and without noise

The biomass which can be estimated is the ‘productive’ biomass, i.e. the variable represented by the multiplication of the active biomass and of the limiting factor. It represents the quantity of biomass which consumes substrates and makes the products.

The figure 15 shows the behaviour of the 3 predictors when there is no noise nor mismatch : there is only little differences between them, as demonstrated in TN48.1 .



**Figure 15 : Behaviour of the Ns and Nb biomass predictors (no noise , no mismatch)
(column : solid or blue line | predictors : dotted or green line)**

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3.2. Sensitivity

From the formulas (A.23) and (A.51) established in TN 48.1, the parameters of the biomass predictors are :

- the dissociation constant k ;
- the stoichiometric factors δ ;
- the time constant $\tau_L = V_L/F_{in}$;
- the equivalent gas/liquid equilibrium constant α ;
- the 'fresh' incoming gas and liquid flow rates G_{in} and F_{in} ;
- the gas and liquid re-circulating ratios R_G and R_L .

The next figures 16 to 23 illustrate the sensitivity of the biomass predictors to each of these parameters. The simulated column is represented by the blue continuous lines and the predictors by the green dotted lines.

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1. Dissociation constant of ammonia : k

The figure 16 shows that a 1 % mismatch on the dissociation constant of ammonia, k, does not affect particularly the biomass estimations for all the predictors.

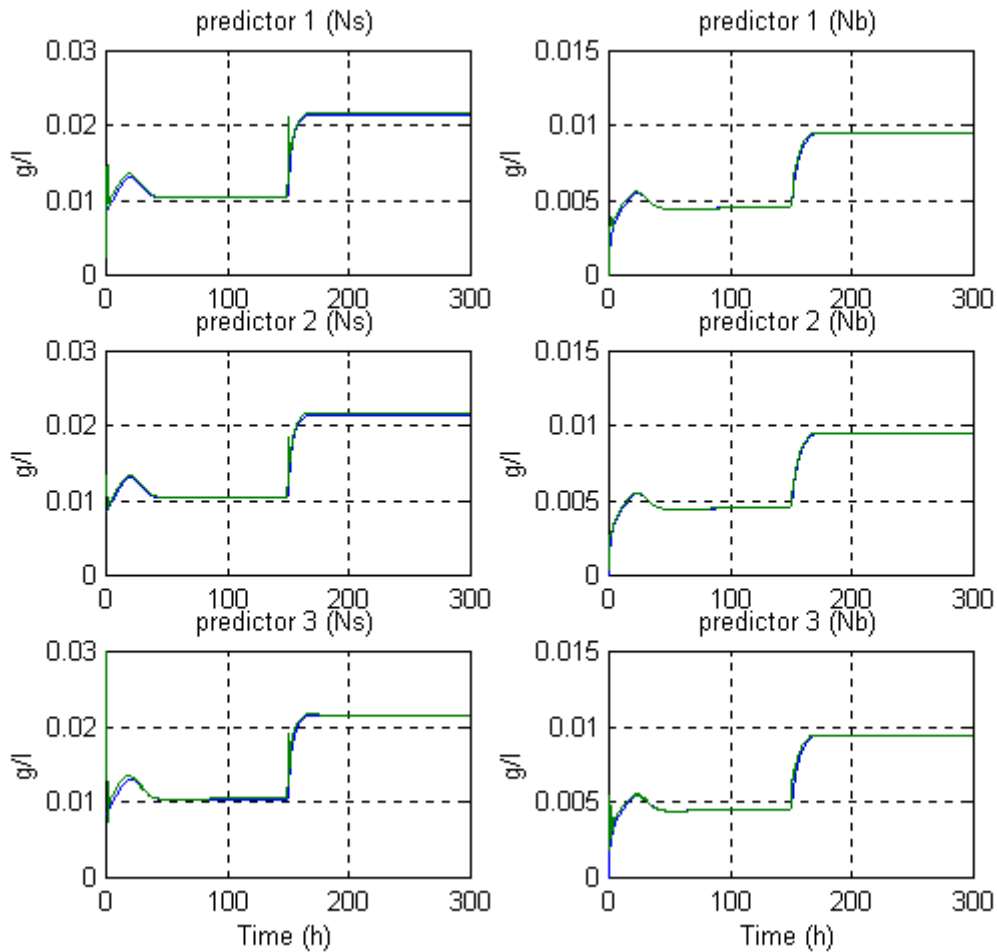


Figure 16 : 1% mismatch on the dissociation constant of ammonia k

2. Stoichiometric factors δ

The figure 17 shows that a 5 % mismatch on the stoichiometric factors δ , causes a 5% error on the biomass estimations for all the predictors.

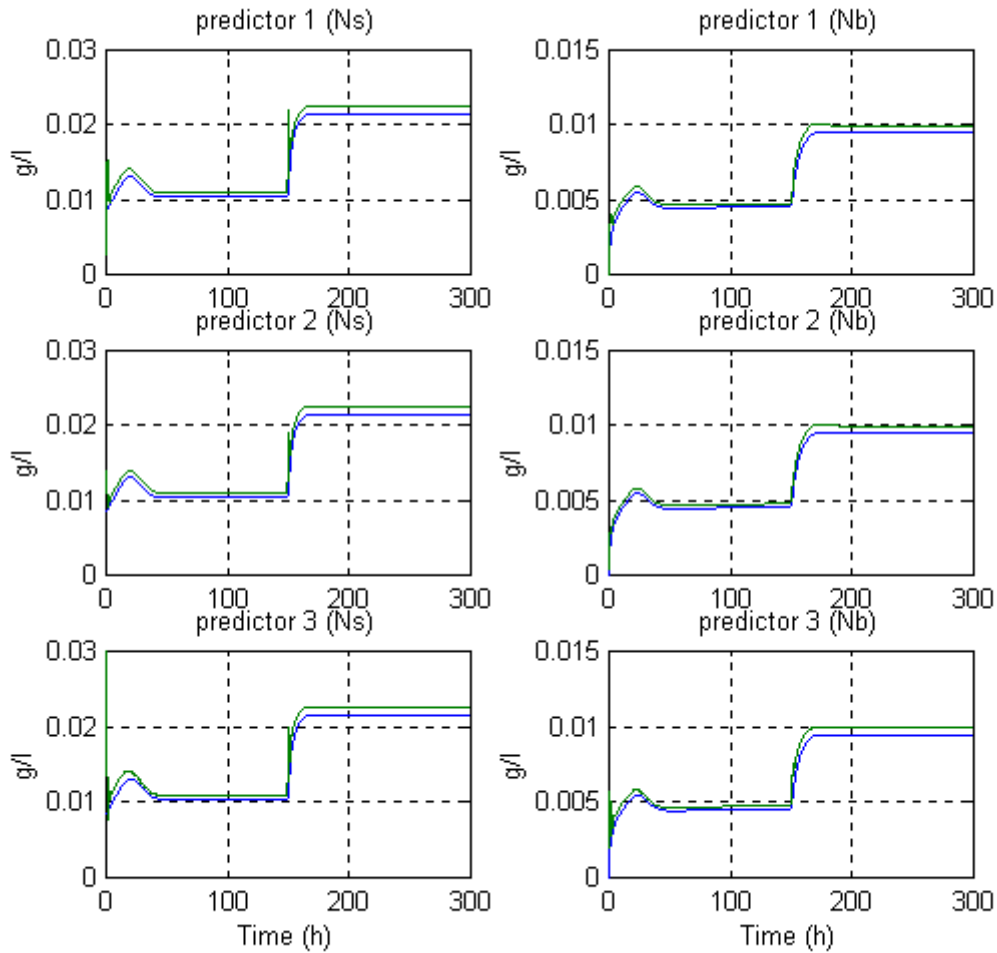


Figure 17 : 1% mismatch on the stoichiometric factors δ

3. Time constant $\tau_L = V_L/F_{in}$

The figure 18 shows that a 5 % mismatch on the time constant τ_L causes a 5% error on the biomass estimations for all the 3 predictors.

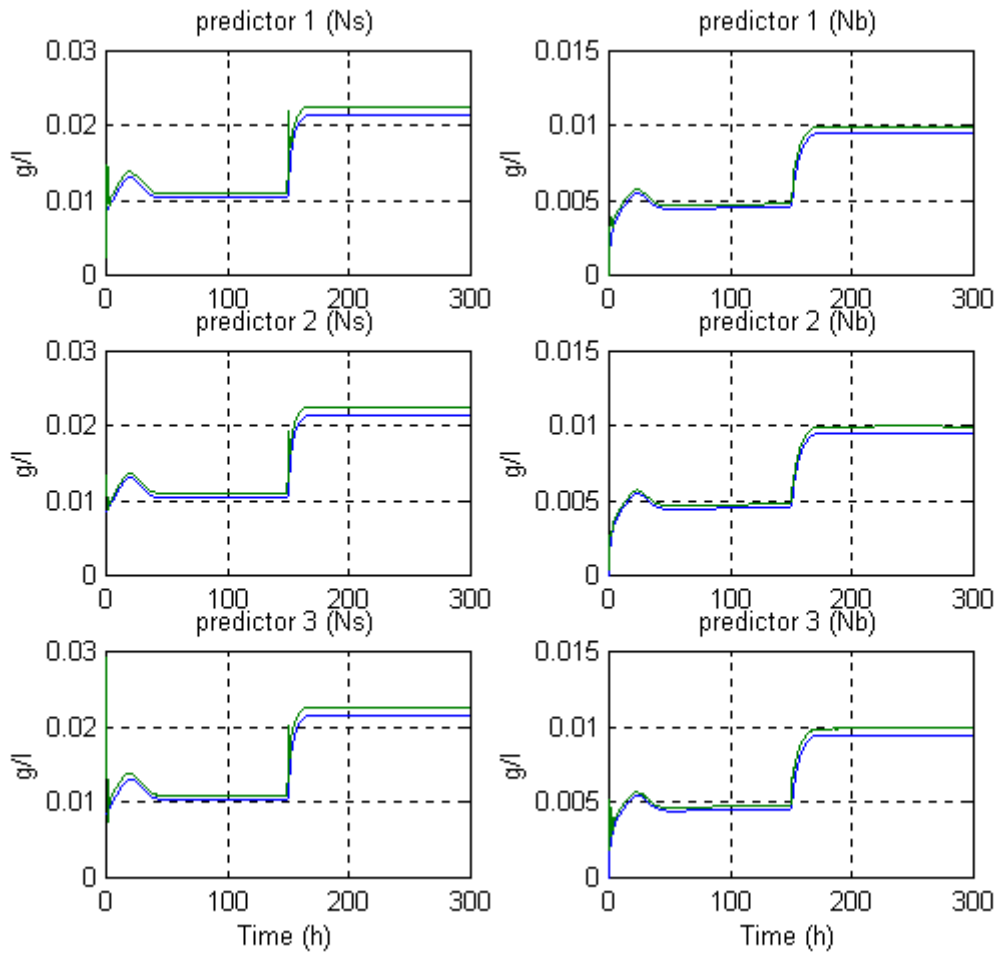


Figure 18 : 5% mismatch on the time constant τ_L

4. Equivalent gas/liquid equilibrium constant α

The figure 19 shows that the impact of the equivalent gas/liquid equilibrium constant, α , is negligible on each of the predictors.

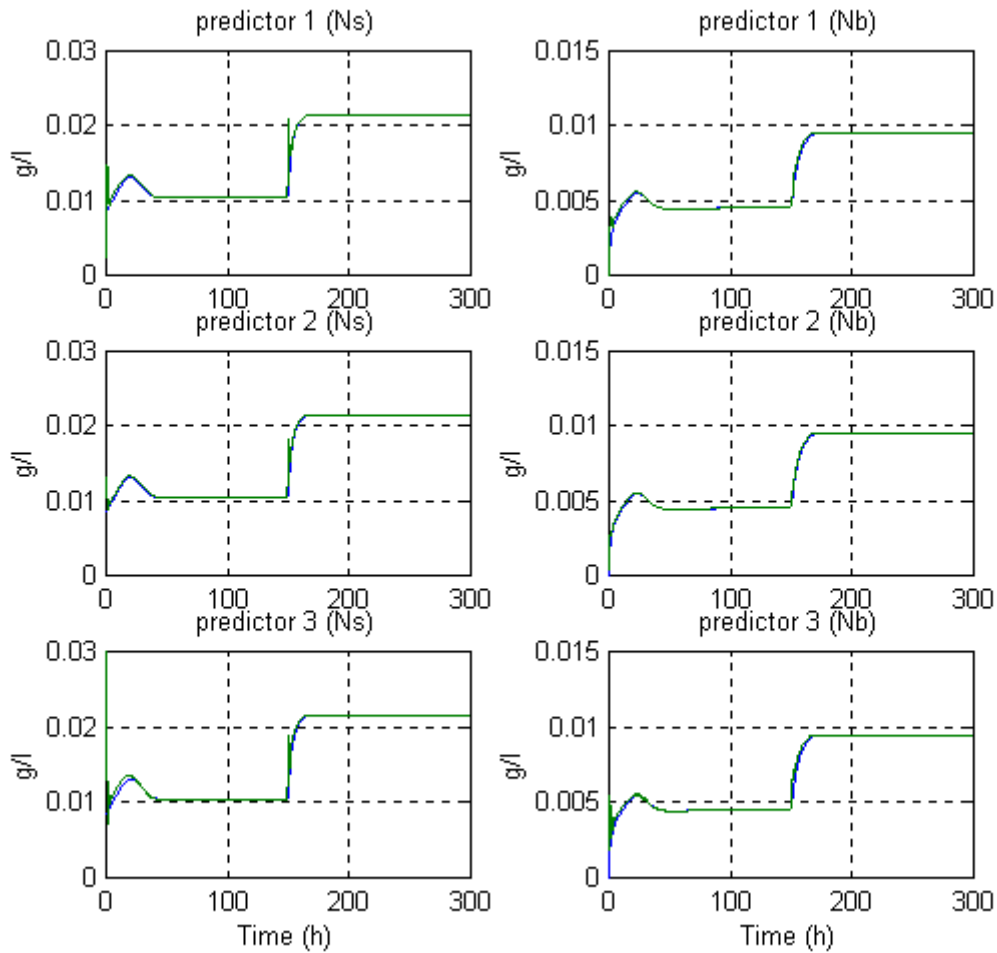


Figure 19 : 5% mismatch on the equivalent gas/liquid equilibrium constant α

5. 'Fresh' incoming gas flow rate G_{in}

The figure 20 shows that the impact of the 'fresh' incoming gas flow rates, G_{in} , is negligible on each of the predictors.

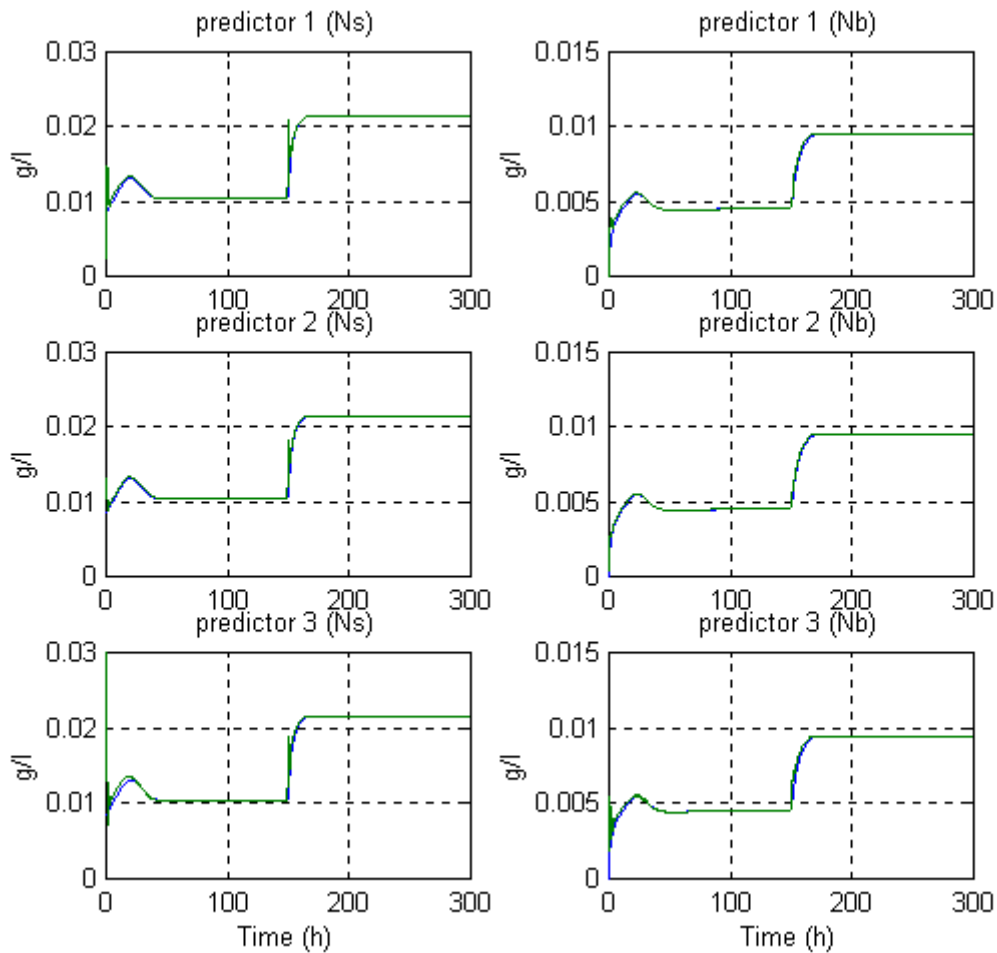


Figure 20 : 5% mismatch on the 'fresh' incoming gas flow rate G_{in}

6. 'Fresh' incoming liquid flow rate F_{in}

The figure 21 shows that the impact of the 'fresh' incoming gas flow rates too, F_{in} , is negligible on each of the predictors.

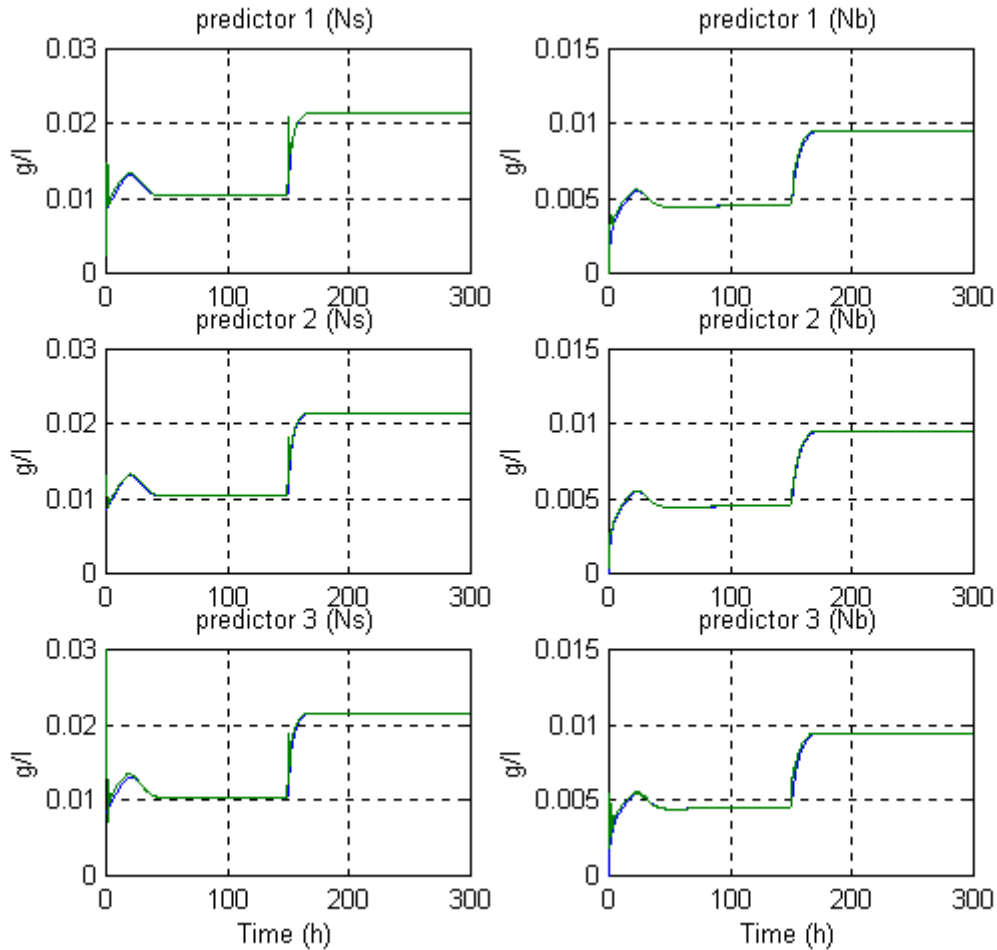


Figure 21 : 5% mismatch on the 'fresh' incoming liquid flow rate F_{in}

7. Gas re-circulating ratio R_G

The figure 22 shows that the impact of the gas re-circulating ratio too, R_G , is negligible on each of the predictors.

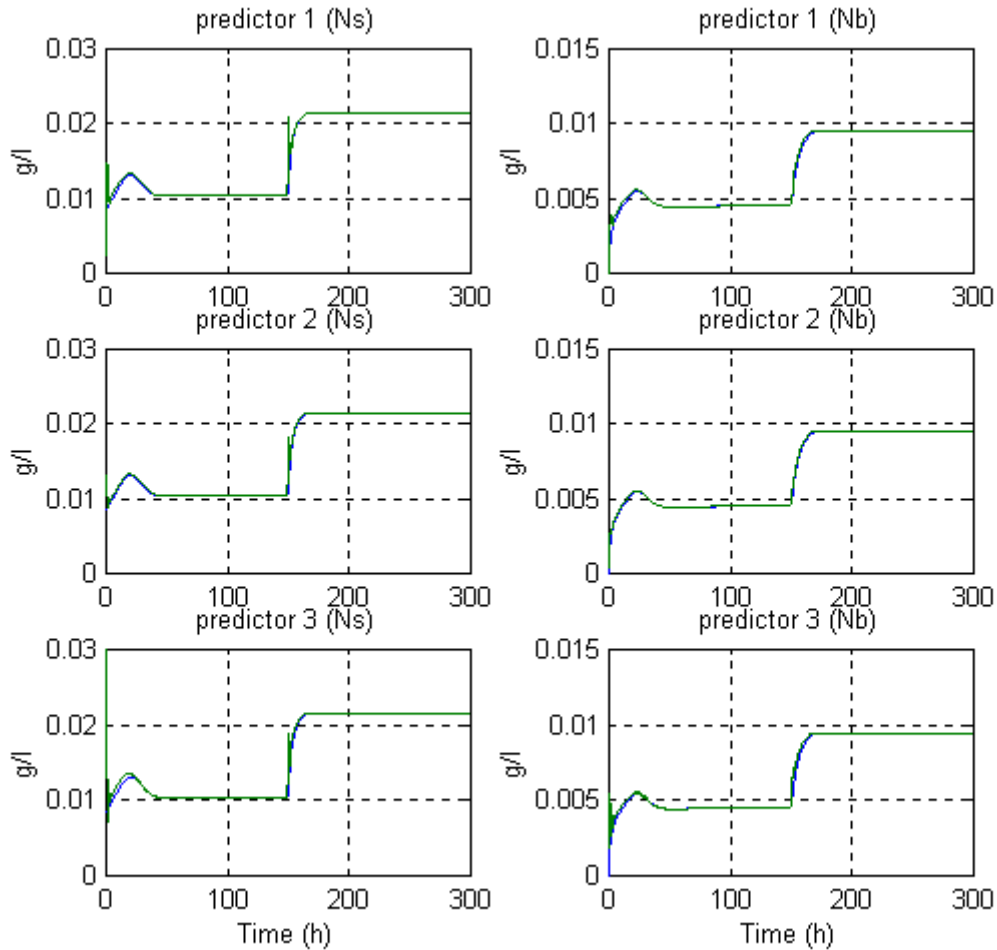


Figure 22 : 5% mismatch on the gas re-circulating ratio R_G

8. Liquid re-circulating ratio R_L

The figure 23 shows that the impact of the liquid re-circulating ratio too, R_L , is negligible on each of the predictors.

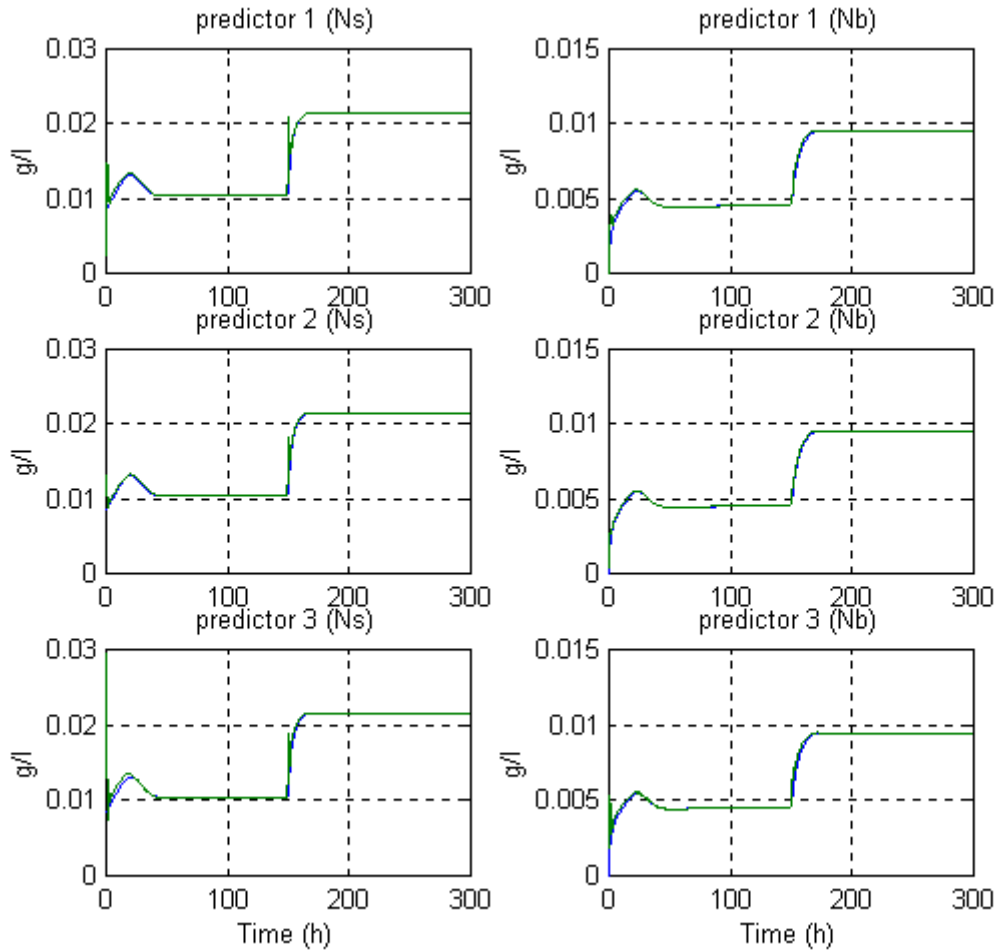


Figure 23 : 5% mismatch on the liquid re-circulating ratio R_L

3.3. Measurements with white noise

When the measurements of nitrate and ammonia are noisy (white noise of amplitude equal to $2 \cdot 10^{-4}$ mol/l, here), the predictor 3 which uses a second derivative is out of work (bottom graph of the figure 24).

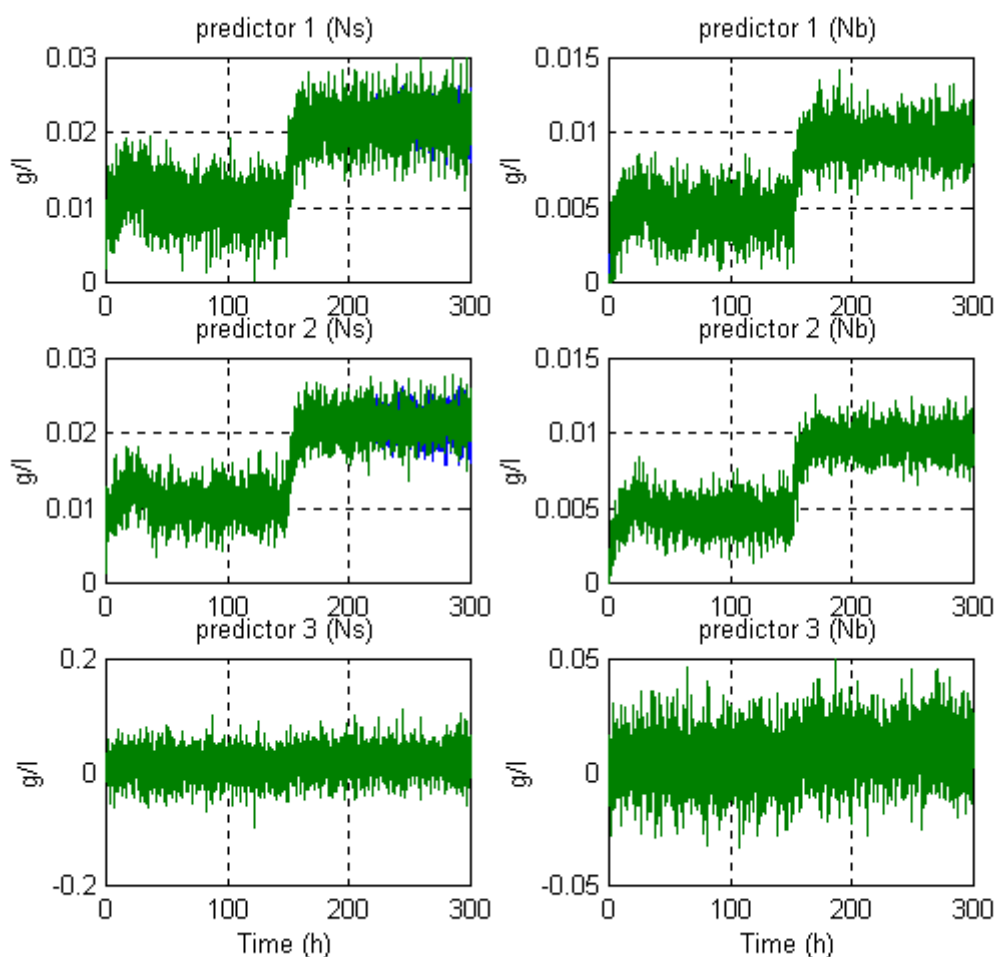


Figure 24 : White noise on nitrate and ammonia measurements : $\pm 10^{-4}$ mol/l

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3.4. Static bias on measurement

The effect of a bias on the measurements of ammonia and nitrate is studied on the model of the predictor 1. The results would be the same for the 2 other predictors. The expression of the mean biomass concentration in the column is recalled hereafter, for the predictor 1 (from (A.23) of TN 48.1) :

$$c_{x1} = \delta_{11} \cdot r_1 + \delta_{12} \cdot r_2$$

$$c_{x2} = \delta_{21} \cdot r_1 + \delta_{22} \cdot r_2$$

$$\text{where } r_1 = \frac{F_{in}}{V_L} \cdot \left(1 + k + \alpha \cdot \frac{G_{in}}{F_{in}} \right) \cdot \left(\left(1 + \frac{V_L}{F_{in}} \cdot p \right) \cdot b_1 - d_{L10} \right)$$

$$r_2 = \frac{F_{in}}{V_L} \cdot \left(\left(1 + \frac{V_L}{F_{in}} \cdot p \right) \cdot b_2 - d_{L20} \right)$$

The stoichiometric factors δ are scalar (dimension less) and their values are :

$$\begin{aligned} \delta_{11} &= -68.5 & \delta_{12} &= -0.7 \\ \delta_{21} &= 0 & \delta_{22} &= 31.6 \end{aligned}$$

The other terms are physical parameters or concentration measurements that are positive. So the Nitrosomonas concentration, c_{x1} , is mainly dependant on r_1 , i.e. on the ammonia measurements, b_1 or d_{L10} , in the incoming or outgoing flow; while the Nitrobacter concentration, c_{x2} , is dependant on r_2 , i.e. on the nitrate measurements, b_2 or d_{L20} . Consequently a static bias on the measurements (b_1 , b_2 , d_{L1} and d_{L2}) will induce a static bias on the biomass predictions of the same order : good sensors with low static bias will give good prediction of biomass concentrations.

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The figure 25 illustrates the impact of a 1% static bias on the ammonia measurement in the 'fresh' incoming liquid flow : it causes a 1% error on the Ns biomass estimations and no error on the Nb biomass ones.

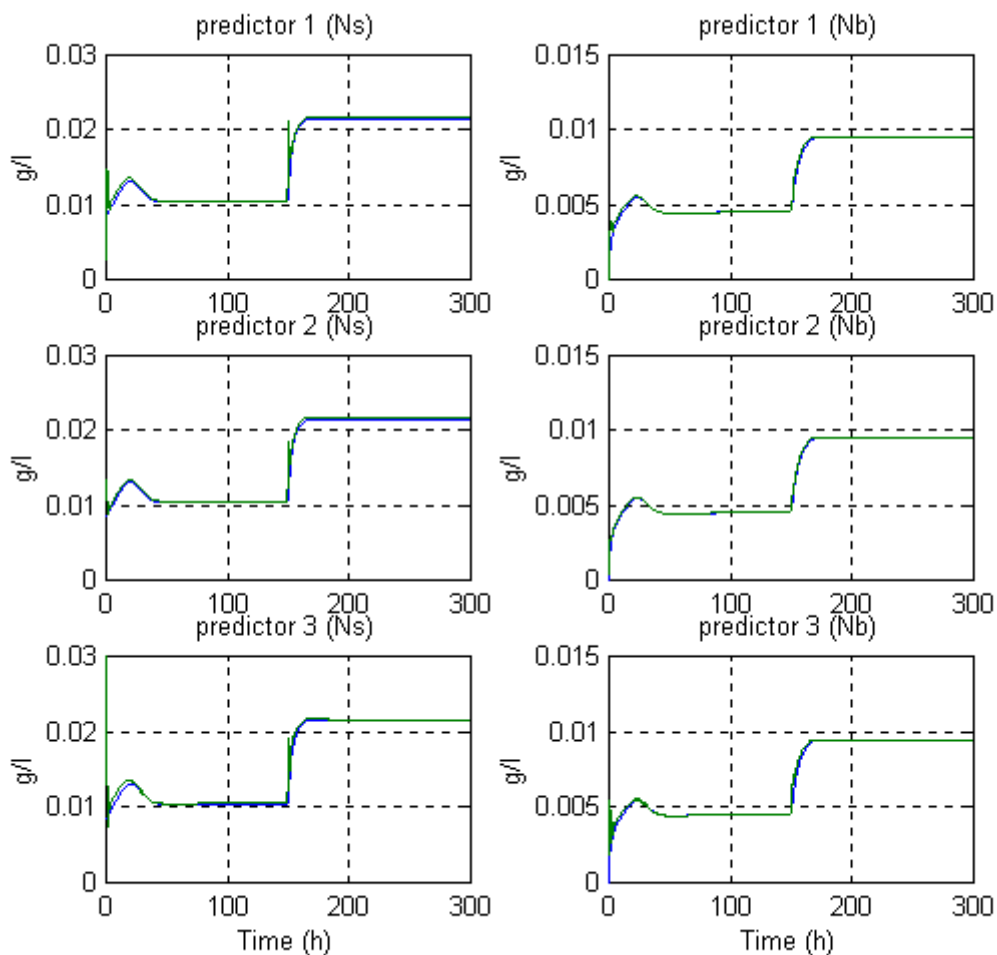


Figure 25 : 1 % static bias on the ammonia measurement in the incoming flow

3.5. Hypothesis H1

The so called hypothesis *H1* has been introduced in the paragraph A.1.3. of TN 48.1 relative to the expression of the variation rate of the nitrite versus the variation rates of ammonia and nitrate. According to this hypothesis, the growth limiting factor and the maintenance limiting factor are identical for each strain :

$$V_{G1} = V_{M1}$$

(Hypothesis *H1* in TN 48.1)

$$V_{G2} = V_{M2}$$

The figure 26 illustrates the case where *H1* is not true : the half maximum maintenance rate saturation constant of the simulated column is the tenth part of the growth one. It causes a bias on all the predicted biomass concentrations.

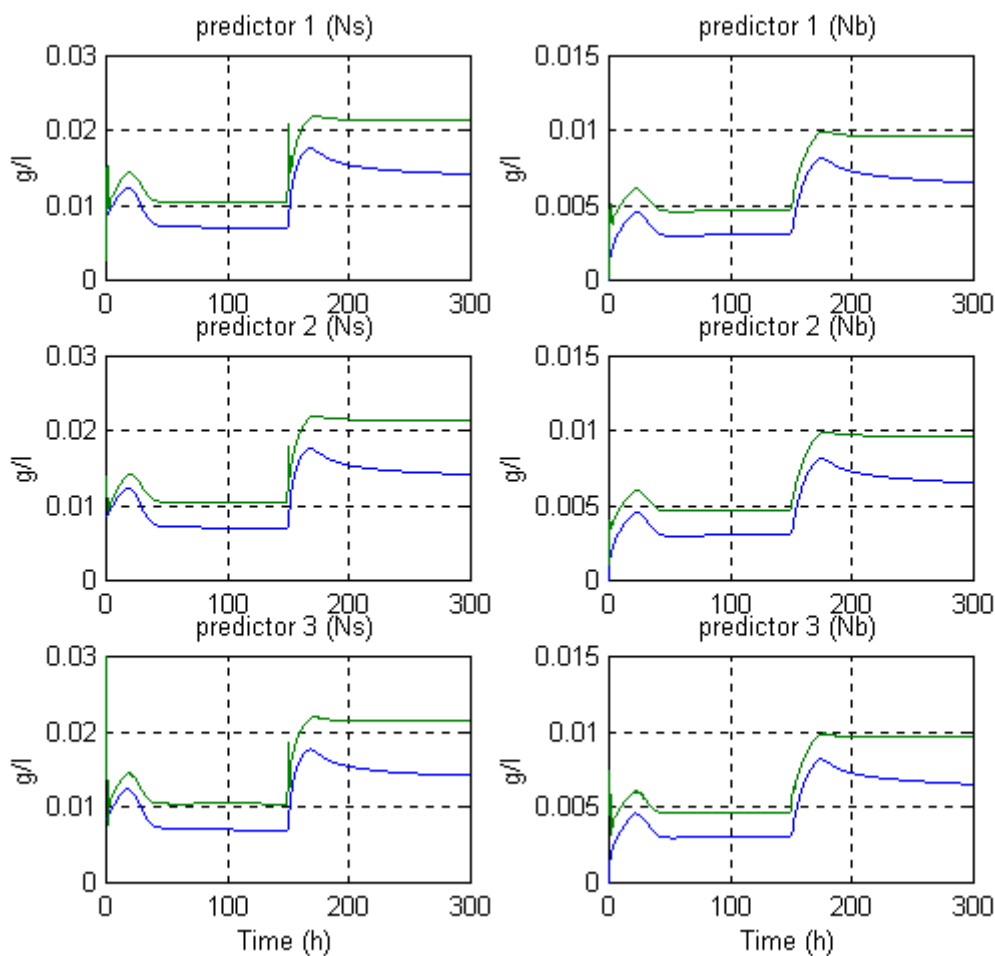


Figure 26 : Case where hypothesis *H1* is not true

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3.6. Choice and expression of the biomass predictor

The predictor 3 is rejected because of its behaviour when there is noise on the measurements. As the 2 first predictors have the same performances, the simpler, i.e. predictor 1, is chosen.

Starting from (A.23) of TN48.1, the formula of the biomass predictor is :

$$\begin{aligned}
 c_{x1} &= \delta_{11} \cdot r_1 + \delta_{12} \cdot r_2 \\
 c_{x2} &= \delta_{21} \cdot r_1 + \delta_{22} \cdot r_2 \\
 \text{where } r_1 &= \frac{1}{\tau} \cdot \left(1 + k + \alpha \cdot \frac{G_{in}}{F_{in}} \right) \cdot \left((1 + \tau \cdot p) \cdot \hat{b}_1 - \hat{d}_{L10} \right) \\
 r_2 &= \frac{1}{\tau} \cdot \left((1 + \tau \cdot p) \cdot \hat{b}_2 - \hat{d}_{L20} \right)
 \end{aligned} \tag{3}$$

in which \hat{d}_{L10} , \hat{d}_{L20} , \hat{b}_1 , \hat{b}_2 and τ have the same meaning as in the nitrite predictor (1) and (2). The coefficients δ are detailed in (A.14) of TN 48.1 .

As the biomass is not easily measured, the identification of the parameters of the biomass predictor is impossible. Nevertheless the results of the biomass predictor could be used for diagnosis, for example.

4. CONCLUSION

In this study, a biomass predictor and a nitrite predictor are proposed, for autotrophic growth, under the hypothesis that the Monod constants are identical for the growth rate and maintenance rate for each of the strains. Nevertheless, in the case of the nitrite predictor, even if this hypothesis is not true, the static bias that is then induced will be compensate by a corrective term whose value will be measured regularly (twice a week) from laboratory analysis. Thanks to this correction, it is expected, and it has to be validated in a next study, that the predicted nitrite will be reliable during transient behaviour, which is the critical period because of possible peak of nitrite.

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. : "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.

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ANNEX

SOFTWARE OF THE PREDICTORS

1. Software of the predictor 1 (Matlab® language) : estim1.m
2. Software of the predictor 2 (Matlab® language) : estim2.m
3. Software of the predictor 3 (Matlab® language) : estim3.m
4. Software of the robustness study (Matlab® language) : robust.m

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A.1. Software of the predictor 1 : estim1.m

```

%*****
%      Biomass and Nitrite estimators  (model 1)      *
%      Version 3.0      July 2000                    *
%                                                    *
%      Estimator model according to TN 48.1          *
%                                                    *
%      The model of the estimator is a mere first order *
%      in which the biomass is constant throughout the volume*
%*****
% . time period of the predictor = period of Matlab simulation*
% . calling programme : 'robust.m'                  *
%*****

% Computation of the transfer of [NH3] at output of the column
%-----
alpha_h = kmis_alfh*alpha(3);% NH3
Kdis_h = kmis_Kdi*Kdis(3);   % NH3
KLa_h = kmis_KLa*KLa(3);    % NH3
VG = kmis_VG*(VA*epsG/epsT + VB*epsG + VC*epsG/epsT); % volume of gas of the column
VL = kmis_VL*(VA*epsL/epsT + VB*epsL + VC*epsL/epsT); % volume of liq of the column
qG = kmis_qG*Gin;
qL = kmis_qL*Fin;

% Computation of the transfer of [NO3] and [NO2] at output of the column
%-----
tauL = kmis_tau*(VA*epsL/epsT + VB*epsL + VC*epsL/epsT)/Fin;

% Coefficients of the linear system binding rate and biomass concentration
%-----
alfa11 = Yx1(3,1) * mumax(1) + Ym1(3,1) * maint(1); % for NH3 and Nitrosomonas
alfa12 = Yx1(3,2) * mumax(2) + Ym1(3,2) * maint(2); % for NH3 and Nitrobacter
alfa21 = Yx1(5,1) * mumax(1) + Ym1(5,1) * maint(1); % for NO3 and Nitrosomonas
alfa22 = Yx1(5,2) * mumax(2) + Ym1(5,2) * maint(2); % for NO3 and Nitrobacter
alfa31 = Yx1(4,1) * mumax(1) + Ym1(4,1) * maint(1); % for NO2 and Nitrosomonas
alfa32 = Yx1(4,2) * mumax(2) + Ym1(4,2) * maint(2); % for NO2 and Nitrobacter

% Coefficients of the linear system binding rates of NH3 NO3 and NO2
%-----
den = alfa11*alfa22 - alfa12*alfa21;
beta1 = kmis_bei*(alfa22*alfa31 - alfa21*alfa32)/den;
beta2 = kmis_be2*(alfa11*alfa32 - alfa12*alfa31)/den;
delta11 = kmis_del*alfa22/den;      delta12 = -kmis_del*alfa12/den;
delta21 = -kmis_del*alfa21/den;     delta22 = kmis_del*alfa11/den;

% Estimator
%=====

% NH3 and NO3
%-----
% Derivative of measures of NH3 and NO3 at column output
[m,n] = size(Te);
dXb = diff(Xb) / dte;
dXb(m,:) = dXb(m-1,:);

% NO2
% ---
% [NO2-] at input of column is assumed null

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

% Initialization for estimation of NO2- concentration in the column
Xi = zeros(1,m);
Xi2 = zeros(1,m);
s1 = zeros(1,m-1);

```

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```

s2 = zeros(1,m-1);

% Estimation of biomass and nitrite
% -----
coef = 1+Kdis_h+alpha_h*qG/qL;
coef1 = beta1*coef;
alph = exp(-dte/tauL);
alph1 = 1-alph;
% initialization of the first order
e = dL_i(1) - beta2*dL_a(1) - coef1*dL_h(1);
xx = e; % static gain equal to 1
for jj = 1:m

% 1. Computation of the (NH3 and NO3-) production/consumption rate
%r1 = (tau_h*dXb(jj,1) + Xb(jj,1) - G1_h*dL_h(jj) - G2_h*dG_h(jj)) ...
%      / G3_h; % [NH3] rate
r1 = (dXb(jj,1) + (Xb(jj,1)-dL_h(jj))/tauL)*coef; % [NH3] rate
r2 = dXb(jj,2) + (Xb(jj,2) - dL_a(jj))/tauL; % [NO3] rate

% 2. Mean productive biomass concentration in the column
Cx(1,jj) = delta11*r1 + delta12*r2;
Cx(2,jj) = delta21*r1 + delta22*r2;

% 3. production rate of nitrite in last tank of the column
r3 = beta1*r1 + beta2*r2;

% 3. concentration of nitrite in last tank of the column (transfer function)
if jj == m, break, end
e = dL_i(jj) - beta2*dL_a(jj) - coef1*dL_h(jj);
xx = alph*xx + alph1*e;
s1(1,jj) = xx;
xx2 = beta2*Xb(jj+1,2) + coef1*Xb(jj+1,1);
s2(1,jj) = xx2;
Xi2(1,jj+1) = xx + xx2;
% 4. concentration of nitrite in last tank of the column (integration of derivative)
Xi(1,jj+1) = Xi(1,jj) + (-Xi(1,jj)/tauL + r3)*dte;
end
end

```

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A.2. Software of the predictor 2 : estim2.m

```

%*****
%      Biomass and Nitrite estimators  (model 2)      *
%      Version 3.0      July 2000                    *
%                                                    *
%      Estimator model according to TN 48.1          *
%                                                    *
%      The model of the estimator is composed of 2 successive*
%      first order (the 2 first order may be different)  *
%      The biomass is assumed constant throughout each volume*
%      The output of each of the first orders is measured  *
%*****
% . time period of the predictor = period of Matlab simulation*
% . calling programme : 'robust.m'                  *
%*****

n1 = ceil(NB/2); % rank of the tank in the middle of part B of the column
RLm = kmis_RL*RL;
RGm = kmis_RG*RG;

% Transfer of [NO3] and [NO2] at middle and output of the column
%-----
tauL1 = kmis_tau*(VA*epsL/epsT + VB*epsL*n1/NB)/Fin/(1+RLm);
tauL2 = kmis_tau*(VB*epsL*(1-n1/NB) + VC*epsL/epsT)/Fin/(1+RLm);

% Transfer of [NH3] at middle and output of the column
%-----
alpha_h = kmis_alph*alpha(3);% NH3
Kdis_h = kmis_Kdi*Kdis(3); % NH3
KLa_h = kmis_KLa*KLa(3); % NH3
VG = kmis_VG*(VA*epsG/epsT + VB*epsG + VC*epsG/epsT); % volume of gas of the column
VL = kmis_VL*(VA*epsL/epsT + VB*epsL + VC*epsL/epsT); % volume of liq of the column
VG1 = kmis_VG*(VA*epsG/epsT + VB*epsG*n1/NB); % volume of gas of the first part of the
column
VL1 = kmis_VL*(VA*epsL/epsT + VB*epsL*n1/NB); % volume of liq of the first part of the
column
VG2 = VG - VG1; % volume of gas of the second part of the equivalent column
VL2 = VL - VL1; % volume of liq of the second part of the equivalent column
qG = kmis_qG * Gin * (1+RGm);
qL = kmis_qL * Fin * (1+RLm);

tau_h = tauL1/(1+alpha_h*qG/(1+Kdis_h)/qL);
G1_h = 1/(1+alpha_h*qG/(1+Kdis_h)/qL);
G2_h = 1/(alpha_h+(1+Kdis_h)*qL/qG);
G3_h = tauL1/(1+Kdis_h+alpha_h*qG/qL);
alpha4_h = alpha_h;
%alpha5_h = 1/(1+KLa_h*VL1/alpha_h/qG)
tau_h2 = tauL2/(1+alpha_h*qG/(1+Kdis_h)/qL);
G1_h2 = G1_h;
G2_h2 = G2_h;
G3_h2 = tauL2/(1+Kdis_h+alpha_h*qG/qL);
%alpha4_h2 = alpha_h;
alpha5_h2 = 1/(1+KLa_h*VL2/alpha_h/qG);

% Coefficients of the linear system binding rate and biomass concentration
%-----
alfa11 = Yx1(3,1) * mumax(1) + Ym1(3,1) * maint(1); % for NH3 and Nitrosomonas
alfa12 = Yx1(3,2) * mumax(2) + Ym1(3,2) * maint(2); % for NH3 and Nitrobacter
alfa21 = Yx1(5,1) * mumax(1) + Ym1(5,1) * maint(1); % for NO3 and Nitrosomonas
alfa22 = Yx1(5,2) * mumax(2) + Ym1(5,2) * maint(2); % for NO3 and Nitrobacter
alfa31 = Yx1(4,1) * mumax(1) + Ym1(4,1) * maint(1); % for NO2 and Nitrosomonas
alfa32 = Yx1(4,2) * mumax(2) + Ym1(4,2) * maint(2); % for NO2 and Nitrobacter

% Coefficients of the linear system binding rates of NH3 NO3 and NO2
%-----
den = alfa11*alfa22 - alfa12*alfa21;
beta1 = kmis_be1*(alfa22*alfa31 - alfa21*alfa32)/den;
beta2 = kmis_be2*(alfa11*alfa32 - alfa12*alfa31)/den;
delta11 = kmis_del*alfa22/den; delta12 = -kmis_del*alfa12/den;

```

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```

delta21 = -kmis_del*alfa21/den;          delta22 = kmis_del*alfa11/den;

% Estimator
%=====

% NH3 and NO3
% -----
% Derivative of measures of NH3 and NO3
[m,n] = size(Te);
dXh = diff(Xh) / dte;
dXh(m,:) = dXh(m-1,:);
dXa = diff(Xa) / dte;
dXa(m,:) = dXa(m-1,:);
Xh = Xh'; Xa = Xa'; dXh = dXh'; dXa = dXa';

% NO2
% ----
% [NO2-] at input of column is assumed null

% Initialization of vectors
% -----
% Initialization for estimation of the mean [productive biomass] in the column
Cx1 = zeros(2,m); % first part of the column
Cx2 = zeros(2,m); % secnd part of the column
% Initialization for estimation of NO2- concentration in the column
Xi = zeros(2,m);

% Estimation of biomass and nitrite
% -----
den = alfa11*alfa22 - alfa12*alfa21;
for jj = 1:m

    % 1. Computation of the NH3 production/consumption rates
    dLe = (dL_h(jj) + RLm*Xh(2,jj)) / (1+RLm);
    dGe = (alpha_h*dL_h(jj) + RGm*(alpha4_h*(alpha5_h2*Xh(1,jj)+Xh(2,jj)))) / (1+RGm);
    r11 = (tau_h*dXh(1,jj) + Xh(1,jj) - G1_h*dLe - G2_h*dGe) ...
           / G3_h; % [NH3] rate in first part
    r12 = (tau_h2*dXh(2,jj) + Xh(2,jj) - (G1_h2 + G2_h2*alpha4_h)*Xh(1,jj)) ...
           / G3_h2; % [NH3] rate in secnd part

    % 2. Computation of the NO3 production/consumption rates
    dLe = (dL_a(jj) + RLm*Xa(2,jj)) / (1+RLm);
    r21 = dXa(1,jj) + (Xa(1,jj) - dLe) / tauL1; % [NO3] rate in first part
    r22 = dXa(2,jj) + (Xa(2,jj) - Xa(1,jj)) / tauL2; % [NO3] rate in secnd part

    % 3. Mean [productive biomass] Cx1 in the first part of the column
    Cx1(1,jj) = delta11*r11 + delta12*r21;
    Cx1(2,jj) = delta21*r11 + delta22*r21;

    % 4. Mean [productive biomass] Cx2 in the secnd part of the column
    Cx2(1,jj) = delta11*r12 + delta12*r22;
    Cx2(2,jj) = delta21*r12 + delta22*r22;
    if jj == m, break, end

    % 4. production rate of nitrite in first and second part of the column
    r31 = beta1*r11 + beta2*r21; % [NO2] rate in first part
    r32 = beta1*r12 + beta2*r22; % [NO2] rate in secnd part

    % 5. concentration of nitrite in first and second part of the column
    dLe = (dL_i(jj) + RLm*Xi(2,jj)) / (1+RLm);
    Xi(1,jj+1) = Xi(1,jj) + ((-Xi(1,jj) + dLe)/tauL1 + r31)*dte;
    Xi(2,jj+1) = Xi(2,jj) + ((-Xi(2,jj) + Xi(1,jj))/tauL2 + r32)*dte;
end

```

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A.3. Software of the predictor 3 : estim3.m

```

%*****
%      Biomass and Nitrite estimators  (model 3)      *
%      Version 3.0      July 2000                    *
%                                                    *
%      Estimator model according to TN 48.1          *
%                                                    *
%      The model of the estimator is composed of 2 successive*
%      first order (the 2 first order may be different) *
%      The biomass is assumed constant in the first volume *
%      and null in the second part of the column      *
%      The output of the column only is measured     *
%*****
% . time period of the predictor = period of Matlab simulation*
% . calling programme : 'robust.m'                  *
%*****

gamma = .5; % volumetric ratio first part / total column
RLm = kmis_RL*RL;
RGm = kmis_RG*RG;
% Transfer of [NO3] and [NO2] at middle and output of the column
%-----
tauL1 = kmis_tau * gamma * (VA*epsL/epsT + VB*epsL + VC*epsL/epsT)/Fin/(1+RLm);
tauL2 = kmis_tau*(1-gamma)*(VA*epsL/epsT + VB*epsL + VC*epsL/epsT)/Fin/(1+RLm);

% Transfer of [NH3] at middle and output of the column
%-----
alpha_h = kmis_alph*alpha(3);% NH3
Kdis_h = kmis_Kdi*Kdis(3); % NH3
KLa_h = kmis_KLa*KLa(3); % NH3
VG = kmis_VG*(VA*epsG/epsT + VB*epsG + VC*epsG/epsT); % volume of gas of the column
VL = kmis_VL*(VA*epsL/epsT + VB*epsL + VC*epsL/epsT); % volume of liq of the column
VG1 = gamma*VG; % volume of gas of the first part of the column
VL1 = gamma*VL; % volume of liq of the first part of the column
VG2 = VG - VG1; % volume of gas of the second part of the equivalent column
VL2 = VL - VL1; % volume of liq of the second part of the equivalent column
qG = kmis_qG * Gin * (1+RGm);
qL = kmis_qL * Fin * (1+RLm);

tau_h = tauL1/(1+alpha_h*qG/(1+Kdis_h)/qL);
G1_h = 1/(1+alpha_h*qG/(1+Kdis_h)/qL);
G2_h = 1/(alpha_h+(1+Kdis_h)*qL/qG);
G3_h = tauL1/(1+Kdis_h+alpha_h*qG/qL);
alpha4_h = alpha_h;
%alpha5_h = 1/(1+KLa_h*VL1/alpha_h/qG)
%tau_h2 = tauL2/(1+alpha_h*qG/(1+Kdis_h)/qL);
%G1_h2 = G1_h;
%G2_h2 = G2_h;
%G3_h2 = tauL2/(1+Kdis_h+alpha_h*qG/qL);
%alpha4_h2 = alpha_h;
%alpha5_h2 = 1/(1+KLa_h*VL2/alpha_h/qG);

% Coefficients of the linear system binding rate and biomass concentration
%-----
alfa11 = Yx1(3,1) * mumax(1) + Ym1(3,1) * maint(1); % for NH3 and Nitrosomonas
alfa12 = Yx1(3,2) * mumax(2) + Ym1(3,2) * maint(2); % for NH3 and Nitrobacter
alfa21 = Yx1(5,1) * mumax(1) + Ym1(5,1) * maint(1); % for NO3 and Nitrosomonas
alfa22 = Yx1(5,2) * mumax(2) + Ym1(5,2) * maint(2); % for NO3 and Nitrobacter
alfa31 = Yx1(4,1) * mumax(1) + Ym1(4,1) * maint(1); % for NO2 and Nitrosomonas
alfa32 = Yx1(4,2) * mumax(2) + Ym1(4,2) * maint(2); % for NO2 and Nitrobacter

% Coefficients of the linear system binding rates of NH3 NO3 and NO2
%-----
den = alfa11*alfa22 - alfa12*alfa21;
beta1 = kmis_be1*(alfa22*alfa31 - alfa21*alfa32)/den;
beta2 = kmis_be2*(alfa11*alfa32 - alfa12*alfa31)/den;
delta11 = kmis_del*alfa22/den; delta12 = -kmis_del*alfa12/den;
delta21 = -kmis_del*alfa21/den; delta22 = kmis_del*alfa11/den;

```

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```

% NH3 and NO3
% -----
% First and second derivatives of measures of NH3 and NO3 at column output
[m,n] = size(Te);
dXb = diff(Xb) / dte;
dXb(m,:) = dXb(m-1,:);
ddXb = diff(dXb) / dte;
ddXb(m,:) = ddXb(m-1,:);

% Initialization of vectors
% -----
% Initialization for estimation of the mean [biomass] in the column
Cx = zeros(2,m);
% Initialization for estimation of NO2- concentration in the column
Xi = zeros(2,m);
Xi2 = zeros(1,m);
s1 = zeros(1,m-1);
s2 = zeros(1,m-1);
% Initialization of coefficients of Laplace function
coef1 = beta1*(1+Kdis_h+alpha_h*kmis_qG/(kmis_qL*Fin));
tau_x = kmis_tau*VL/Fin/2;
rdelta = sqrt(1-4*VL1*VL2/(VL/Fin*(1+RLm)));
tetal = tau_x*(1+rdelta);
teta2 = tau_x*(1-rdelta);
alph_L1 = exp(-dte/tetal); % coef of the Laplace function for the first tank
alph_L1 = 1-alph_L1;
alph_L2 = exp(-dte/teta2); % coef of the Laplace function for the second tank
alph_L2 = 1-alph_L2;
xeta0 = alpha_h*Gin*kmis_qG/(1+Kdis_h)/Fin/kmis_qL;
xeta = (1+RGm)/(1+RLm)*xeta0;
eps1 = xeta*(1-xeta0)*VL2/Fin-xeta0*VL/Fin;
eps2 = -xeta0*VL1*VL2/(1+RLm)/Fin/Fin;

% Estimation of biomass and nitrite
% -----
% initialization of the second order
e = dL_i(1) - beta2*dL_a(1) - coef1*dL_h(1);
e1 = e; % initialization of the past value of e1 (static gain = 1)
o1 = e1; % initialization of the past value of o1 (static gain = 1)
e2 = Xb(1,1); % initialization of the past value of e2 (static gain = 1)
x2 = e2; % initialization of the past value of x2 (static gain = 1)
x2p = x2; % initialization of the past value of x2 for derivative computation
do2p = (x2 - x2p)/dte; % initialization of approximate first derivative
for jj = 1:m
% 1. Computation of the NH3 production/consumption rate
dLeh = (dL_h(jj) + RLm*Xb(jj,1)) / (1+RLm);
dGeh = (alpha_h*dL_h(jj) + RGm*(alpha4_h*Xb(jj,1))) / (1+RGm);
r1 = (tau_h*tauL2*ddXb(jj,1) + (tau_h+tauL2)*dXb(jj,1) + Xb(jj,1) - G1_h*dLeh - G2_h*dGeh)
...
/ G3_h; % [NH3] rate
% 2. Computation of the NO3 production/consumption rate
dLea = (dL_a(jj) + RLm*Xb(jj,2)) / (1+RLm);
r2 = (tauL1*tauL2*ddXb(jj,2) + (tauL1+tauL2)*dXb(jj,2) + Xb(jj,2) - dLea)/tauL1; % [NO3]
rate
% 3. Mean productive biomass concentration in the column
Cx(1,jj) = delta11*r1 + delta12*r2;
Cx(2,jj) = delta21*r1 + delta22*r2;
% 4. production rate of nitrite in first and second part of the column
if jj == m, break, end
r3 = beta1*r1 + beta2*r2; % [NO2] rate in first part
% 5. concentration of nitrite in first and second part of the column
dLei = (dL_i(jj) + RLm*Xi(2,jj)) / (1+RLm);
Xi(1,jj+1) = Xi(1,jj) + ((-Xi(1,jj) + dLei)/tauL1 + r3)*dte;
Xi(2,jj+1) = Xi(2,jj) + ((-Xi(2,jj) + Xi(1,jj))/tauL2)*dte;
% 6. concentration of nitrite in last tank of the column (Laplace function)
% 6.1. transfer of the combination of the inputs of the column
e = dL_i(jj) - beta2*dL_a(jj) - coef1*dL_h(jj); % input of transfer H1
e1 = alph_L1*e1 + alph_L1*e1;
o1 = alph_L2*o1 + alph_L2*e1; % output of transfer H1
s1(1,jj) = o1;
% 6.2. taking into account the outputs of the column
xx2 = beta2*Xb(jj+1,2) + coef1*Xb(jj+1,1);
% 6.3. filtered derivative of the measured concentration of ammonia
e2 = alph_L1*e2 + alph_L1*Xb(jj+1,1);
x2 = alph_L2*x2 + alph_L2*e2;
do2 = (x2 - x2p)/dte; % approximate first derivative
ddo2 = (do2 - do2p)/dte; % approximate second derivative
x2p = x2;

```

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```

do2p = do2;
o2 = coef1*(do2*eps1+ddo2*eps2); % output of transfer H2
s2(1,jj) = xx2 + o2;
Xi2(1,jj+1) = o1 + xx2 + o2;
end

```

A.4. Software of the robustness study : robust.m

```

%*****
%      Biomass and Nitrite estimators      *
%      Version 3.0      July 2000          *
%                                           *
%      Estimator model according to TN 48.1 *
%                                           *
%      Robustness study                    *
%                                           *
%*****
% . time period of the predictor = period of Matlab simulation*
%*****

clear

% Initialization of the mismatch coefficients
kmis_alpha = 1;
kmis_Kdi = 1;
kmis_KLa = 1;
kmis_VG = 1;
kmis_VL = 1;
kmis_qG = 1;
kmis_qL = 1;
kmis_tau = 1;
kmis_bel = 1;
kmis_be2 = 1;
kmis_nh3 = 1;
kmis_RL = 1;
kmis_RG = 1;
kmis_del = 1;

titre_mis = 'No noise ; No mismatch';

imis = 5;      % 5% mismatch on k
imis = 6;      % -5% mismatch on k
imis = 10;     % 50% mismatch on VG (all the estimators are independant of VG)
imis = 2;      % 5% mismatch on VL or (VL1 and VL2)
imis = 9;      % 5% mismatch on KLa
imis = 16;     % 1% mismatch on k and noise
imis = 11;     % -5% mismatch on tauL or (tauL1 and tauL2)
imis = 1;      % 5% mismatch on tauL or (tauL1 and tauL2)
imis = 7;      % 1% mismatch on k
imis = 13;     % 1% mismatch on beta1 (consumtion rate factor of NH3)
imis = 14;     % 1% mismatch on beta2 (consumtion rate factor of NO3)
imis = 8;      % 5% mismatch on alpha
imis = 3;      % 5% mismatch on qL
imis = 4;      % 5% mismatch on qG
imis = 19;     % 5% mismatch on RG
imis = 18;     % 5% mismatch on RL
imis = 17;     % growth limiting factors different from maintenance limiting factors
imis = 12;     % noise with no mismatch
imis = 15;     % 1% mismatch on [NH3] in the incoming liquid flow
imis = 20;     % 5% mismatch on delta (stoichiometric factor of NH3 and NO3 rates)
imis = 0;      % no mismatch
    if imis == 17
        load s15c5_0
        load s15c5_0e
    elseif (imis == 12 | imis == 16)
        load s14c5_b
        load s14c5_bf
    else
        load s14c5_0
        load s14c5_0e
    end
end
if imis == 1
    kmis_tau = 1.05;

```

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```

    titre_mis = '+5% mismatch on the time constant tauL';
elseif imis == 2
    kmis_VL = 1.05;
    titre_mis = '+5% mismatch on the volume of liquid VL';
elseif imis == 3
    kmis_qL = 1.05;
    titre_mis = '+5% mismatch on the liquid flow rate qL';
elseif imis == 4
    kmis_qG = 1.05;
    titre_mis = '+5% mismatch on the gas flow rate qG';
elseif imis == 5
    kmis_Kdi = 1.05;
    titre_mis = '+5% mismatch on k_dissociation';
elseif imis == 6
    kmis_Kdi = .95;
    titre_mis = '-5% mismatch on k_dissociation';
elseif imis == 7
    kmis_Kdi = 1.01;
    titre_mis = '+1% mismatch on k_dissociation';
elseif imis == 8
    kmis_alph = 1.05;
    titre_mis = '+5% mismatch on gas/liquid equilibrium constant';
elseif imis == 9
    kmis_alph = 1.05;
    titre_mis = '+5% mismatch on KLa_NH3';
elseif imis == 10
    kmis_VG = 1.5;
    titre_mis = '+50% mismatch on VG';
elseif imis == 11
    kmis_tau = .95;
    titre_mis = '-5% mismatch on the time constant tauL';
elseif imis == 12
    titre_mis = 'noise with no mismatch';
elseif imis == 13
    kmis_be1 = 1.01;
    titre_mis = '+1% mismatch on beta1 (consumtion rate factor of NH3)';
elseif imis == 14
    kmis_be2 = 1.01;
    titre_mis = '+1% mismatch on beta2 (consumtion rate factor of NO3)';
elseif imis == 15
    kmis_nh3 = 1.01;
    titre_mis = '+1% mismatch on [NH3] in the incoming flow rate';
elseif imis == 16
    kmis_Kdi = 1.01;
    titre_mis = '+1% mismatch on k_dissociation and white noise on measurements';
elseif imis == 17
    titre_mis = 'growth limiting factors different from maintenance limiting factors';
elseif imis == 18
    kmis_RL = 1.05;
    titre_mis = '+5% mismatch on liquid recirculating ratio RL';
elseif imis == 19
    kmis_RG = 1.05;
    titre_mis = '+5% mismatch on gas recirculating ratio RG';
elseif imis == 20
    kmis_del = 1.05;
    titre_mis = '5% mismatch on delta (stoichiometric factor of NH3 and NO3 rates)';
end
titre_mis

if std(diff(Te)) > 1e-6
    message = ' Sampling period non constant'
    break
end
dte = Te(2)-Te(1)

% Data acquisition of the filtered signals
% -----
dG_h = sige(:,1);
dL_h = kmis_nh3*sige(:,2);
dL_a = sige(:,4);
dL_i = sige(:,3);
Xb = sige(:,5:6);           % NH3 and NO3 at end of the column (for estimator 1 and 3)
Xh = [sige(:,7), Xb(:,1)]; % NH3 at end and middle of the column (for estimator 2)
Xa = [sige(:,8), Xb(:,2)]; % NO3 at end and middle of the column (for estimator 2)

% Estimation of nitrite and biomass with estimator 1
% =====
tic, estim1, toc

```

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```

% Plot
pou = 3;          % plot of the nitrite concentrations (process and estimation)
itracbio = 1;    % 1 --> biomass concentrations; 0 --> intermediate values of [NO2]
t_est1
nomfic = ['est1_',num2str(imis)];
eval(['save ',nomfic,' Te Xi Xi2 Cx Xmoy imis titre titre_mis'])

message = 'Open a new plotting window and strike a key'
pause

% Estimation of nitrite and biomass with estimator 2
% =====
tic, estim2, toc

% Plot
pou = 32;        % plot of the nitrite concentrations (process and estimation)
t_est2
nomfic = ['est2_',num2str(imis)];
eval(['save ',nomfic,' Te Xi Cx1 Cx2 Xmoy1 Xmoy2 Xmoy VL1 VL2 imis titre titre_mis'])

message = 'Open a new plotting window and strike a key'
pause

% Estimation of nitrite and biomass with estimator 3
% =====
tic, estim3, toc

% Plot
pou = 3;          % plot of the nitrite concentrations (process and estimation)
itracbio = 1;    % 1 --> biomass concentrations; 0 --> intermediate values of [NO2]
t_est3
nomfic = ['est3_',num2str(imis)];
eval(['save ',nomfic,' Te Xi Xi2 Cx Xmoy VL1 VL2 imis titre titre_mis'])

```

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