MELISSA

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TECHNICAL NOTE : 73.1

Nitrite control of the nitrifying compartment

ROBUSTNESS STUDY AND C SOFTWARE

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0	0	April 2003	Draft
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<u>Abbreviations or notations:</u>

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
PC : Personal Computer
PLC : Programmable Logical Computer
CV : Controlled Variable
MV : Manipulated Variable
CST : Completely Stirred Tank

GENERAL INFORMATION CONCERNING THE TECHNICAL NOTES OF THE SERIAL NUMBER 73

All the technical notes of the serial number 73 concern the NO_2 control of the nitrification column :

TN 73.1 : Study of the controller of NO2. Description of the software of the estimator and controller.

TN 73.2 : Elaboration of the estimator of the state used by the internal model of the control.

TN 73.3 : Attempt of automatic conversion of the software from Matlab language into C language for the target computer of the pilot plant.

TN 73.4 : Simplification of the matrices of the state system.

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 and biomass 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 predictive horizon of the control.

The approach is now to consider the column as 3 ideally stirred tanks (parts: A, B or fixed bed, and C). Then the state becomes much bigger (its size is multiplied by factor 3) : only components of part C are measured, components of the 2 other parts needing to be estimated. Particularly the biomass in the fixed bed and the NO_2 in A, B, C are estimated.

Since a previous study (TN 64.4), the control has been reviewed in an attempt to minimize the bias on the Controlled Variable.

2. PRINCIPLE OF THE CONTROL

The core of the control is a scenario, which allows forecasting the behaviour of the nitrite on a horizon H (typically 10 hours) that follows a sampling time (figure 1). The scenario which is defined by the concentrations at process input and by a modifiable liquid flow rate that are kept constant on H, is applied to the estimated state. It gives a foreseen behaviour of NO_2 whose extremum is compared with the constraint. The scenario is tested repeatedly with another flow rate until the extremum matches the constraint. Then the corresponding flow rate is the found value of the Manipulated Variable.

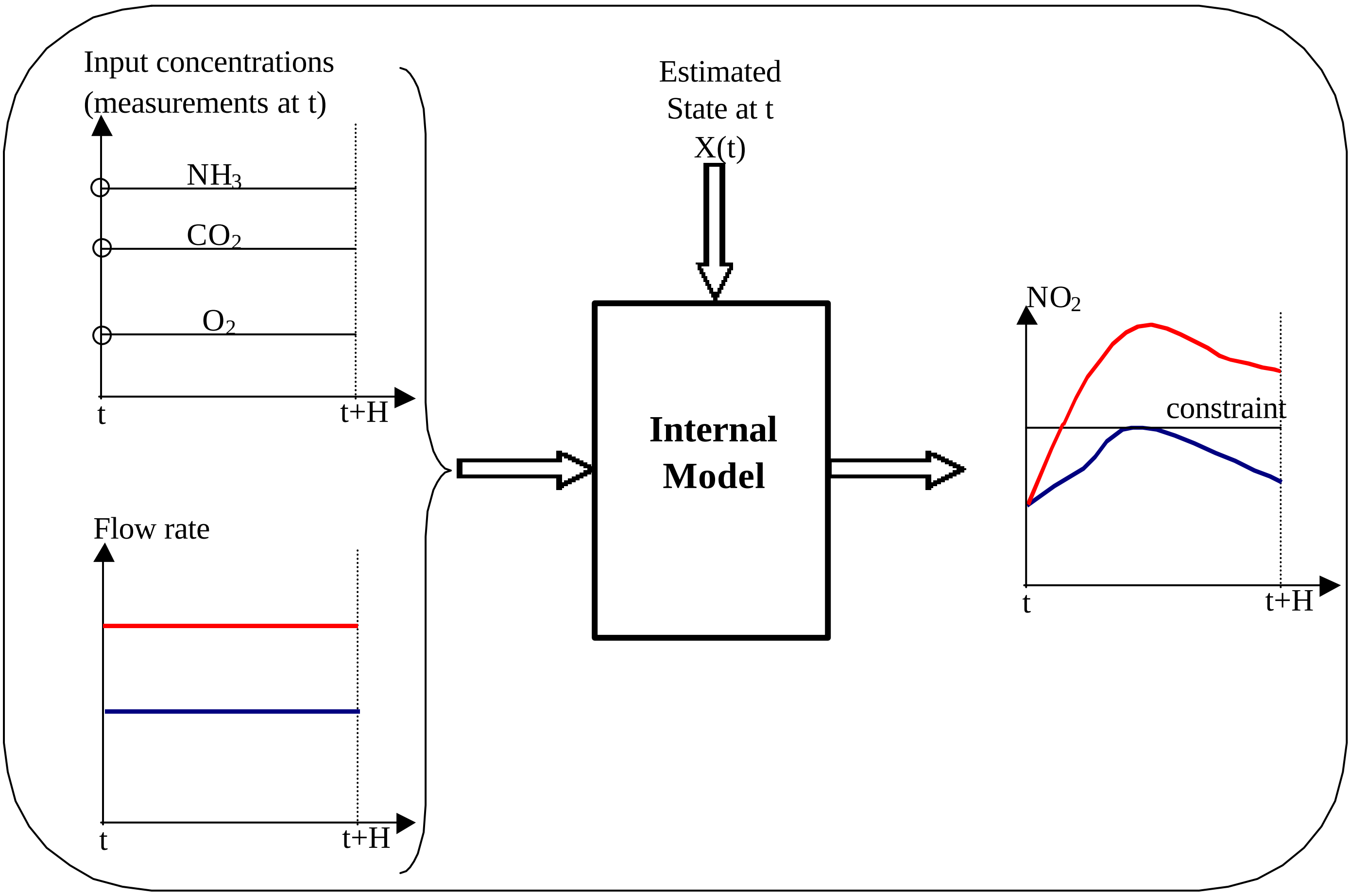

Figure 1 : Principle of the control
t : sampling time
H : forecast horizon

Despite the simplified state of the internal model, the behaviour of NO_2 of the model on horizon H is not very far from the one of the process, except during the 2 hours that follow the step of load. This is another justification of the choice of the internal model (Annex 1).

As previously said, the repeated scenario is partly defined with the liquid flow rate for which an initial value has to be chosen. In order to reduce the computational time, the following rule is applied to make the choice.

<u>Rule for choosing the initial value of flow rate in the scenario :</u>
First, three kinds of flow have to be distinguished :

1. <u>The 'requested' flow</u>. It is the flow requested by an operator or by the controller of the MELISSA loop. This requested flow do not take into consideration the production of NO_2.
2. <u>The 'reference' flow</u>. The 'requested' flow is time variable and the changes occur by step. Now a positive step produces a peak of NO_2. In order to avoid this peak, a positive step of 'requested' flow will be smoothen by a first order 'reference' flow. And a negative 'requested' flow will be unchanged to give the 'reference' flow, as it does not produce a peak of nitrite.
3. <u>The 'control' flow</u>. It is the MV (Manipulated Variable) computed by the control to avoid the CV (Controlled Variable) overshooting its constraint.

Then the initial value in the scenario is the 'reference' flow. The extremum of the corresponding behaviour of NO2 is compared to the constraint. If it does not fit, a new value of flow is computed according to the distance to the objective. If it fits, i.e. if the extremum is under the constraint, the iteration is stopped and the MV is equal to the 'reference' flow. In this way, the introduction of the 'reference' flow spares computational time. Simulations show also it reduces the noise on the MV.

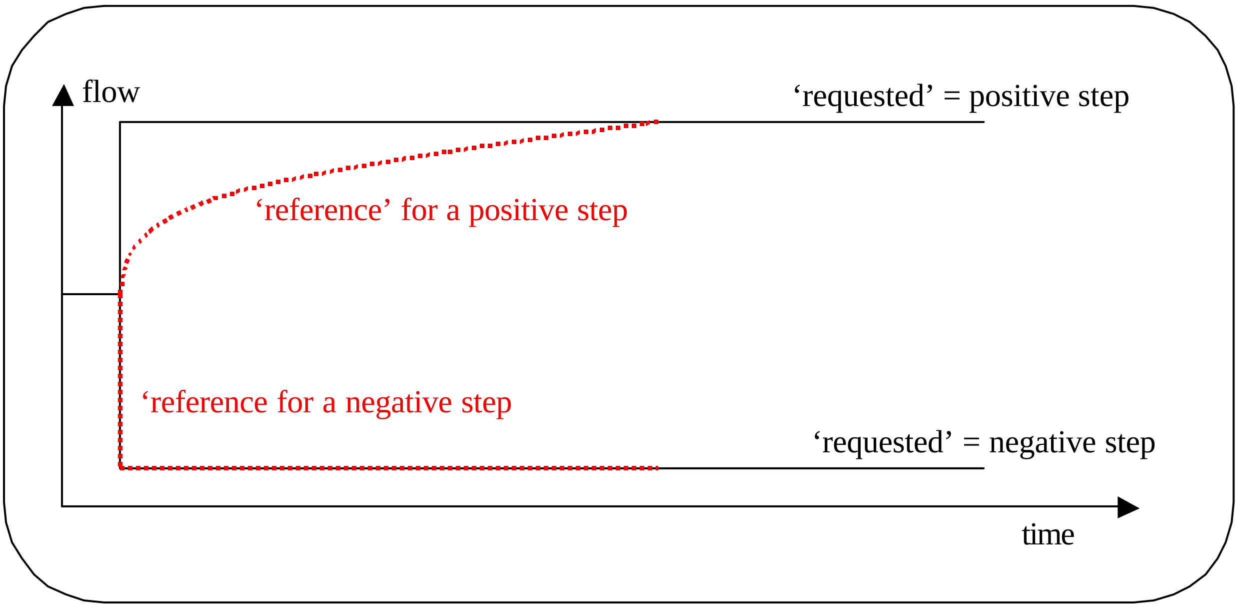

Figure 2 : 'Requested' and 'Reference' flow rate

Actually, as explained with more details in annex 2, the 'reference' curve is composed of 2 first order trajectories with 2 time constants : a rather small one and a great one. The first part is a quick first order but when the process output is close to the 'requested' value, then the ference' curve becomes slow in order to smoothen the MV.

3. ROBUSTNESS

3.1. Introduction

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

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;
- constraint on NO_2 set to 3 10^{-4} mol/l, arbitrarily on the simulator.
- 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.

The concentration of total ammonia at column input is constant (2.5 10^{-2} mol/l) all along the simulation.

At beginning of a simulation, the 'controlled' and 'requested' flows are equal to 0.4 l/h. At t=0.2 h, the 'requested' flow is increased to 0.6 l/h.

Figure 3 illustrates the reference behaviour of the control of this process when there is no noise nor mismatch. On the top graph the constraint (3 10^{-4} mol/l), the NO_2 concentration at column output and the NO_2 estimation are plotted with green, blue and red lines respectively. On the bottom graph, the 'requested' flow and the MV are plotted with blue and green lines respectively.

Because of the dead zone, after time t=10 h, the 'control' flow is slightly increasing and the NO_2 approaches its constraint very slowly.

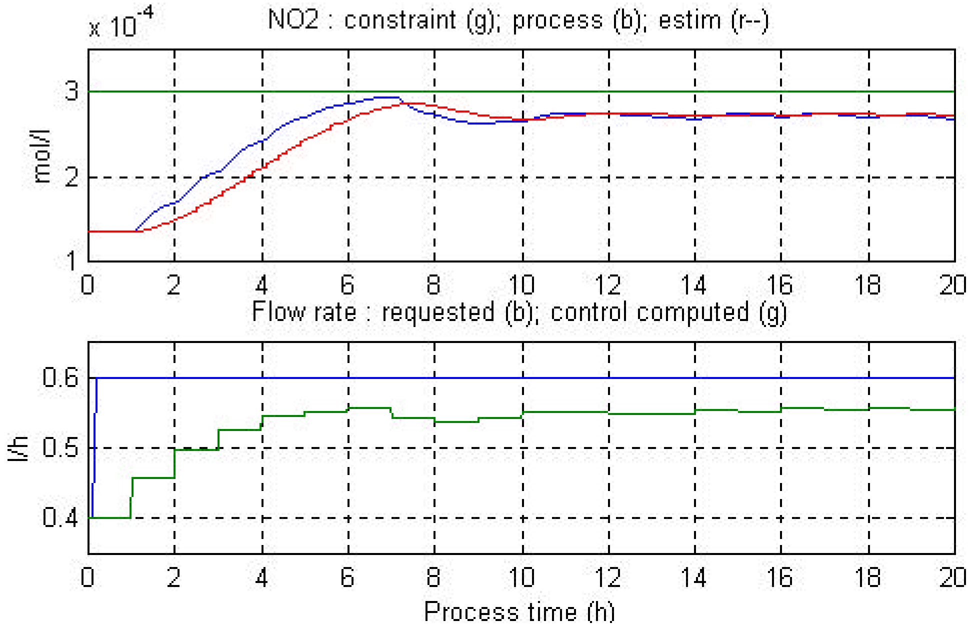

Figure 3 : Closed loop simulation with no mismatch and no noise

3.2. Noise on NH_3 and NO_3 measurements

The measurements are filtered with a low pass filter. The coefficient of the filter has to be tuned in order to realize the best compromise between reduction of noise and dephasing : a high coefficient will produce a high noise reduction but also a great dephasing (that implies a great delay in the control answer), and inversely. On the simulator the coefficient is set to 0.9 . This is a parameter that can be changed on the parameters file associated to the control software.

In the simulation of figure 4, a white noise has been added on NO_3 measurements at column output with a standard deviation of 10^{-4} mol/l (about 0.5 % of the mean signal).

As already mentioned in TN 73.2, the noise on NO_2 estimation is high (standard deviation is about 10 % of the mean value). Different simulations show that this amplitude of noise is bearable. But a noise ten times as great is no more bearable because the MV becomes very noisy and vary continuously between 0 and its 'requested' value.

The absolute standard deviation on NO2 estimation can be expressed from absolute standard deviation on measurements of NH3 at column input and NO3 at column output as follows :

$$\sigma_{(NO2)} = K \cdot \left(\sigma_{(NH3\_inpu)t} + \sigma_{(NO3\_output)}\right)$$

where K depends on the coefficient of the low pass filter (1)

here $K \approx 0.2$

This relation shows that the effect of noise on measurements of NH_3 at column input is the same as for NO_3 at column output.

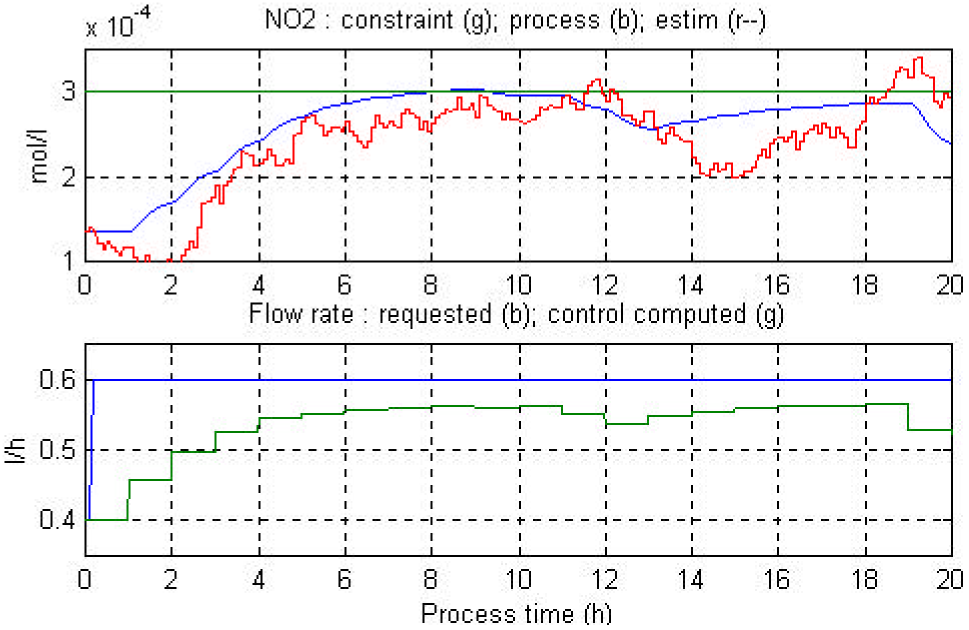

Figure 4 : Closed loop simulation with noise on NO_3 at column output

3.3. Noise on O_2 measurement

The results of figure 5 show that a noise whose standard deviation σ is 10^{-5} mol/l (about 5 %) on O2 in the liquid at column output is quite bearable. An important increase of noise amplitude will have no drastic consequence on the Manipulated Variable.

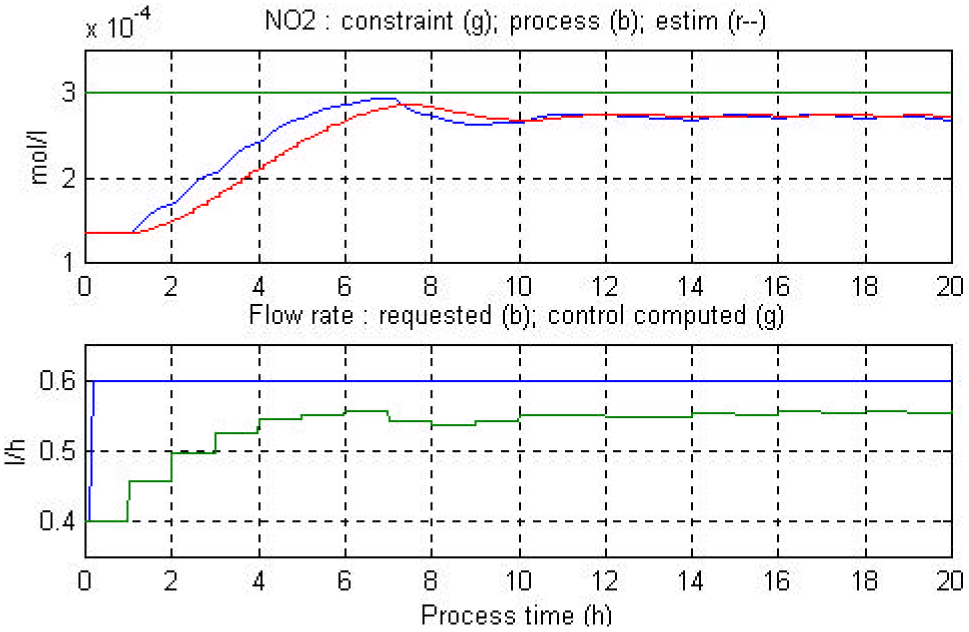

Figure 5 : Noise on O2 in liquid output (s = 10^{-5} mol/l = 5 % of mean value)

3.4. Mismatch on dissociation constant of NH_3

As it has been seen in the robustness study of the estimator, a mismatch on the dissociation constant k has a low consequence. So it has for the control (fig. 6 where the constant of the controller is 10 % higher than the corresponding constant of the process) : the behaviour of the Manipulated Variable (and consequently of the closed loop system) is quite similar of the reference behaviour of the simulation without noise nor mismatch (fig. 3).

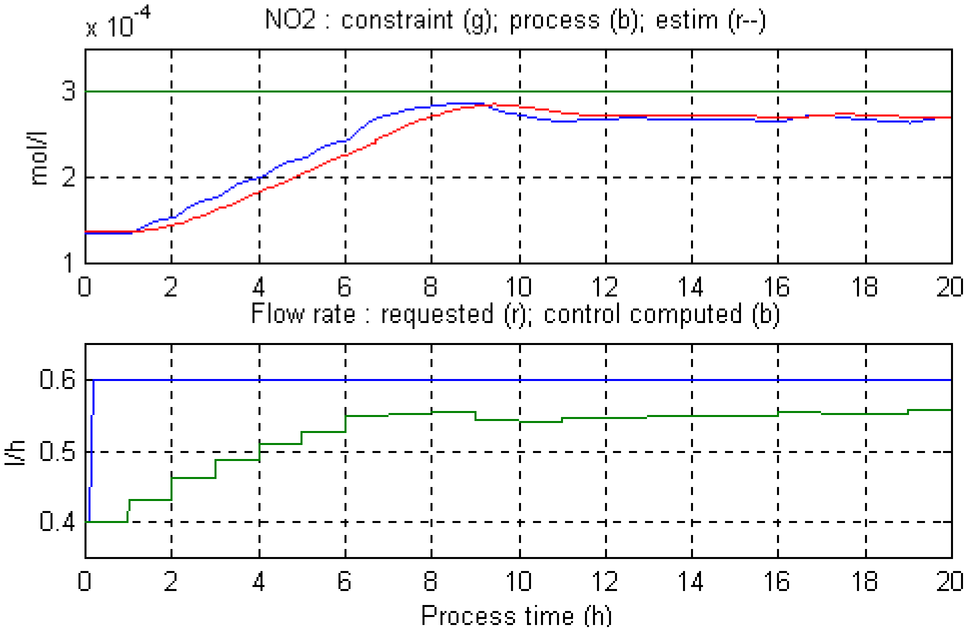

Figure 6 : Mismatch on dissociation constant k (k_control = 1.1*k_process)

3.5. Mismatch on limiting concentrations

3.5.1. Limiting concentrations of Nitrosomonas growth and maintenance

The impact of the limiting concentrations is low on the control as it can be seen on figure 7 where the limiting concentrations of the internal model are 50 % higher than those of the process.

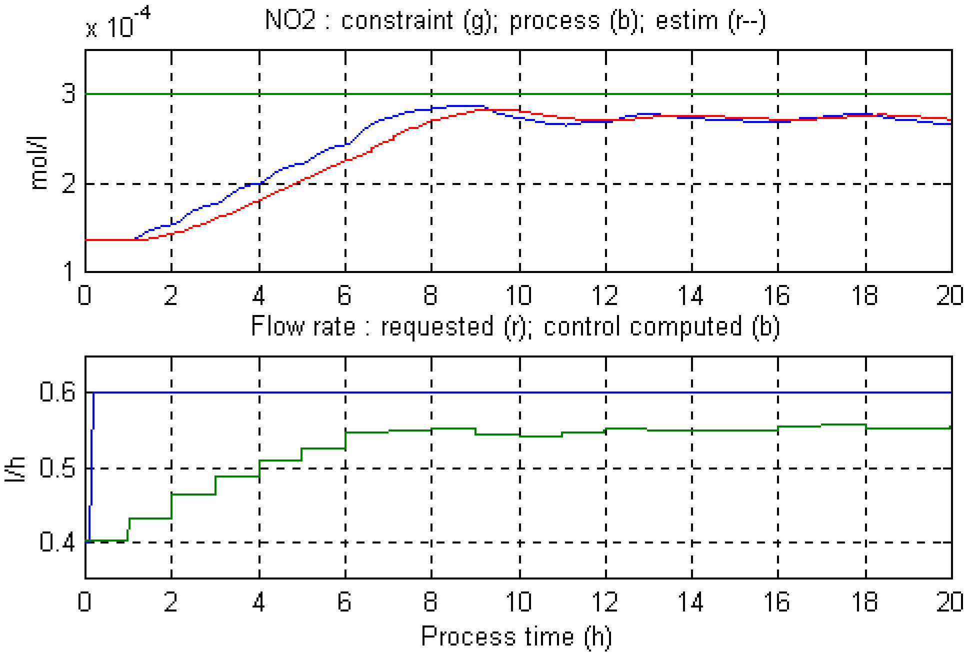

Figure 7 : Mismatch on limiting concentrations Kl of Ns (Kl_control = 1.5*Kl_process)

3.5.2. Limiting concentrations of Nitrobacter growth and maintenance

In that case, the Nitrobacter biomass is overestimated. Hence the NO2 production is underestimated and the CV tends to the constraint very slowly (fig. 8).

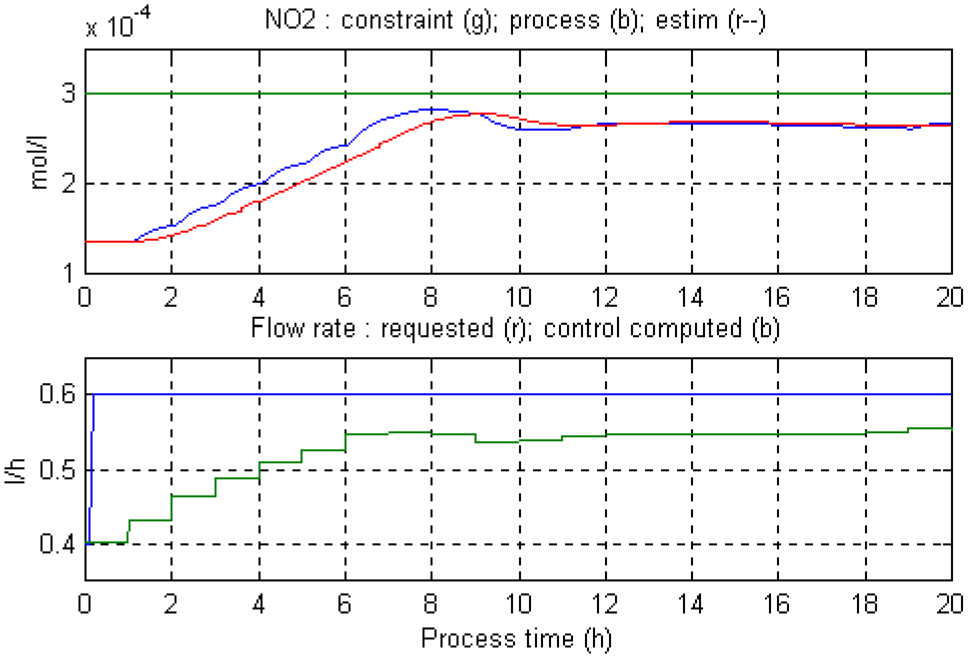

Figure 8 : Mismatch on limiting concentrations Kl of Nb (Kl_control = 1.5*Kl_process)

3.6. Mismatch on specific growth and maintenance rates

3.6.1. Specific growth rate

A 10 % increase on specific growth rate µ involves a very slight underestimation of NO_2. An overshoot could be possible : the NO2 process (blue line on figure 9) is nearly trespassing the constraint (green line).

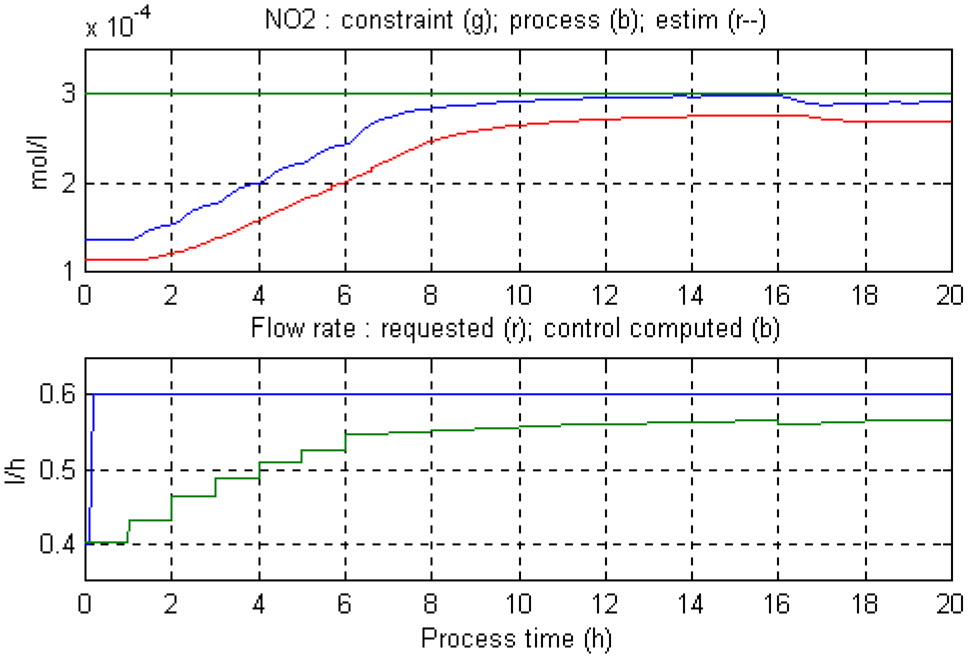

Figure 9 : Mismatch on specific growth rate m (m_control = 1.1*m_process)

3.6.2. Specific maintenance rate

A 10 % increase on specific maintenance rate ‘m’ involves a very slight overestimation of NO_2. Hence the CV approaches its constraint more slowly (fig. 10).

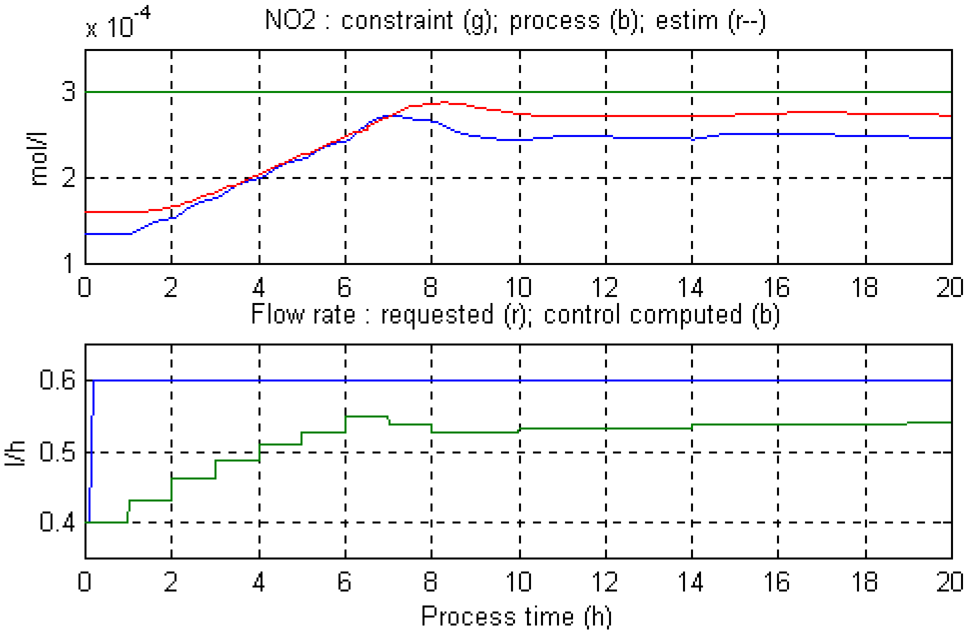

Figure 10 : Mismatch on specific maintenance rate m (m_control = 1.1*m_process)

3.7. Mismatch on the gas/liquid transfer KLa

As it has been shown in a previous study (TN 64.3), the influence of KLa is highly non linear on the NO_2 production regarding the volume of the fixed and the load.
In the present example, the ammonia load is rather high. So a reduction by half of the value of KLa in the internal model overestimates the NO_2 production on the scenario horizon, which implies a bias on the CV (fig 11).

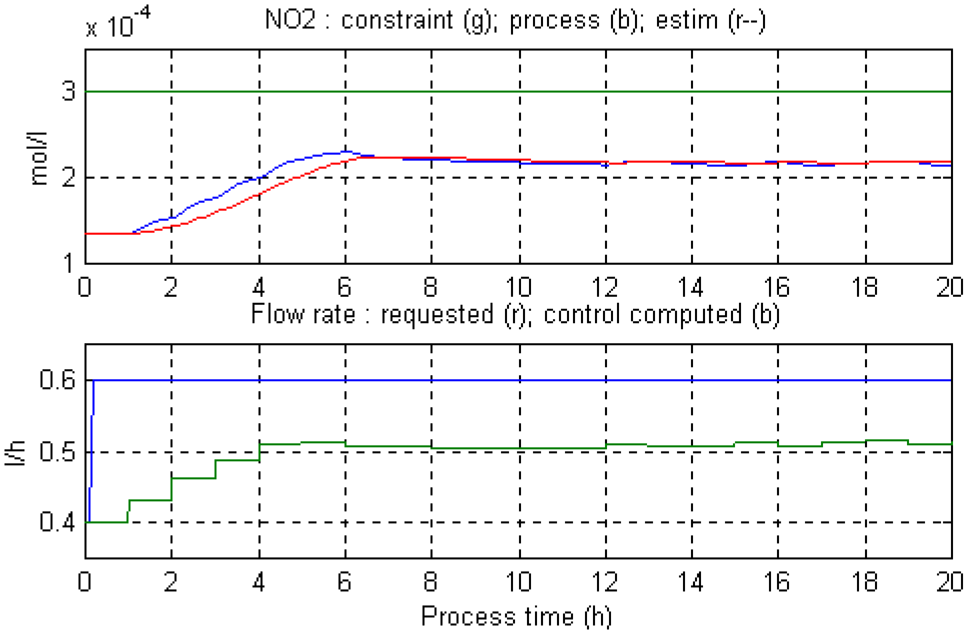

Figure 11 : Mismatch on gas/liquid transfer KLa (KLa_control = 0.5*KLa_process)

3.8. Bias on sensor

When a bias exists on a sensor, the NO_2 estimation can be corrected with a compensation term (cf. TN 73.2). In this simulation a bias of 10^{-4} mol/l has been added on the measurement of NH_3 and corrected with a compensation term of same value (because absolute value of β_1 is close to 1 in (7bis) of TN 73.2). Nevertheless the biomass estimation is disturbed and can not be corrected in the same way with a compensation term because measurement of biomass is impossible, even from time to time. But control is not affected drastically (fig. 12).

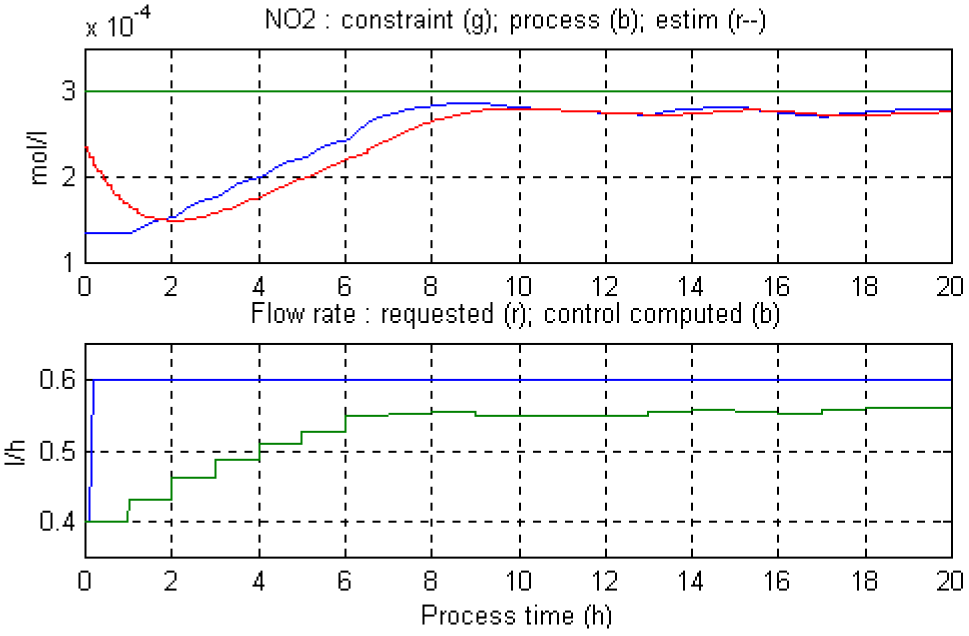

Figure 12 : Bias on NH3 sensor (NH3_meas=NH3_pro + 10^{-4} mol/l)

4. CONTROL SOFTWARE

4.1. Introduction

The control programme has been first built in Matlab® language for practical reasons and then translated into C language in order to be able to be implemented on any machine (PC or PLC). Message code and spy array are introduced to help implementing and maintenance work.

4.2. Functions of the control programme

The programme is conceived as a module with only one gateway connected to the computer system for exchanging data at a given period of time.
The 2 main functions of the programme are :

1. estimation of the state of the internal model;
2. control itself based on a scenario method.

These 2 main functions run at different sampling periods of time : 0.1 and 1 h for the estimator and the control, respectively. The shorter value (0.1 h) is the period for exchanging data with the computer system. Between 2 sampling of control (1 h), the estimated state is low pass filtered to reduce the noise of estimation.

The different sub-routines of the programme are detailed in the following table 1.

<table>
<tr><th>Name</th><th>Function of the sub-routine</th></tr>
<tr><td>nctrl</td><td>: Gateway from computer system</td></tr>
<tr><td>| -acq_par</td><td>: Acquisition of the parameters from disc file ‘f_ctrl_3.txt’</td></tr>
<tr><td>| -estim_3</td><td>: Main function of estimation of state of internal model</td></tr>
<tr><td>| | -estim_NX</td><td>: Estimation of nitrite and biomass concentrations</td></tr>
<tr><td>| | | -order</td><td>: Second and third order filter</td></tr>
<tr><td>| -con_3</td><td>: Main function of control itself</td></tr>
<tr><td>| | -extremum</td><td>: Computation of the extremum of NO2 on horizon H of the scenario</td></tr>
<tr><td>| | -integ_im</td><td>: Integration of state for scenario method</td></tr>
<tr><td>| | | -linterp</td><td>: Linear interpolation</td></tr>
<tr><td>| | | -im_nitr2</td><td>: State derivative of the internal model</td></tr>
<tr><td>| | | | -stasysim</td><td>: Computation of matrices of the internal model</td></tr>
<tr><td>| | | | | -transbi</td><td>: Transfer parameters of the bi_phasis compounds</td></tr>
<tr><td>| | | | -irate</td><td>: Limiting coefficients for growth and maintenance rate of biomass</td></tr>
</table>

Table 1 : Name and function of the sub-routines of the programme

4.3. Arguments of the gateway routine

This section describes the arguments of the main C routine (named *nctrl*) that are exchanged with the external environment. This routine *nctrl* has to be called by the machine (PC or PLC) system at given period of time. This period is the sampling period of the estimator. It is set to 0.1 hour.

The routine *nctrl* has 5 arguments that are listed in the Table 2.

The 2 first arguments are output arrays; the 2 following ones are inputs (1 array and 1 scalar).

The last argument ‘flag_ini’ is an input/output argument. Its function is very important as it implies the initialization of all the arrays of the programme when its value is 0. Its returned value that is set by *nctrl* routine is 1. It has to be set to 0 by the supervisor system when and only when an initialization is needed, particularly at starting of the control.

Name	Definition
x	Outputs vector of control
errors	Number and code of errors occurred in a run of the programme
u	Inputs vector of control
flag_sav	Flag for saving spy files ‘f_x.txt’ and ‘f_xef.txt’ when set to 1 by the external environment
flag_ini	Initialisation flag when set to 0 by the external environment

Table 2 : Description of the arguments of the gateway routine

Description of the inputs vector ‘u’ :

The vector ‘u’ is composed of 21 components described in the table 3.

When a component of ‘u’ can not be measured, it should be replaced by a constant value set from the keyboard by the operator.

Index	Unit	Description
0	l/h	Measured liquid flow rate or setpoint of the FRC of the liquid pump
1	mol/l	O_2 concentration in the gas input stream
2	mol/l	CO_2 concentration in the gas input stream
3	mol/l	NH_3 concentration in the gas input stream
4	mol/l	O_2 concentration in the liquid input stream
5	mol/l	total CO_2 concentration in the liquid input stream
6	mol/l	total NH_3 concentration in the liquid input stream
7	mol/l	unused (room for NO_2 concentration if not null)
8	mol/l	NO_3 concentration in the liquid input stream
9	mol/l	PO_4 concentration in the liquid input stream
10	mol/l	SO_4 concentration in the liquid input stream
11	mol/l	O_2 concentration in the liquid output stream
12	mol/l	total CO_2 concentration in the liquid output stream
13	mol/l	total NH_3 concentration in the liquid output stream
14	mol/l	NO_3 concentration in the liquid output stream
15	mol/l	PO_4 concentration in the liquid output stream
16	mol/l	SO_4 concentration in the liquid output stream
17	l/h	Measured gas flow rate or setpoint of the FRC of the gas pump
18	l/h	‘Required’ liquid flow rate
19	mol/l	Maximum constraint of NO_2
20	mol/l	Compensation term for estimator

Table 3 : Description of the components of the vector ‘u’

Description of the outputs vector ‘x’ :

The vector ‘x’ contains a lot of internal variables of the estimator and of the controller itself and has to be saved by the supervisor from one call to the next one. It is roughly described in the table 4 and is composed of 3 groups of components :

- x1 contains 81 components : the nitrite, biomass and state estimations and also internal variables of the estimator ;
- x2 contains 49 components : the MV, the behaviour of NO_2 on the scenario horizon H ;
- x3 is a saving of the inputs vector ‘u’ from a call to the next one and has the same size as ‘u’.

Limits of indices in x (C convention)	Description
0 to 20	Raw estimated state (concentrations of compounds in liquid phase of the parts A, B and C of the column)
21 to 37	Estimated NO_2 and biomass and internal variables of the estimator
38 to 80	Array for delayed inputs
81 to 87	MV and internal variables of the controller itself
88 to 129	Temporal evolution of NO_2 on the horizon H

130 to 150	Saving of ‘u’ for next call of the programme by the supervisor

Table 4 : Description of the components of the vector ‘x’

With the C convention for index (where the index of the first component is 0), the MV is the component of index 81 and the estimation of NO2 is the component of index 25.

4.4. Parameters of the control

The parameters of the control are saved in an ASCII file ‘f_ctrl_3.txt’ that is read by the *nctrl* routine at initialization (each time *flag_ini* is equal to 0). The parameters file is attached to the software package.

Name	Definition
dt_c	Sampling period of controller
dt_e	Sampling period of estimator
H	Horizon of simulation of the scenario
T_s	Vector of periods of time on H
stepmax	Maximum step of the iterative algorithm in routine ‘con_3’
zone_c	Vector of parameters of the zone defined around the nitrite constraint
coefil	Coefficient of the low pass filter of the inputs
Par_im0	Vector of parameters of the internal model of the control
Vv_e	Vector of volumes for the estimator time constants
beta_e	Vector of coefficients of the linear system binding rates of NH3 NO3 and NO2
delta_e	Vector of coefficients of the linear system binding rates of NH3 NO3 and the biomass
ind_3e	Vector of indices for the estimator
i_ctrl	Flag for running estimator and controller (if 1) or estimator alone (if 0)
boundin	Bounds of the validity domain of the components of the vector of inputs ‘u’

Table 5 : Description of the parameters of the control

4.5. Code of message

Message or error detection coming from the programme are returned to the supervisor by means of a code number at end of each run.

The table 6 gives the message corresponding to a code number and the subroutine where the message comes from.

Code	Content of Message	Origin
10,11, 12	Identity of volumes will imply division by 0 in routine ‘ord volumes have to corrected before restarting the programme.	acq_par
20	Input liquid flow rate is null. Estimation is frozen	estim_NX
21	Input liquid flow rate is null at initialization. Restart the programme when liquid flow is no more null.	estim_NX
22	Negative value of time constant ‘tauB’	estim_NX
23	Negative value of time constant ‘teta’	estim_NX
24	Negative value of time constant ‘teta1’	estim_NX
25	Negative value of time constant ‘teta2’	estim_NX

26	Negative value of time constant ‘teta	estim_NX
27	Ammonia consumption rate cannot be positive (non reversible reaction)	estim_NX
28	Nitrate production rate cannot be negative (non reversible reaction)	estim_NX
29	Nitrosomonas concentration cannot be negative	estim_NX
30	No interval found for dichotomy method	con_3
31	No interval found for dichotomy method : max number of iterations has been trespassed	con_3
32	No convergence for dichotomy method	con_3
400+j	The concentration of the component ‘j’ of the state vector is negative	integ_im
500+j	The value of the component ‘j’ of the inputs vector ‘u’ is outside its validity domain.	nctrl
70	Complex square root	transbi
71, 74	The first order approximation is not justified in part A of the column	transbi
72, 75	The first order approximation is not justified in part B of the column	transbi
73, 76	The first order approximation is not justified in part C of the column	transbi
90,91, 92	Identity of time constants implies division by 0. The volumes have to corrected before restarting the programme.	order
95,96	The components of the vector x are not monotonic ascending	linterp

Table 6 : Code number, content and origin (routine) of the message

4.6. Method of integration on the scenario horizon

The computation of the outputs of the state system during the horizon H of the scenario is done by integration of the derivative of the state system. The Euler method has been chosen because of the simplicity of the algorithm and despite its big computational time (big computational time is acceptable because the period of the control is long : 1 hour).

When the concentration of a compound reaches its limit, the system becomes non linear and the Euler method, which has no variable step, may have difficulty to deal with and the solution may be a negative concentration. So, at each integration step, each solution that is negative or zero is forced to be equal to the tenth of the limiting concentration. In fact this value is assumed to be the lowest value that is physically possible. This rule is applied in the routine ‘integ_im’.

4.7. Constraints on internal variables of the estimator

4.7.1. Constraints on NO_2 estimation

Due to the noise, the output of the estimator may be a negative value of NO_2 concentration, which is physically impossible.

When such an event occurs, the output of the estimator is forced to the tenth value of the limiting concentration of NO_2 for the growth of the Nitrobacter biomass. This rule is applied in the routine ‘estim_NX’.

4.7.2. Constraints on variation rates and biomass estimation

As the growth and maintenance reactions are not reversible, the consumption of NH_3 must be negative or zero and the production rate of NO_3 must be positive or zero. When this is not the case, because of the noise, the rate is forced to zero and an error message is emitted. This rule is applied in the routine ‘estim_NX’.

Consequences on the biomass estimation :

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 recalled in relation (8) of TN 73.2 :

$$c_{Xk} = \delta_{k1} \cdot r_1 + \delta_{k2} \cdot r_2$$

$$\text{where } \delta_{k1} \text{ and } \delta_{k2} \text{ are function of the stoechiometry and limiting factors}$$

$$r_1 = \text{consumption rate of } NH_3$$

$$r_2 = \text{production rate of } NO_3$$

For Nitrobacter (k=2), $\delta_{k1} = 0$. Now δ_{k2} and r_2 are positive. Then c_{Xk} is positive.

For Nitrosomonas (k=1), both δ_{k1} and δ_{k2} are negative. Now r_1 and r_2 have opposite signs. Then c_{Xk} could be negative. In that case, it is forced to 0 and an error message is emitted. This rule is applied in the routine ‘estim_NX’.

5. CONCLUSION

On simulator, the robustness of the controller is checked for the main parameters. The noise on the NH3 and NO3 measurements has to be very low : 0.5 % of the mean value.

The control has now to be validated on the pilot.

6. REFERENCE

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

7. ANNEX 1 : SCENARIO ON HORIZON H

As said in introduction (section 1), the column of the internal model is assumed to be composed of 3 CST's (part A, B or fixed bed, and C). But the column of the process is slightly different as it is supposed to be modelled with 4 CTS's : 1 for part A, 1 for part C and 2 for the fixed bed. That implies a difference of behaviour of the 2 columns : the column of the internal model never represents the process one. But how big is the difference?

For the control, the most important feature is the behaviour of NO_2 as it determines the value of the Manipulated Variable. So the difference between the 2 columns can be evaluated by comparing the 2 behaviours of NO_2 at output. The comparison is explained hereafter (figure A1.1).

First the process is simulated on a response time (at the end of the simulation the response of the process is complete) : from 0 to tsim of fig. A1.1 . The simulated process is the same as the one described in section 3 and a step of load occurs at starting.

The NO_2 and the biomass are estimated by means of the estimator all along the simulation (sampling period of the estimator : 0.1 h).

The simulation horizon is sampled each every 1 h from t=1 to t=6 h (which gives 6 samples).

At each sample, the internal model is launched on the horizon H of the scenario. Its input data are the process measurements and the estimations of this sample. The behaviour of the NO_2 on this horizon H is compared to the NO_2 process that follows the sample during the duration H : (the 6 samples are plotted on figure A1.2, one per graph).

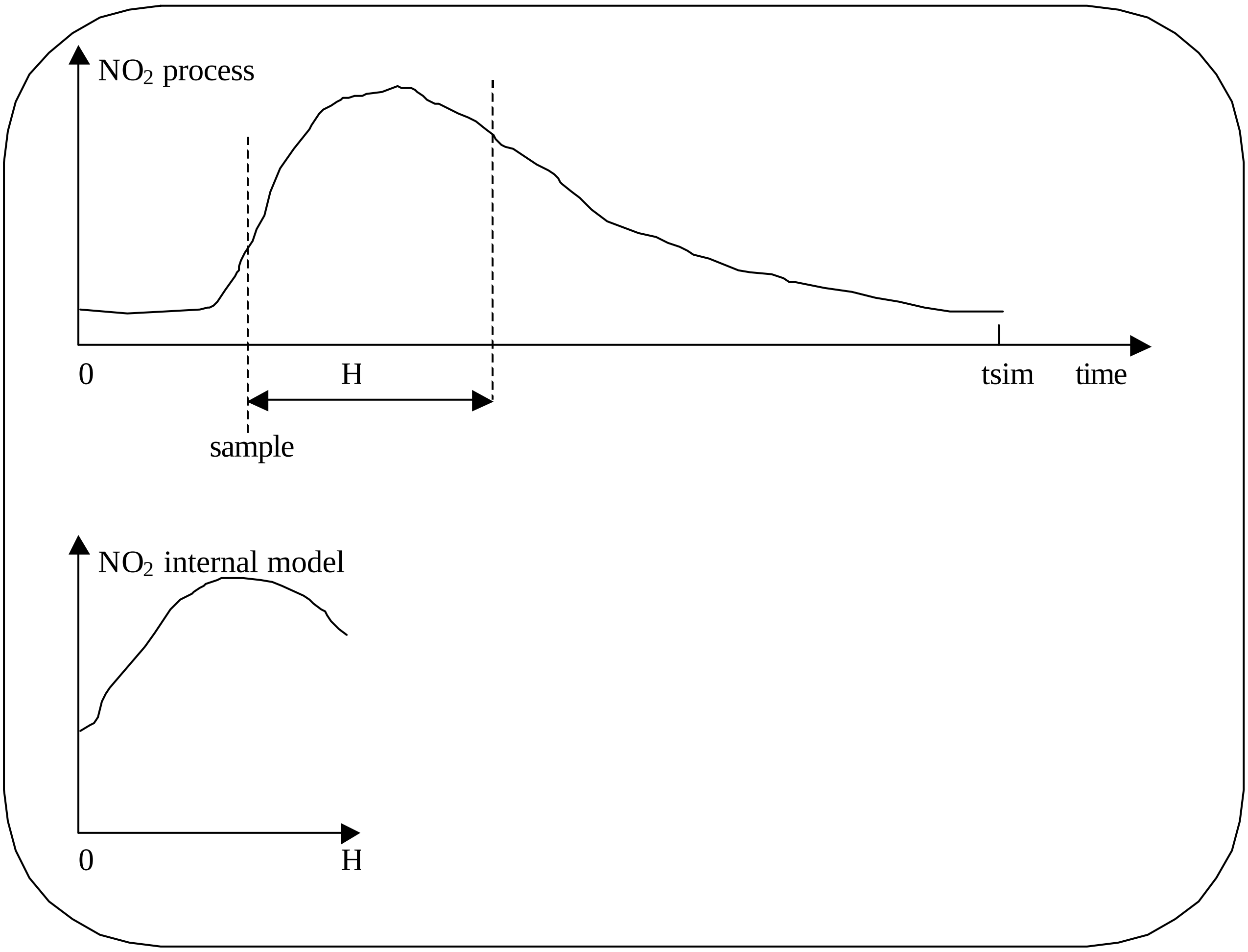

Figure A1.1 : Comparison internal model / process.
If the internal model is equal to the process, the 2 curves are the same on H

The figures A1.2 shows the NO_2 of the internal model on the horizon H (10 h) and of the process during the same period of time.
It can be observed that for the first hour that follows the step of load, the NO_2 of the scenario is about 30 % lower than the one of the process. For the following hours, the gap smaller and the NO_2 of the scenario can be assumed close to the one of the process. So the biggest difference between the 2 columns occurs during the hour that follows a step of load. But thanks to the first order reference trajectory (next annex) the impact of this difference is smoothed.

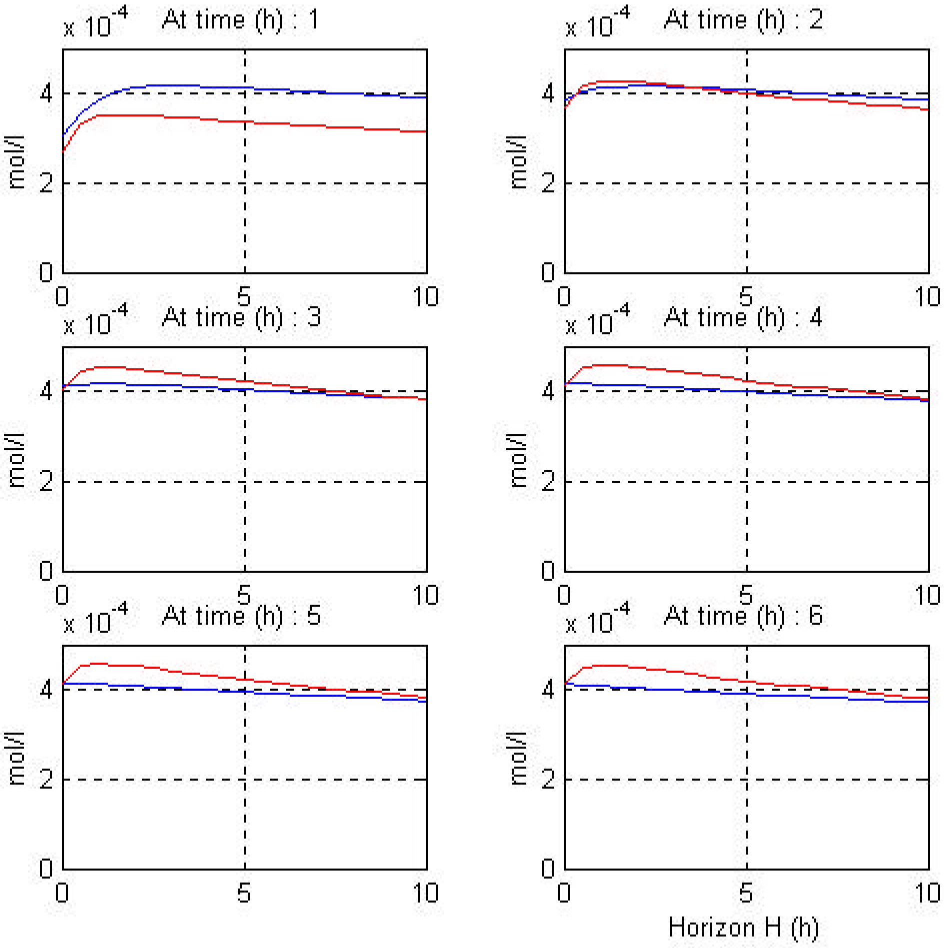

Figure A1.2 : Comparison: NO_2 of internal model on H / NO_2 of process.
Process (blue line); Model on horizon H (red line)

8. ANNEX 2 : REFERENCE TRAJECTORY AND DEAD ZONE

As said in section 2, if a step of 'requested' flow is positive, 'the reference' trajectory is a first order curve (figure A2.1). The time constant of this first order is variable : when the measured flow rate is far from its constraint, the first order is quick with a short time constant and inversely, when the measured flow rate is within a threshold around the constraint (i.e. when it is inside the dead zone), the time constant is big. Moreover, inside the dead zone, the time constant varies according to the distance to the constraint : the shorter it is, the bigger is the time constant. This makes the MV less sensitive to the noise when the measured flow is near its 'requested' value.

Outside the dead zone the time constant τ_1 does not vary.

Inside the dead zone the time constant τ_2 is a quadratic function of the distance x of the measured flow to its 'requested' value (figure A2.2) :

$$\tau_2 = a \cdot (d - x)^4 + \tau_1$$

with d : width of the dead zone

x : distance between the measured and 'requested' flow rate

a : numerical constant

In the present study :

τ_1 = 3 h;

d = 0.1 l/h;

a = 9.7 10^5 (expressed in the adequate unit);

Then, x = d $\Rightarrow$ $\tau_2 = \tau_1$ (continuity on the dead zone border)

and x = 0 $\Rightarrow$ τ_2 = 100 h (big time constant if the measured flow is on its ‘requested value’)

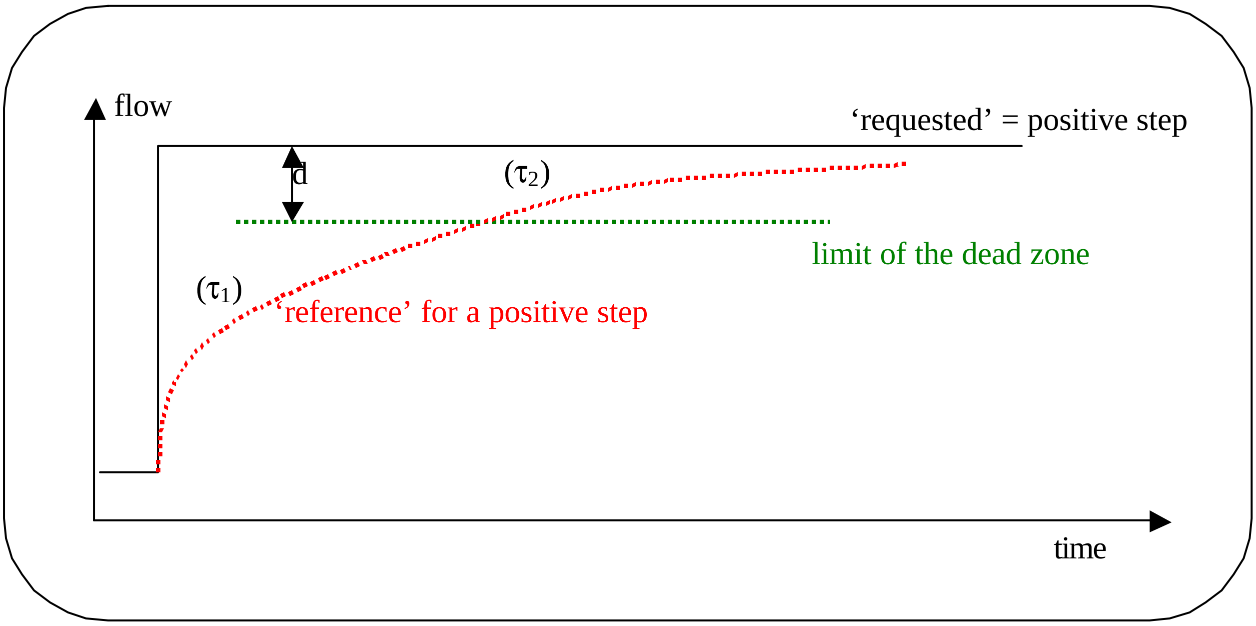

Figure A2.1 : Reference trajectory and dead zone

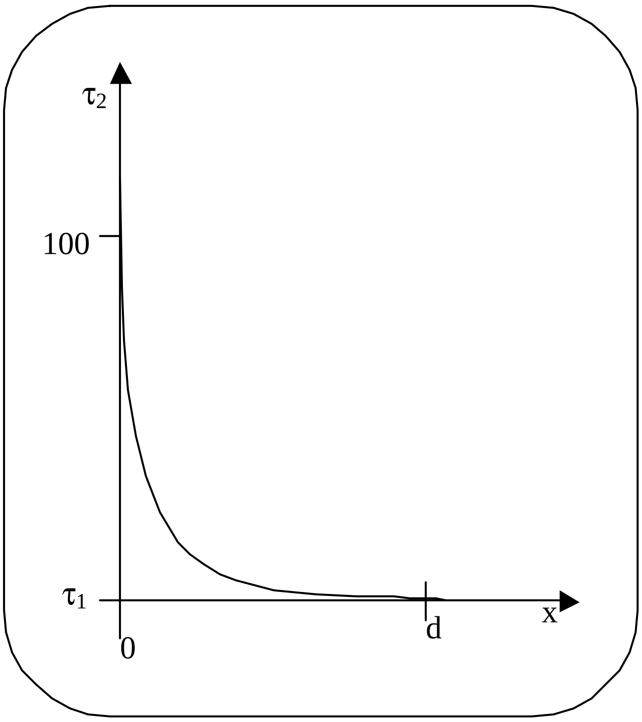

Figure A2.2 : Time constant τ_2 versus the distance x ($0 \le x \le d$)

9. ANNEX 3 : INITIAL VALUES AND PARAMETERS OF THE PROCESS

9.1. Initialization file of the variables of the process 'i_sim.m'

```
%*********************************************************************
%       Control of the Nitrifying compartment                        *
%       Version 1.2     November 2002                                *
%                                                                    *
%       i_sim.m   Initialization of the simulation                   *
%                                                                    *
%*********************************************************************

clear all
global Ae_3 Be_3 Ce_3 De_3 E_3
global A_c B_c C_c D_c E_c
global MAG MAL MBG MBL MEG MEL
global Fin1
global Fin1_c
global integ_prog inoise

% Simulation parameters
  tdeb=0;
  tmax=.1;
  tolr=1e-10; % low tolerance for noise on NO3=5% of the load and NO2=1.3 10-4 mol/l
  tolr=1e-8;  % normal tolerance for general case
  tola=1e-16;
  tfin=20;
  nbptx = 50000;
```

```
% Simulation horizon
  dt = .1;        % (h) simulation period of the inputs
  T = [0:dt:tfin]';
  [m,n] = size(T);
% Type of test
% ============
  typtst = 5;     titre = 'Variable step of liquid flow rate';
  typtst = 12;    titre = 'Step of NO2 constraint; NH3 and Q constant';  % (NB=1)
  typtst = 3;     titre = 'Step of ammonia (low load)';
  typtst = 1;     titre = 'Step of ammonia (high load)';
  typtst = 14;    titre = 'Step of ammonia (high load)';  % NB=2; high load
  typtst = 11;    titre = 'Step of requested flow rate (high load)';  % Mix of typtst=0 & 2
(NB=1; high load)
  typtst = 13;    titre = 'Step of ammonia (low load)';   % NB=2; low load
  typtst = 15;    titre = 'Steps of ammonia and liquid flow (opposite effects)';  % NB=2; low
load
  typtst = 0;     titre = 'Test of software';  % NB=1
  typtst = 10;    titre = 'Step of ammonia (high load)';  % Mix of typtst=0 & 1 (NB=1; high
load)
  typtst = 16;    titre = 'Step of liquid flow';  %like 15 without NH3 step;NB=2; low load
  typtst = 20;    titre = 'Test equi. to UAB-26.03.03)';  % study of step flow UAB on March
26th 2003 with low NO2
  typtst = 4;     titre = 'Step of liquid flow rate (low load)'; % NB=2; low load
  typtst = 2;     titre = 'Step of liquid flow rate (high load)';  % NB=2; high load
  titre=['Test ',num2str(typtst),'; ',titre];
% Initializing global parameters
% ==============================
  Gin_3 = 60;       % incoming gas flow rate (l/h) (email by Julio Perez on October 28th 2002)
  % The recirculating L flow is set to 0.77 l/h (previous value of flow through Spiru).
  % Then the residence time in Spiru = 100 h
  % The volume of the Nitri compart is modified to keep its residence time unchanged
  % The volume of Rhodo is set to 9 l : minimum for Fr=400 W/m2 and a biomass production of
.118 g/h
  %Fcirc = .4;   % Recirculating L flow rate (arbitrary value) (l/h)
  %share2 = 1 ;   % sharing ratio of liquid at output of compart 2 (Rhodo) towards Nitri
  %Fin_3 = Fcirc*share2;% liquid flow rate through Nitri(l/h)
  Fin_3 = .4;% liquid flow rate through Nitri(l/h) (email by Julio Perez on October 28th 2002)
% Parameters of compart.
% ======================
  Matom = [12; 1; 16; 14; 32; 31];  % C H O N S P atomik mass
  i_sim_3
  Fin1 = Fin_3;  % global Fin1   is used to run computation of the state matrices Ae,Be ...
  Fin1_c = Fin_3;% global Fin1_c is used to run computation of the state matrices A_c,B_c ...
% Choice of the integration programme
% ===================================
  integ_prog = 1; % 0 --> Integration customized with Euler method
                  % 1 --> Simulink S_function integration tools
% Checking the estimator or the control separately
% (test of estimator with 'sim_con' : itest_e = 1; i_ctrl = 0;)
% ================================================
  itest_e = 1; % 1 --> Estimator is running in 'tst_im'
  if NB_3>1, itest_e = 1; end % Estimated state cannot be replaced by process state in
'tst_im'
  i_ctrl = 0; % 1 --> Control is running in 'nctrl'
               % 0 --> Estimator alone is running in 'nctrl'
% Initializing indices used for the measurement of NH3 & NO3 at column output
% ============================================================================
  i1 = (NB_3+2)*NG_3+(NB_3+1)*(NG_3+NL_3); % output vector indices in part C of Nitri (L
compounds only)
  %i1 = (NB_3+2)*NG_3+(NB_3+0)*(NG_3+NL_3); % output vector indices in last tank of B of Nitri
(L compounds only)
  ind_3c1 = i1+[1:NG_3,NG_3+2:NG_3+NL_3]; % output vector indices in part B or C of Nitri (L
compounds only)
% Initializing indices (in control data input vector): vector 'ind_3e'
% used for the estimator
% ====================================================================
  i1=[1, ...                % index of flow rate
      1+2*NG_3+[0:2], ...   % indices of NH3_Ltotal NO2 NO3 at column input
      1+3*NG_3+NL_3+[0,1]]; % indices of NH3 NO3 at column output
   i2=1+2*NG+NL+[1:NG];      % indices of of O2 CO2 NH3 in the L output flow;
   i3=1+3*NG+NL+[1:NL-1];    % indices of of NO3 PO4 SO4 in the L output flow;
```

```
  ind_3e = [length(i1),length(i2),length(i3),i1,i2,i3]; % vector of indices 'ind_3e' for the
estimator
% Sizing state and input vectors
% ==============================
  dimd_e = 10; % for sizing the buffer of delayed signal in 'estim_3.m'
  dimx_e = 3*(NG+NL)+4*dimd_e+20; % see size of vector 'x_out' in 'estim_3.m'
  dimi_c = 3*NG_3+2*NL_3+4; % see size of vector 'u' in 'estim_3.m'
% Parameters of controller and estimators
% =======================================
  i_con
  dimx_c = 7+2*length(T_s);
% Choice of the initial load
% ===========================
  lNH3 = 1.0e-2; % (mol/h of NH3 total) high ammonia load
  if (typtst == 0 | typtst == 3 | typtst == 4 | typtst == 13 | ...
      typtst == 15 | typtst == 16)
    lNH3 = lNH3 / 10;  % decreasing the ammonia load
  end
% Initial concentrations in gas and liquid inputs
% ===============================================
  load init\f_init  % loading CG0_3 CL0_3 (example from the global simulator
                    % where NO2 and NO3 not null at input of the column
                    % and where NH3_G is null at input of the column)
  if typtst == 20 % test UAB on March 26th 2003
    CG0_3(1)=1/22.4*.2; % (mol/l) : conc of O2 in air
  end
  CL0_3(NG_3+1) = 0;% NO2 set to 0 at input of the column
  CL0_3(NG_3+2) = 0;% NO3 set to 0 at input of the column
  %CG0_3(NG_3) = alpha_3(NG_3)*CL0_3(NG_3); % (modif 22.11.02) Gas/Liquid at thermodynamic
equilibrium
  lNH3_example = Gin_3*CG0_3(NG_3) + Fin_3*CL0_3(NG_3)*(1+Kdis_3(NG_3)); % mol/h of NH3 total
of the example
  % all the concentrations of the example are made proportional to the chosen load
  CL0_3 = CL0_3 * lNH3 / lNH3_example;
  %CG0_3(NG_3) = alpha_3(NG_3)*CL0_3(NG_3); % Gas/Liquid at thermodynamic equilibrium
  lNH3_check = Gin_3*CG0_3(NG_3) + Fin_3*CL0_3(NG_3)*(1+Kdis_3(NG_3)) % mol/h of NH3 total
% Initial concentrations of N2 and H2O in gas (input or output)
% =============================================================
  fm_O2 = CG0_3(1)*VM;                    % O2  (molar fraction)
  fm_CO2 = CG0_3(2)*VM;                   % CO2 (molar fraction)
  fm_H2O = 5.796e-2;                      % H2O (molar fraction)
  fm_N2 = 1 - fm_O2 - fm_CO2 - fm_H2O;    % N2  (molar fraction)
  cN2_3  = fm_N2  / VM;       % mol/l
  cH2O_3 = fm_H2O / VM;       % mol/l
% Steady state of column
% ======================
  [X0_3, Y0_3, dX0_3] = stesta_3( ...
   NL_3, NG_3, NS_3, NB_3, NX_3, NO_3, NI_3, NV_3, WX_3, WYG_3, WYL_3, ...
   iO2_3, iCO2_3, iNH3_3, iNO2_3, iSub_3, iXNs_3, iXNb_3, iXag_3, ...
   KlNs_3, KlNb_3, KmNs_3, KmNb_3, mumax_3, maint_3, Yx_3, Yx1_3, Ym1_3, ...
   CG0_3, CL0_3, indG_3, indL_3, RG_3, RL_3, fG_3, fL_3, VA_3, VnB_3, VC_3, ...
   epsL_3, epsG_3, epsT_3, alpha_3, Kdis_3, KLa_3, Gin_3, Fin_3);
  if isempty(X0_3)
    disp(' X0_3 empty')
    break
  end
  X0_3L_disp=reshape(X0_3(1:(NG_3+NL_3)*(NB_3+2)),NG_3+NL_3,NB_3+2)
  X0_3S_disp=reshape(X0_3((NG_3+NL_3)*(NB_3+2)+[1:2*NS_3*(NB_3+2)]),2*NS_3,NB_3+2)
% Temporal inputs of column
% =========================
  dG = ones(size(T))*CG0_3'; % incoming G [O2,CO2,NH3] conc (mol/l)
  dL = ones(size(T))*CL0_3'; % incoming L [O2,CO2,NH3,NO2,NO3,HPO4,SO4] conc (mol/l)
  Fint = ones(size(T))*Fin_3'; % input liquid flow rate (l/h)
  Gint = ones(size(T))*Gin_3'; % input gas flow rate (l/h)
  if (typtst == 0 | typtst == 1 | typtst == 3 | typtst == 10| ...
      typtst == 13| typtst == 14)
    t0 = .2;
    ind = find(T>=t0);
    ii = NG_3; % index of ammonia in liquid input
    dL(ind,ii) = 1.5*CL0_3(ii)*ones(size(ind)); % increasing step of ammonia load
    %dG(:,NG_3) = alpha_3(NG_3)*dL(:,NG_3); % (modif 22.11.02) Gas/Liquid at thermodynamic
equilibrium
```

```
    %Fint(ind) = .5325*ones(size(ind)); % increasing step of liquid flow rate
  elseif (typtst == 2)
    t0 = .2;
    ind = find(T>=t0);
    Fint(ind) = 1.5*Fin_3*ones(size(ind)); % increasing step of required liquid flow rate
    %t0 = 6; t1=8;
    %ind = find(T>=t0 & T<t1);
    %Fint(ind) = 1.0*Fin_3*ones(size(ind)); % decreasing step of required liquid flow rate
  elseif (typtst == 4 | typtst == 11)
    t0 = .2;
    ind = find(T>=t0);
    Fint(ind) = 1.5*Fin_3*ones(size(ind)); % increasing step of required liquid flow rate
  elseif (typtst == 12)
    t0 = .1;
    ind = find(T>=t0);
    Fint(ind) = 2*Fin_3*ones(size(ind)); % increasing step of required liquid flow rate
  elseif (typtst == 15)
    t0 = .2;
    ind = find(T>=t0);
    ii = NG_3; % index of ammonia in liquid input
    dL(ind,ii) = 1.5*CL0_3(ii)*ones(size(ind)); % increasing step of ammonia load
    t0 = 1;
    ind = find(T>=t0);
    Fint(ind) = .15*ones(size(ind)); % decreasing step of (required) liquid flow rate
  elseif (typtst == 16)
    t0 = .2;
    ind = find(T>=t0);
    Fint(ind) = .15*ones(size(ind)); % decreasing step of (required) liquid flow rate
  elseif (typtst == 5)
    DeltaQ = .4; % l/h
    t0 = 4;
    ind = find(T>=t0);
    Fint(ind) = (Fin_3+DeltaQ)*ones(size(ind)); % increasing step of required liquid flow rate
    titre = ['Step of flow: ', num2str(DeltaQ), ' l/h'];
  elseif (typtst == 20) % test UAB on March 26th 2003
    t0 = .2;
    ind = find(T>=t0);
    Fint(ind) = 1.5*Fin_3*ones(size(ind)); % increasing step of (required) liquid flow rate
  end
% Temporal compensation term for NO2 estimation
% ==============================================
  compens = 0*(1e-4); % (mol/l) initial compensation term
  compenst=ones(size(T))*compens; % temporal evolution of the compensation term
% Initial measurements for control
% ==================================
  % Input 'u' (column vector)
  %       u(1)                        (l/h) liquid flow rate
  %       u(1+[1:NG])                 (mol/l) conc. in the Gas input flow
  %       u(1+NG+[1:NG+NL])           (mol/l) conc. in the Liquid input flow
  %       u(1+2NG+NL+[1:NG,NG+[1:NL-1]])(mol/l) conc. of O2 CO2 NH3 NO3 PO4 SO4 in the L
output flow
  %       u(3NG+2NL+1)                (l/h)   gas flow rate
  %       u(3NG+2NL+2)                (l/h)   required liquid flow rate
  %       u(3NG+2NL+3)                (mol/l) NO2 setpoint (or NO2 max constrain)
  u0_c = [Fint(1);
          dG(1,:)';
          dL(1,1:NG_3)'.*(1+Kdis_3);
          dL(1,NG_3+[1:NL_3])';
          Y0_3(ind_3c1).*[(1+Kdis_3);ones(NL_3-1,1)];
          Gint(1);
          Fint(1);
          0;         % arbitrary value for NO2 setpoint before calling estimator 'estim_3'
          compens];  % initial compensation term for NO2 estimation before calling estimator
'estim_3'
% NO2 setpoint
% ============
  % Initial state x of estimator
  [x_L0,x_NX0,X0_c] = estim_3([],[],u0_c,0,dt_e,Vv_e,RL_c, ...
                NG_3,NL_3,NS_3,KlNs_c,KlNb_c,Kdis_c,KLa_c,alpha_c, ...
                beta_e,delta_e,ind_3e,dimd_e,dimi_c);
  spNO2 = x_NX0(5); % (mol/l)
  if (typtst == 2 | typtst == 10 | typtst == 14)
```

```
    spNO2 = 3e-4; % (mol/l)
  elseif (typtst == 4)
    spNO2 = 1.8e-4; % (mol/l)
  elseif (typtst == 11)
    spNO2 = 2.5e-4; % (mol/l)
  elseif (typtst == 13)
    spNO2 = 2.3e-4; % (mol/l)
  elseif (typtst == 20) % test UAB on March 26th 2003
    spNO2 = 3e-5; % (mol/l)
  end
  spNO2t = ones(size(T))*spNO2; % time NO2 setpoint (mol/l)
  if (typtst == 12)
    t0 = 1.9;
    ind = find(T>=t0);
    spNO2t(ind) = 3e-4*ones(size(ind)); % increasing step of NO2 setpoint (mol/l)
  end
  u0_c(dimi_c-1)=spNO2t(1); % setting the NO2 constraint
  % Arbitrary initial state for 'im_nitri' (to be Matlab 5.3 compliant)
  % X0_c = zeros(NX_3*(NB_c+2),1);
  if length(u0_c) ~= dimi_c,
    disp('Wrong sizing of the input vector for control')
    arret = 1;
  end
disp(' *** Nitri Control - End of initialization ***')
% CG0 = [O2 CO2 NH3]
% CL0 = [O2 CO2 NH3 NO2 NO3 PO4 SO4]
% X0  = [O2 CO2 NH3 NO2 NO3 PO4 SO4 XA_Ns XA_Nb XG_Ns XG_Nb] for each tank
```

9.2. Initialization file of the parameters of the process 'i_sim_3.m'

```
%********************************************************************************
%       Nitrifying column control at UAB pilot plant                   *
%       Version 2.6     November 2002                                  *
%                                                                      *
%       State system according to TN 44.2                              *
%          . dissociation of CO2 and NH3                               *
%          . column = NB+2 CST's in series                             *
%                                                                      *
%       Modifications in March 2000                                    *
%          . vector KlNs and KlNb moved into scalar                    *
%          . Monod type law for maintenance in 'irate.m'               *
%                                                                      *
%       i_sim_3.m   Initialization of the process model                *
%                                                                      *
%********************************************************************************

arret = 0;

% Column parameters (pilot column at UAB)
%------------------
NB = 2;         % number of stirred tanks in part B (fixed bed):TN63.1 p.20 (LGCB)
VA = 1.48;      % volume of part A (l)
VB = 6.17;      % volume of part B (l)
VC = 0.45;      % volume of part C (l)
epsL = .33;     % volume ratio of liquid
epsG = .04;     % volume ratio of gas
epsT = epsG + epsL;
fG = 0;         % ratio of backward flow in a tank (gas phase)
fL = 0;         % ratio of backward flow in a tank (liquid phase)
d_beads = .0041;% (m) diameter of the beads  (TN 27.2 p.13 by LGCB)
d_column= .120; % (m) diameter of the column (TN 27.2 p.13 by LGCB)
RG = 0;         % recycling ratio of gas    (email by Julio Perez on Oct 28th 2002)
RL = 6;         % recycling ratio of liquid (email by Julio Perez on Oct 28th 2002)
VnB = VB / NB;  % volume of an equivalent stirred tank
Temp = 303;     % K (TN35.1 ADERSA)
pH = 8;         % TN35.1 ADERSA

% General parameters
% ------------------
```

```
NG = 3;         % number of bi-phases substrates (in the L and G phases)
NL = 4;         % number of mono-phase substrates in the liquid phase
                % (HNO2 HNO3 H3PO4 H2SO4)
NS = 2;         % number of strains of bacteria (Ns and Nb)
NX = NG+NL+2*NS;% nb of coef of state vector Xi for any tank
NO = NX+NG;     % nb of outputs for any tank
NI = 2*NG + NL;
NV = NI * (NB + 2);

% Kinetic parameters
% ------------------
Nls = 4;                        % nb of limiting substrates
Nis = 2;                        % nb of inhibitory substrates
%          Ns         Nb
mumax = [5.7e-2 ;   3.6e-2];    % max specific growth rate (1/h)
maint = [3.38e-3;   7.92e-3];   % maintenance coeffcient (1/h*(mol/gbio))
KlNs  = [5.05e-6           ;    % half saturation constant for growth : O2   (mol/l)
         6.625e-5          ;    % half saturation constant for growth : NH3  (mol/l)
         1e-10            ];    % no limitation with HCO3- for growth  (mol/l)
KlNb  = [           1.7e-5 ;    % half saturation constant for growth : O2   (mol/l)
                    3.6e-4 ;    % half saturation constant for growth : NO2- (mol/l)
                    1e-10 ];    % no limitation with HCO3- for growth  (mol/l)
In =    [1e30       1e30   ;    % inhibitory substrate : NO2- (mol/l)
         1e30       1e30]  ;    % inhibitory substrate : NO3- (mol/l)
if typtst == 20 % test UAB on March 26th 2003
  KlNs(2,1)=KlNs(2,1)/10;       % in order to reach the low NH3 conc. of the UAB test
  KlNb(2,1)=KlNb(2,1)/10;       % in order to approach the very low NO2 conc. of the UAB test
end
%if typtst == 2 % test for yearly meeting
%  KlNb(2,1)=KlNb(2,1)*5;       % (Yearly meeting) in order to have high NO2 conc. to be
detected
%end
KmNs  = 1*KlNs;         % half saturation constant for maintenance : O2; NH3   (mol/l)
KmNb  = 1*KlNb;         % half saturation constant for maintenance : O2; NO2-  (mol/l)

% Stoechiometry matrices (TN 27.1 p.39, LGCB)
% -------------------------------------------
% 1. stoechiometry matrix of the growth reactions
%          Ns         Nb
Yx1  =  [-5.4269   -6.5106 ;    % O2
         -1        -1      ;    % CO2
         -4.5341   -0.1994 ;    % NH3
          4.3347   -15.1714;    % NO2H
          0         15.1714;    % NO3H
         -0.0089   -0.0089 ;    % PO4H3
         -0.0035   -0.0035 ];   % SO4H2
Yx11 =  [ 3.8433   -0.4914 ;    % H2O
          1         1      ];   % biomasse Nitri (Nitrosomonas and Nitrobacter)

% 2. stoechiometry matrix of the maintenance reactions
%          Ns         Nb
Ym1  =  [-1.5      -0.5    ;    % O2
          0         0      ;    % CO2
         -1         0      ;    % NH3
          1        -1      ;    % NO2H
          0         1      ;    % NO3H
          0         0      ;    % PO4H3
          0         0      ];   % SO4H2
Ym11 =  [ 1         0      ];   % H2O

% change of unit of Yx1 :
Scompn = [1     1.6147 .3906 .1994 .0035 .0089]; % stoechio composition biomass nitri
M_nitri = Scompn*Matom;
Yx1 = Yx1 / M_nitri; % (mol substrate / g biomass)
Yx11= Yx11/ M_nitri; % (mol substrate / g biomass)

Yx(1,1) = 1/Yx1(3,1);   % yield for (global) growth of Ns (g X/mol NH3)
Yx(2,1) = 1/Yx1(4,2);   % yield for (global) growth of Nb (g X/mol NO2-)
% 3. stoechiometry matrix of the chemical compounds (atoms C H O N S P):
% atom : C         H         O         N         S         P
MSC = [  0         0         2         0         0         0       ;  % O2
         1         0         2         0         0         0       ;  % CO2
```

```
         0         3         0         1         0         0       ;  % NH3
         0         1         2         1         0         0       ;  % NO2H
         0         1         3         1         0         0       ;  % NO3H
         0         3         4         0         0         1       ;  % PO4H3
         0         2          4         0         1         0       ]; % SO4H2
MSC1= [  0         2         1         0         0         0       ]; % H2O
% 4. checking the stoechiometry of the global chemical equations (atoms C H O N S P):
if 1
  mass_balance=[M_nitri*[Yx1;Yx11]]'*[MSC;MSC1;Scompn];
  if ~all(all(abs(mass_balance) <= 2e-4 ))
    format short e
    disp('Mass is unbalanced in stoechiometry of growth reactions')
    disp('  C            H            O            N            S            P')
    disp(mass_balance)
    arret = 1;
  end
  mass_balance=[Ym1;Ym11]'*[MSC;MSC1];
  if ~all(all(abs(mass_balance) <= 1e-16 ))
    format short e
    disp('Mass is unbalanced in stoechiometry of maintenance reactions')
    disp('  C            H            O            N            S            P')
    disp(mass_balance)
    arret = 1;
  end
end

% Nominal gas and liquid flow rates
% ---------------------------------
Gin = Gin_3;    % l/h
Fin = Fin_3;    % l/h

% Gas/liquid transfer parameters
% ------------------------------
KLa = [51; 51; 500];    % O2 CO2 NH3   (1/h) before TN 73.1
voidage = .385;      % degree of voidage (L Poughon's email on 5th Nov 2002)
voidage = epsG+epsL; % degree of voidage (L Poughon's conversation on 14th Nov 2002 at MELISSA
meeting in Paris)
uG = Gin*(1+RG)*1e-3/3600/(voidage*pi*d_column^2/4); % superficial velocity of Gas
uL = Fin*(1+RL)*1e-3/3600/(voidage*pi*d_column^2/4); % superficial velocity of Liquid
coef = 1.12; % corrective factor for temperature (TN 63.2 p.7 by LGCB)
KLax = coef*1481*(uG).^0.5979*(d_beads/d_column)^(-0.1153);  % TN 63.2 p.30 by LGCB
KLax=150; % to allow NB=5 with high load
KLa = KLax*ones(NG,1)  % O2 CO2 NH3   (1/h) for TN 73.1

% Physico-chemical constants
% --------------------------
[kpart,Kab,ksi_bid] = i_physic(Temp,pH);
% partition coefficients
kpartN = kpart([2,4,6],1);   % O2 CO2 NH3 (T = Temp K,non ionic form)
% dissociation coefficient (for NH3)
Kb = Kab(3,1);          % basicity cst  at T = 'Temp' K
Ke = Kab(4,1);          % ionic product at T = 'Temp' K
KNH3 = Kb*10^(-pH)/Ke;  % [NH4+] = KNH3 * [NH3]solvated
% dissociation coefficient for CO2
KCO2 = Kab(1,1)/(10^(-pH))*(1+Kab(2,1)/(10^(-pH))); % [HCO3-]+[CO3--] = KCO2 * [CO2]solvated
% dissociation coefficient (for H3PO4)
Ka = 6.166e-8;                    % (at T=298K, from TN 27.2,LGCB)
xx = 10^(-pH)/Ka;   KPO4 = 1+xx;  %[PO4]total = f([HPO4=])
% dissociation vector for the biphase substrates
Kdis = [0; KCO2; KNH3]; % O2  CO2  NH3
% liquid/gas thermodynamical equilibrium constants
VM = 22.4 * Temp / 273;  % molar volume (l/mol)
alpha = kpartN / 55.56 / VM;

% Computation of the state system of the nitrifying compartment
%--------------------------------------------------------------
[Ae_3,Be_3,Ce_3,De_3,E_3] = stasys_3(NG, NL, NB, Gin, Fin, RG, RL, fG, fL, ...
                                     VA, VnB, VC, epsL, epsG, epsT, ...
                                     alpha, Kdis, KLa);

% Initialization of vector of indices
%------------------------------------
```

```
iO2  = 1:NG+NL:(NB+1)*(NG+NL)+1; % indices of O2 L in the state vector
iCO2 = iO2  + 1;                 % indices of HCO3- in the state vector
iNH3 = iCO2 + 1;                 % indices of NH3 L in the state vector
iNO2 = iNH3 + 1;                 % indices of NO2 in the state vector
iNO3 = iNO2 + 1;                 % indices of NO3 in the state vector
iPO4 = iNO3 + 1;                 % indices of PO4 in the state vector
iSO4 = iPO4 + 1;                 % indices of SO4 in the state vector
iSub = 1:(NG+NL)*(NB+2);         % ind. of subs. in state vector
iXNs = 1 : 2*NS : 2*NS*(NB+1) + 1;
iXNs = iXNs + (NG+NL)*(NB+2); % ind. of act. biomass Ns in the state vector
iXNb = iXNs + 1;              % ind. of act. biomass Nb in the state vector
iXag = (NG+NL)*(NB+2) + 1 :(NG+NL+2*NS)*(NB+2); % ind. of active and global
indG0 = 1:NG;         indG = indG0;
indL0 = NG+1:2*NG+NL; indL = indL0;
for ii = 1:NB+1
  indG = [indG, indG0+ii*NI];   % ind. of Gas concen. in the output vector
  indL = [indL, indL0+ii*NI];   % ind. of Liq concen. in the output vector
end

% Noise
%------
% 1. Weight vector of the noise on the derivative of the state vector
WX0 = 0*5*[0    0    1e-6   1e-6    1e-6  0    0];
WX = WX0;
for ii = 1:NB+1
  WX = [WX, WX0];
end

% 2. Weight vector of the noise on the output vector
%WYG0 = 0*5*[0    0    0 ];
%WYL0 = 0*5*[0    0    1e-5/(1+KNH3)   0    1e-5  0    0];
%WYG = WYG0;
%WYL = WYL0;
%for ii = 1:NB+1
%  WYG = [WYG, WYG0];
%  WYL = [WYL, WYL0];
%end
WYG = zeros(1, NG*(NB+2));
WYL = zeros(1, (NG+NL)*(NB+2));
if typtst == 0 % noise added on part B of the column where measurements are supposed to be
done
  WYG0 = 0*2*[0    0    0 ];
  WYL0 = 0*2*[0    0    1e-5/(1+KNH3)   0    1e-5  0    0];
  WYG(1,NG*NB+[1:NG]) = WYG0;
  WYL(1,(NG+NL)*NB+[1:NG+NL]) = WYL0;
else % noise added on part C of the column
  WYG0 = 0*5*[0    0    0 ];
  WYL0 = 0*5*[0    0    1e-5/(1+KNH3)   0    1e-5  0    0];
  WYG(1,NG*(NB+1)+[1:NG]) = WYG0;
  WYL(1,(NG+NL)*(NB+1)+[1:NG+NL]) = WYL0;
end

% Checking the mass balance of atoms C H O N S P
%-----------------------------------------------
% 1. Stoechiometry matrices of compounds in Gas Liquid and Solid phases :
MSG = MSC(1:NG,:);  % O2 CO2 NH3 : Gas
MSL = MSC;
MSL(1:NG,:) = diag(1+Kdis)*MSL(1:NG,:); % O2 CO2 NH3 : solvated and ionic forms
MSS = Scompn ./ (M_nitri*ones(size(Matom')));  % CHONSP atom/g biomass
MSS = [MSS; MSS];                              % CHONSP atom/g biomass
% 2. matrices of volume of tanks
Vg = [ VA*epsG/epsT;
       VnB*epsG*ones(NB,1);
       VC*epsG/epsT];
Vl = [ VA*epsL/epsT;
       VnB*epsL*ones(NB,1);
       VC*epsL/epsT];

% Saving the specific variables of the Nitrifying compartment
% ==========================================================
NL_3 = NL;     NG_3 = NG;     NS_3 = NS;
NB_3 = NB;     NX_3 = NX;     NO_3 = NO;     NI_3 = NI;     NV_3 = NV;
```

```
Kdis_3 = Kdis;
Fin_3 = Fin; Gin_3 = Gin; RG_3 = RG;      RL_3 = RL;
fG_3 = fG;     fL_3 = fL;     VA_3=VA;       VnB_3=VnB;     VB_3=VB;  VC_3=VC;
epsL_3=epsL; epsG_3=epsG; epsT_3=epsT;
WX_3 = WX;     WYG_3 = WYG; WYL_3 = WYL;
iO2_3 = iO2; iCO2_3 = iCO2; iNH3_3 = iNH3; iNO2_3 = iNO2;
iSub_3 = iSub; iXNs_3 = iXNs; iXNb_3 = iXNb; iXag_3 = iXag;
KlNs_3 = KlNs; KlNb_3 = KlNb; KmNs_3 = KmNs; KmNb_3 = KmNb;
mumax_3=mumax; maint_3=maint;
Yx_3=Yx;       Yx1_3=Yx1;   Ym1_3=Ym1;   Yx11_3=Yx11; Ym11_3=Ym11;
indG_3=indG; indL_3=indL;
MSG_3=MSG;     MSL_3=MSL;     MSS_3=MSS;       MSC_3=MSC;   MSC1_3=MSC1;
Vg_3 = Vg;     Vl_3 = Vl;     alpha_3=alpha; KLa_3=KLa;
pH_3 = pH;

if arret
  disp(' *=*=* Nitri : initialization aborted *=*=*')
  break
end
disp(' *** Nitri - End of initialization ***')
```