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MELISSA

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TECHNICAL NOTE : 48.3

Nitrite and Biomass Predictors
of the Nitrifying Compartment
Phase III: First Validation

Version : 1
Issue : 0

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0	0	February 2002	Draft
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	"Nitrite and biomass predictors of the nitrifying compartment-Phase III"		
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Abbreviations :

N_s : Nitrosomonas

N_b : Nitrobacter

FFT : Fast Fourier Transform

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NOTATION

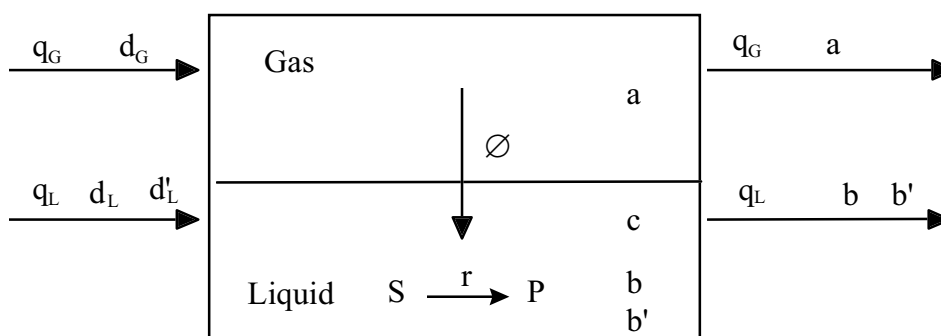
The notation is the one of TN 44.2 or TN48.1 and is recalled hereafter, for each substrate of the problem and for each tank of the column :

- 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)**

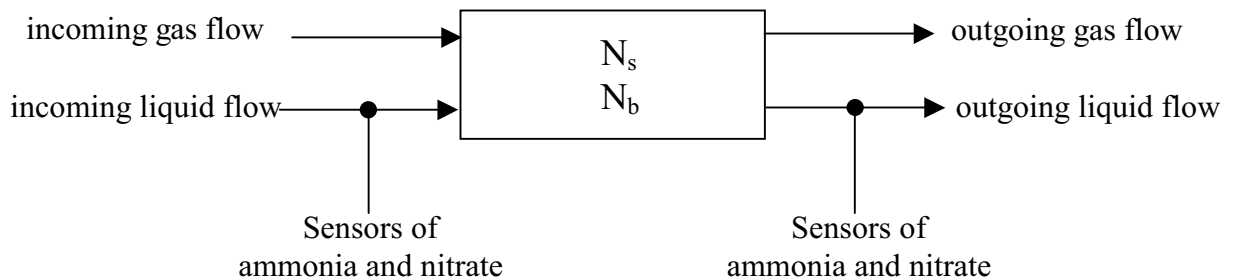
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1. INTRODUCTION

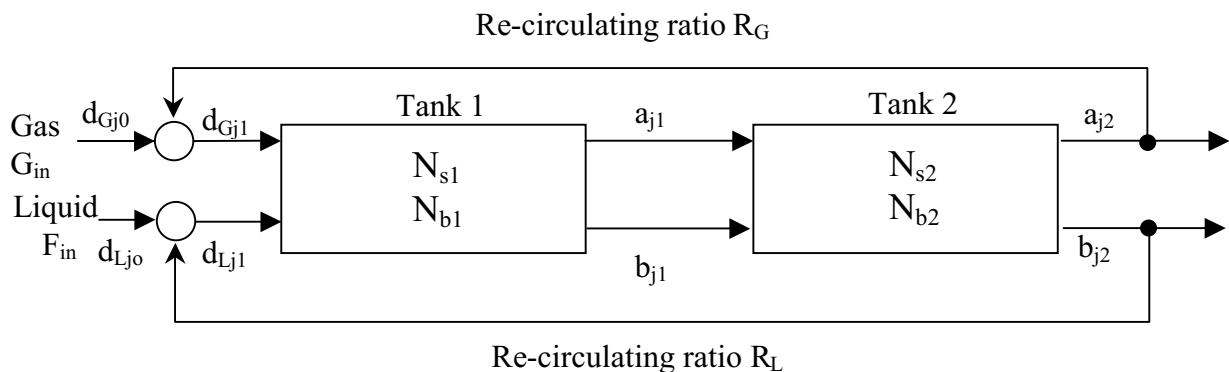
1.1. Recall

In the previous study reported in Technical Note 48.1, three candidates of predictors have been 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).



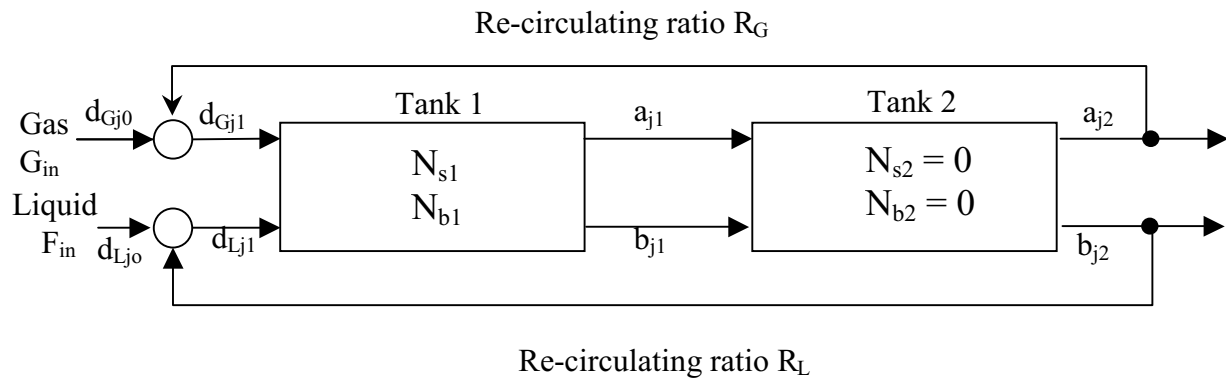
Scheme 1 : Model of the predictor 1



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

The robustness study of TN 48.2 has shown that the predictor 2 is satisfactory but requires a supplementary sensor of ammonia and one of nitrate in the middle of the column. So the resulting nitrite predictor will be composed of the 2 concurrent predictor 1 and 3 :

- predictor 1 for a starting column (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.

1.2. Objective of the study

During more than 8 months, from October 10th 1999 to June 30th 2000, UAB has performed a lot of various tests on the nitrifying column. Although these tests were not specifically designed for the validation of the nitrite estimator because at that moment the estimator was not built yet, it appeared that it could be instructive to make a first evaluation of the nitrite predictor on this experiment.

As the study will show it, the results are promising. One can just regret that the instant of the steps of ammonia are not exactly registered for the validation of the estimator. Nevertheless a great part of the experiment can be used on that purpose.

The data recorded in the file of the experiment 'data_from_tn43_3.xls' have been transformed and completed in order to fit the inputs of the nitrite estimator. The way the necessary data have been rebuilt is detailed in annex.

2. COMPARISON ESTIMATION VERSUS MEASUREMENT

The parameters of the estimator have been set according to the conditions of the experiment:

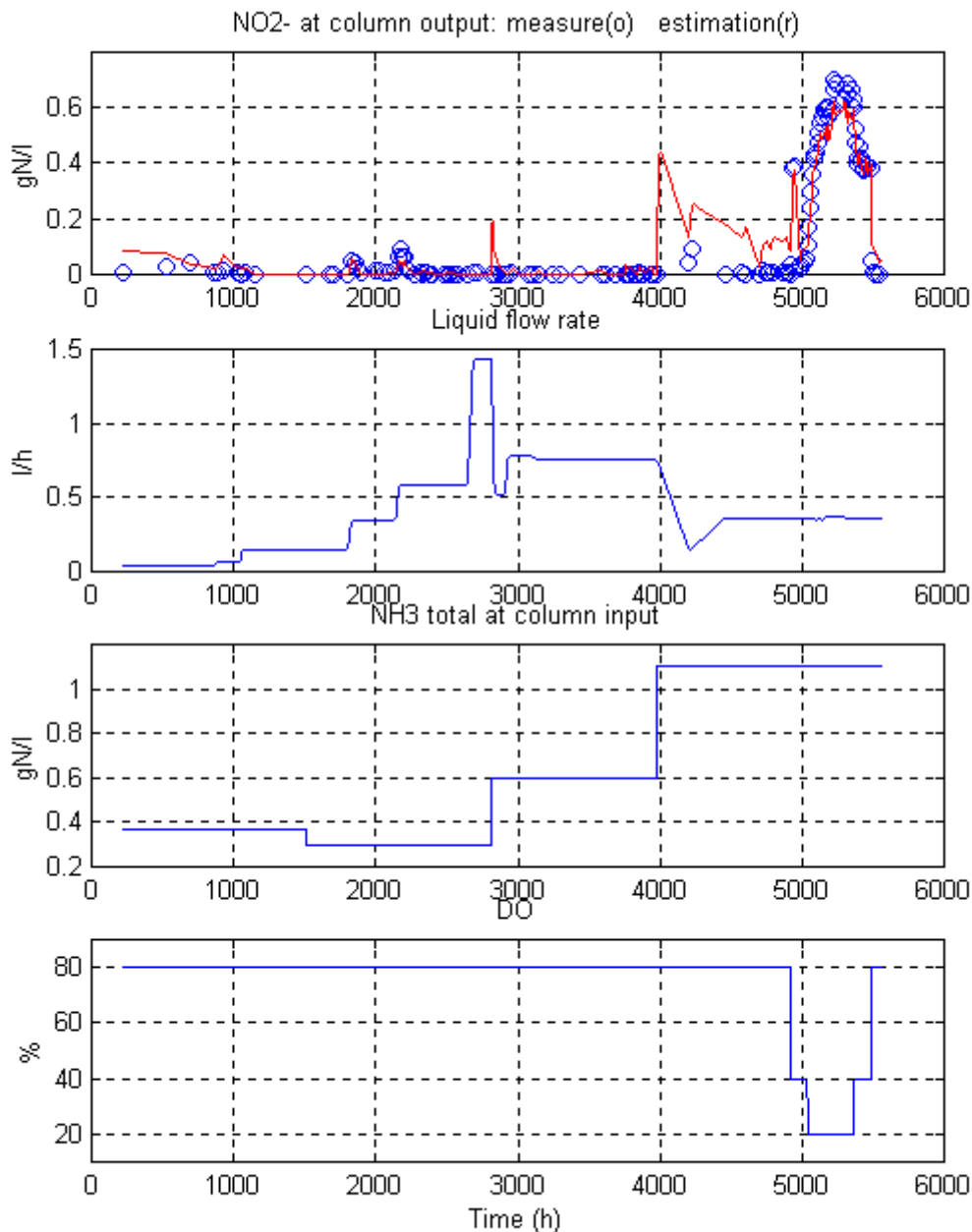
- pH = 8.1 as in TN 43.3 .
- Temperature = 30 or 28 °C according to the concerned part of experiment. During the test where the temperature is varying, the corresponding parameter of the estimator is set to a mean value because the estimator is supposed not to be function of variable temperature.
- The gas flow rate and the gas re-circulating ratio, G_{in} and R_G , are set to 1.8 l/h and 99, which gives an aeration flow rate equal to 180 l/h as in TN 43.3
- The liquid re-circulating ratio, R_L , is set to 6 as in TN 43.3 .
- Volume of liquid of the column, $V_L = 3.76$ l .

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- The maximum specific growth rates and maintenance coefficients for N_5 and N_6 are those of TN27.2 by LGCB.

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The whole experiment, plotted on the figure 1, consisted in steps of liquid flow rate (second graph), steps of ammonia (measured as total ammonia plus ammonium in the third graph), steps of dissolved oxygen (DO in the fourth graph) and steps of temperature between time $t=3450$ and $t=4000$ h (not plotted). The first graph shows the nitrite estimation with predictor 1 whose temperature is set to a constant value equal to 30 °C. For some parts of the experiment the nitrite estimation fits well and for the other parts it does not. Details are given in the following figures.

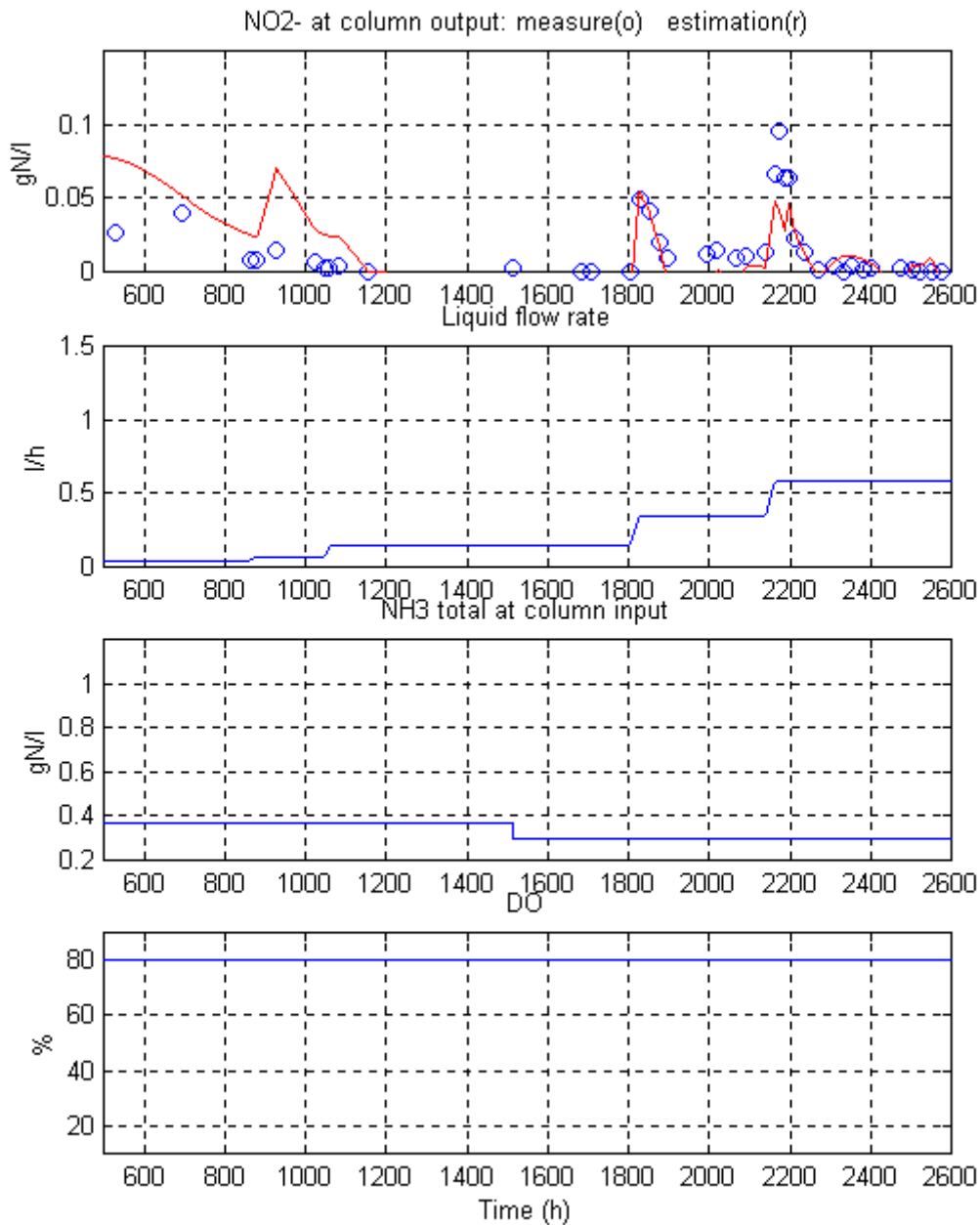


UAB experiment from October 10th 1999 to June 30th 2000

Figure 1

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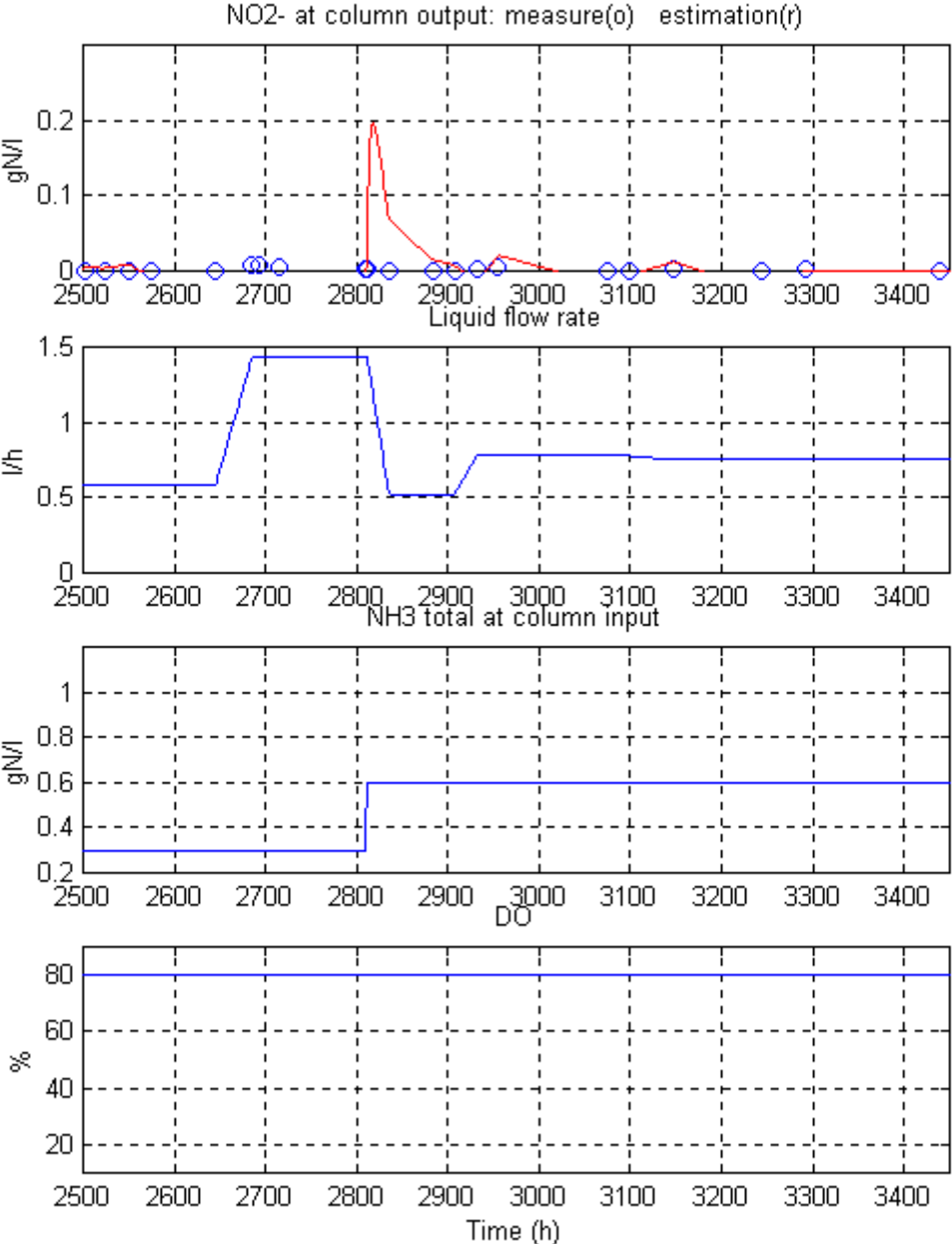
The figure 2 shows the beginning of the experiment with increasing steps of input flow rate. The nitrite is overestimated at the step at time $t=875$ h, correctly estimated at $t=1800$ h and underestimated at $t=2150$ h. The explanation of the gap could be the time period of the ammonia and nitrate measurements that is much bigger than the requested one (the ideal time period is justified in the further section 3).



First increasing steps of input flow rate
Figure 2

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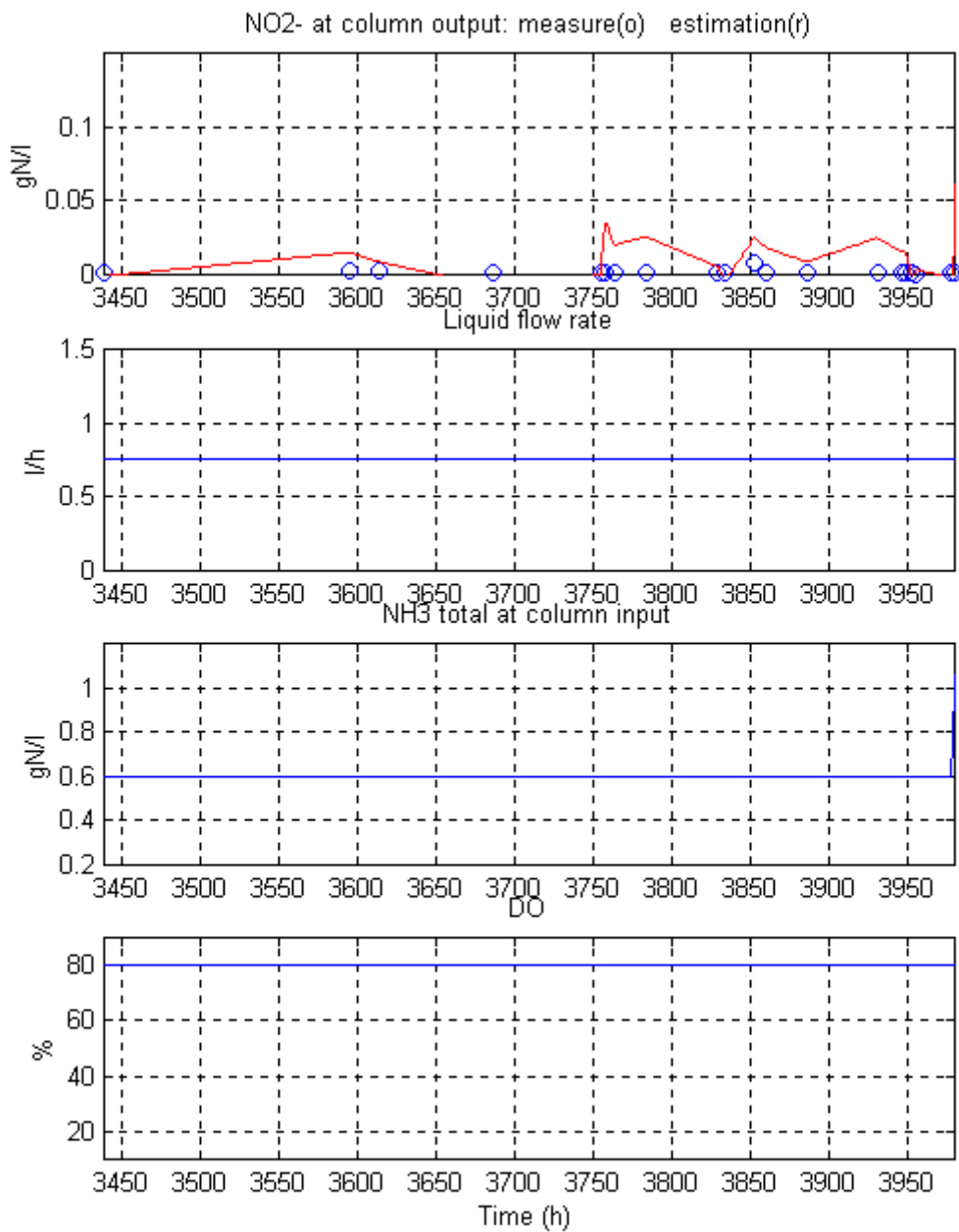
The figure 3 shows the next steps of input ammonia and flow rate. When the input concentration is doubled at time $t=2800$ h, the estimator gives a big peak of nitrite that does not appear in the measurement. There is no explanation, except that there is too much uncertainty about what was done exactly at that moment : the input flow was set to zero (from 8th to 14th February 2000) and the moment, when steps of flow and ammonia concentration were done, is not exactly recorded .



Steps of input NH3 and flow rate
Figure 3

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The figure 4 shows the variation of temperature. This parameter is set to constant value equal to 27 °C in the estimator. The gap is about 10^3 mol/l (14 ppm N).

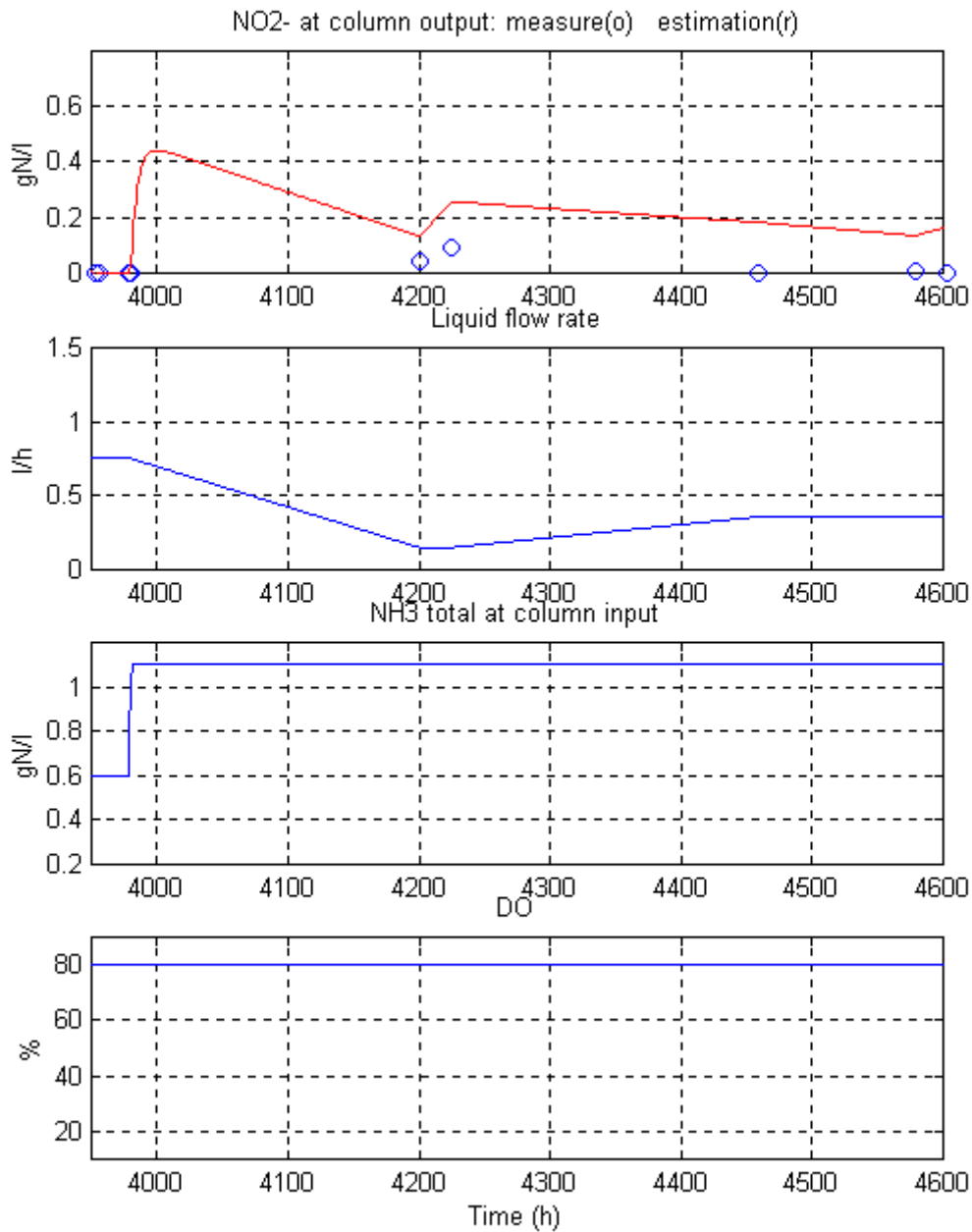


Variations of temperature

Figure 4

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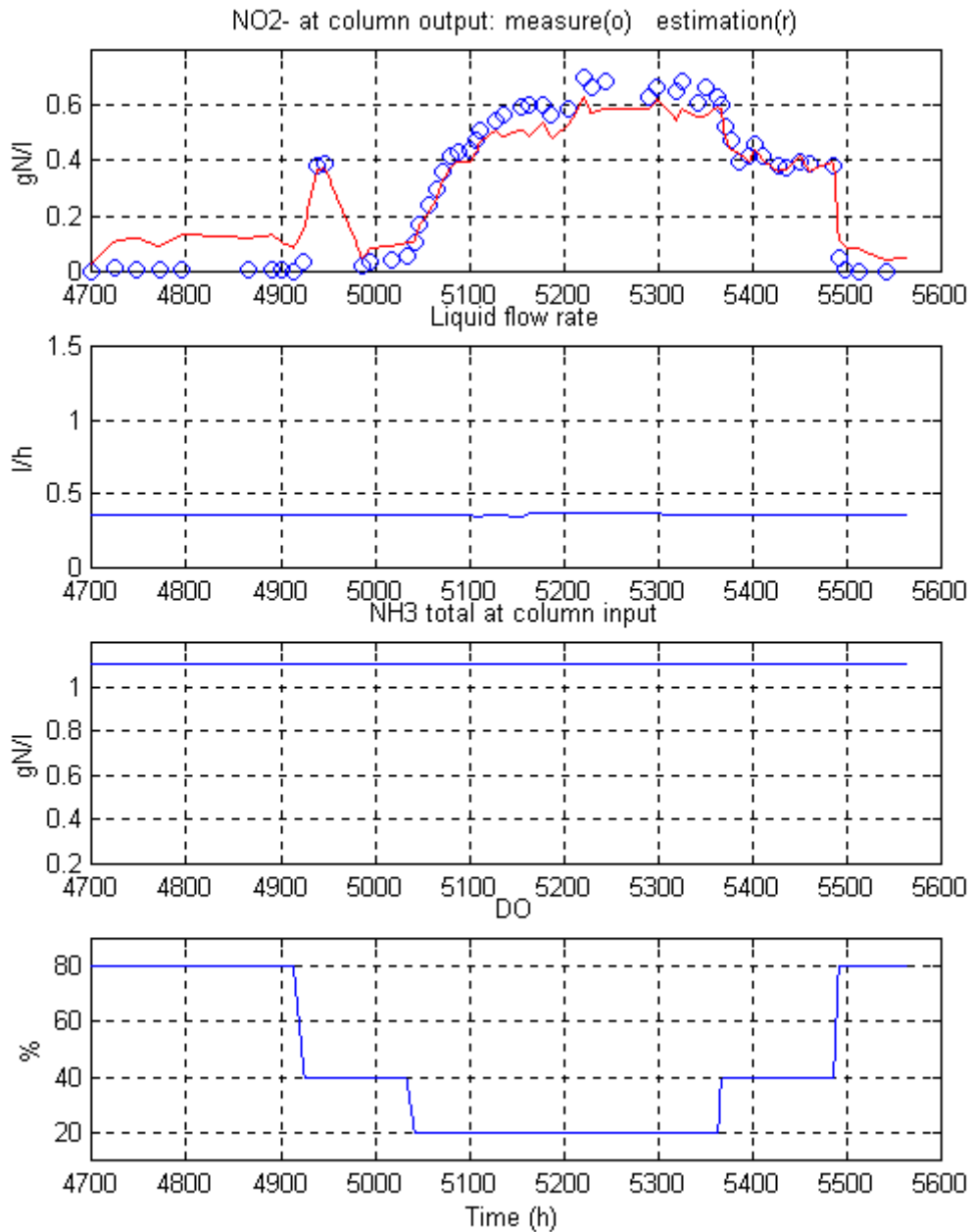
The figure 5 shows step of input ammonia. There is no explanation for the gap.



Step of input NH3
Figure 5

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The figure 6 shows the steps of dissolved oxygen. The estimation fits the measurement well.



Variation of the Dissolved Oxygen

Figure 6

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3. SPECIFICATIONS OF THE VALIDATION TESTS

The specifications concern the sampling periods of the variables to be collected.

3.1. Sampling period of ammonia and nitrate measurements

Theoretical justification

The choice of the sampling period is based on the expression of the nitrite concentration for the predictor 1 (from (A.20) of TN 48.1) :

$$b_3 = s_2 - s_1$$

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

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

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

So the nitrite concentration, b_3 , is the algebraic sum of the 2 functions s_1 and s_2 :

- s_1 is a typical first order transfer with time constant τ_L .
- s_2 , which is function of the ammonia and nitrate at column output, b_1 and b_2 .

It can be checked in the figure 7 that the nitrate behaviours as a first order. But the order of ammonia is higher : a FFT of the signal would show high frequencies in the spectrum.

According to the Shannon theorem applied to first order, the sampling period T_s is around the tenth of the time constant (or residence time).

Numerical application

In the present case, this rule cannot be applied because of s_2 , a function whose order is higher than 1. So the sampling period has to be shorted as illustrated in simulation of figures 9 and 10 : for a long residence time (22 h), $T_s = 1$ h max; for a short residence time (3.8 h), $T_s = .5$ h max,

So, in order to choose a common value for all the tests, the sampling period of the ammonia and nitrate measurements will be 0.5 h.

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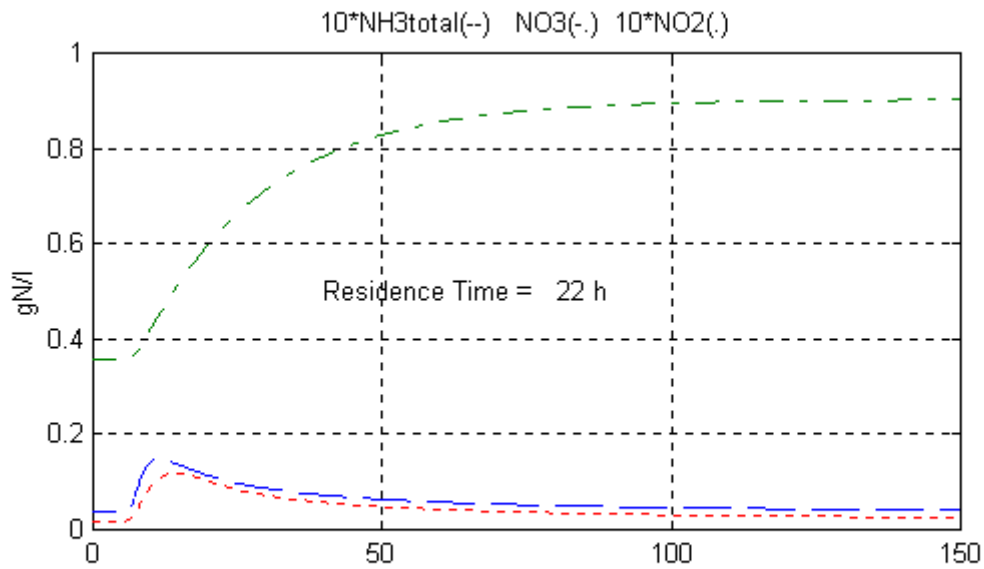
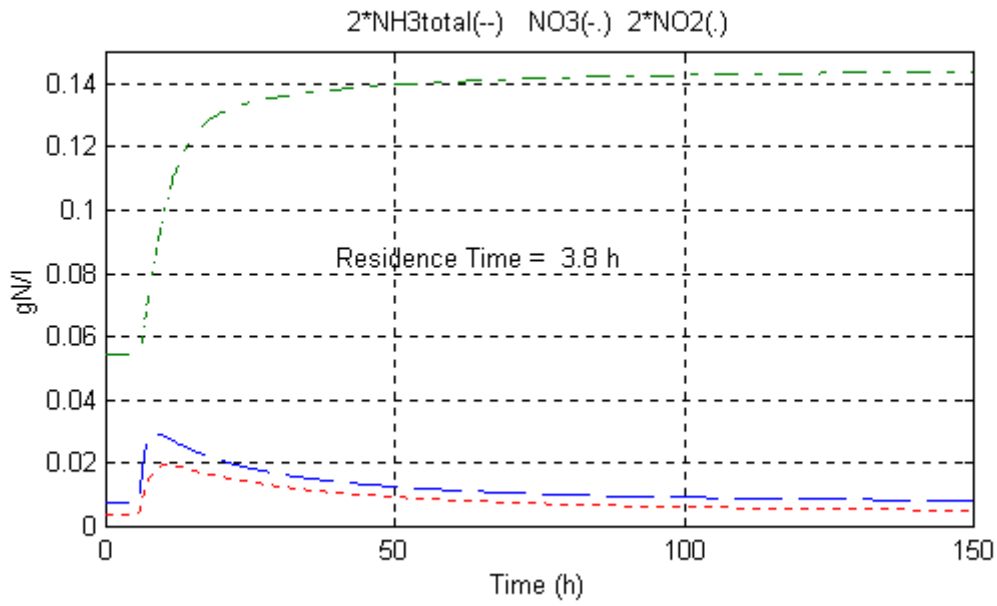


Figure 7 : Simulations at column output at different Residence Times

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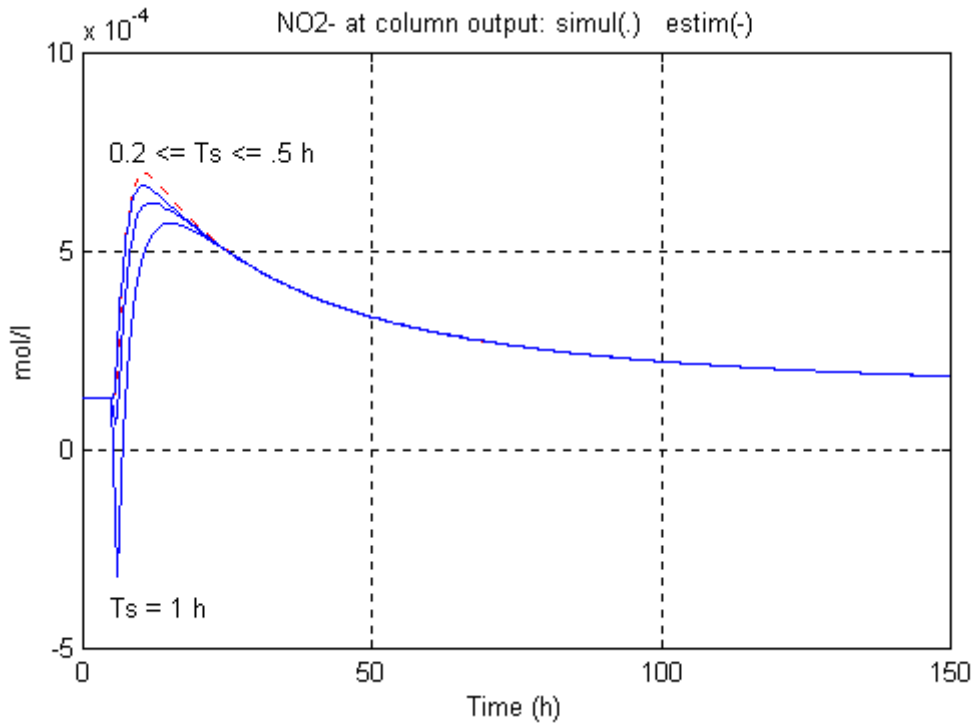


Figure 8 : Impact of the sampling period (T_s) of NH_3 and NO_3 when the residence time is 3.8 hours

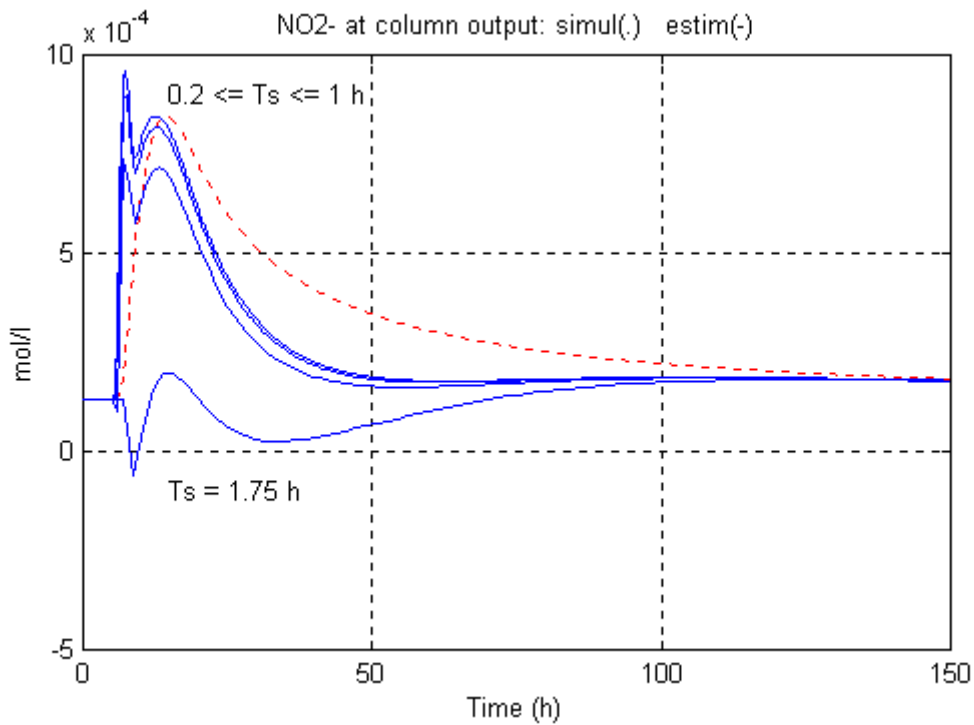


Figure 9 : Impact of the sampling period (T_s) of NH_3 and NO_3 when the residence time is 22 hours

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3.2. Practical conditions of the validation tests

Considering the 2 extreme simulations of figure 7, it can be observed that the duration of a test is independent of the liquid flow rate and is about 100 h. So the time between two successive excitations of the process is expected to be 100 h (4 days).

As already said, the sampling period of ammonia and nitrate has to be 0.5 h.

As the titration of nitrite is not easy, the sampling period T of this variable has to be as long as possible and not constant all along the test : T equal to 1 h during the 12 first hours following the excitation, and T equal to 1 day, beyond. In order to have the value of the nitrite when the excitation is done, a measurement has to be done at that moment.

As the validation of the estimator is considered to be done for the dissolved oxygen disturbances, the only remaining excitations are steps of load of ammonia :

- positive step of liquid flow rate with constant concentration of ammonia.
- positive step of ammonia in the input liquid flow.

The variables to be measured versus the time are :

- concentrations of ammonia and nitrate at the input and output of the column.
- input liquid flow and the re-circulation liquid flow.
- input gas flow and re-circulating gas flow.
- concentration of ammonia in the input gas flow, if any (concentration of ammonia in the output gas flow is negligible).

Except for nitrite, the sampling period of all the measured variables is 0.5 h. Nevertheless if a variable is generally constant (as the ammonia concentration in the input flow) its recording can be simplified to the value itself and the time interval on which it is constant.

4. CONCLUSION

Although the data extracted from the UAB experiment from October 10th 1999 to June 30th 2000 have made possible a first validation of the nitrite estimator when the nitrite concentration is high (during Dissolved Oxygen tests), complementary tests are still necessary when concentration of nitrite is low. This study allowed to define more precisely the operational conditions of the validation tests (see section 3 for details).

These conditions are gathered hereafter.

Sampling periods

In order to estimate correctly the peak of nitrite, the sampling period of ammonia and nitrate is fixed to 0.5 h.

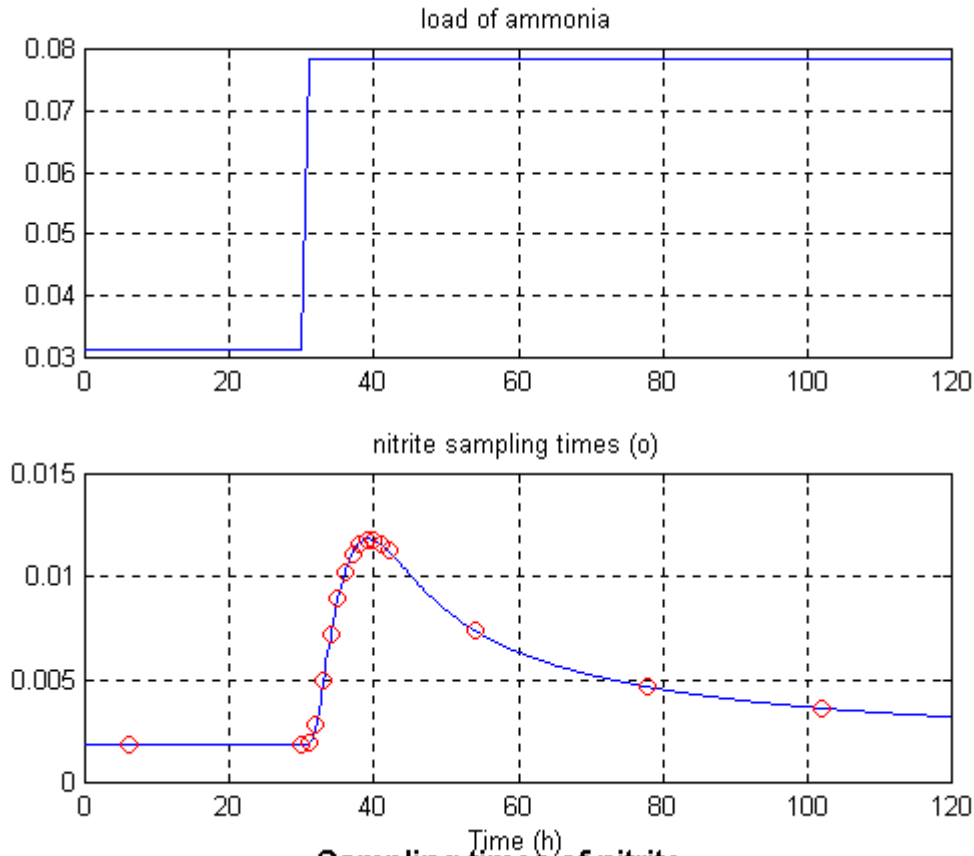
The sampling period of nitrite is fixed to

- 1h during the 12 first hours of the transient following the excitation ;
- 1 day until the end of the test (i.e. until the process recovers its steady state).

Each test is expected to last 4 days.

The figure 10 illustrates the sampling times of nitrite at column output.

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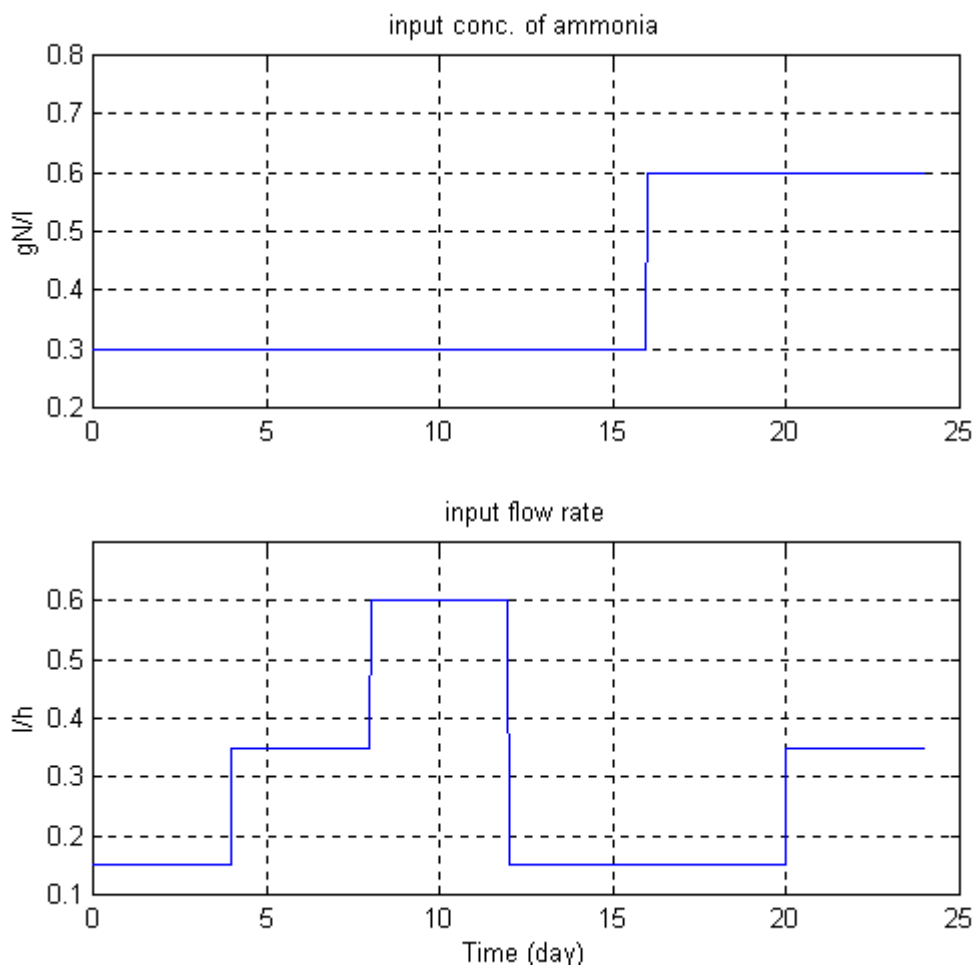
Sampling times of nitrite
Figure 10

Excitation of the process

In order to validate the estimator in the range of low concentrations of nitrite (20– 50 ppm), the steps of ammonia concentration and of flow rate are deduced from the previous experiment (October 1999 – June 2000). The values of the steps amplitude and the moments of their variation are proposed in the figure 11.

The first step, at time $t=4$ days in the figure 11, can be realized as soon as the column is at steady state.

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Protocol for validation of estimator
Figure 11

Data collection

The variables to be measured versus the time are :

- concentrations of ammonia and nitrate at the input and output of the column.
- input liquid flow and the re-circulation liquid flow.
- input gas flow and re-circulating gas flow.
- concentration of ammoniac in the input gas flow, if any (concentration of ammoniac in the output gas flow is negligible).

Because of the different sampling periods, the data have to be saved into 2 groups (2 ASCII files or 2 leaves of an EXCEL file) :

- one group for the variables collected every half an hour.
- one group for the nitrite measurements.

The delay, if any, between the sampling and the results of analysis has to be mentioned.

As soon as a test is terminated, the data will be sent to ADERSA in order to check that the foreseen protocol allows to validate the estimator and to make corrections if necessary.

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5. REFERENCES

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ANNEX

Reconstruction of data from UAB experiment

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A1. Method used for the reconstruction of data

The main feature of the data file 'data_from_tn43_3.xls' is that the measured variables are sampled versus the number of residence time and not versus the time itself. As the nitrite estimation is time variable, the reconstruction of data was necessary before using them for the estimation.

The time has been rebuilt from the data 'to' and 'nto' , saved in the pre-quoted file, with the formula :

$$Ts(ii) = Ts(ii-1) + to(ii)*dnto(ii-1)$$

where :

- $Ts(ii)$: instant of the sampling 'ii'
- $to(ii)$: residence time of the sampling 'ii'
- $dnto(ii) = nto(ii+1) - nto(ii)$
- $nto(ii)$: number of residence time of the sampling 'ii'

The initial instant $Ts(1)$ has been set to 0 on October 10th 1999.

Comparing this so rebuilt time with the calendar time of the experiment, it can be noted that the input flow rate of the column has been set to 0 during about a total number of 20 days on the whole experiment. Particularly, taking into account the evolution of 'to' and 'nto' compared to the calendar time, it can be deduced that the liquid flow rate was set to 0 from 8th to 14th February 2000, from 9th to 15th March 2000, on the 25th and 26th 2000. This information of null flow rate is not given to the estimator because the model cannot take it into account.

The input flow rate has been rebuilt taking into account 'to' and the volume of liquid $V_L=3.76$ l.

Based on the figures of the TN 43.3, the steps of ammonia have been set on the following 'nto' :

- for the step 0.37 → 0.30 gN/l , $nto = 31.84$.
- for the step 0.30 → 0.60 gN/l , $nto = 215.83$.
- for the step 0.60 → 1.10 gN/l , $nto = 445.21$.

The accidents mentioned in the pre-quoted file have been plotted in order to try to explain the behaviour of the estimator, but without success.

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A2. Software for the reconstruction of data

```

%*****
%      Biomass and Nitrite estimators      *
%      Version 3.1      January 2002      *
%
%      Estimator model according to TN 48.1      *
%
%      Off line estimations through real data      *
%      UAB data from October 10th 1999 to June 30th 2000      *
%
%*****
% . time period of the predictor = 0.1 or 1 hour      *
% . data are restored to fit that time period      *
%*****

clear

% Initialisation of the parameters and constants of the estimators
i_est
dte = 1; % sampling period of estimators (h).
        % For model 3, dte=.1 h is necessary for the integrative method
(otherwise, unstable)
clear Fin

itest = 2; % Data from UAB, TN43.3
if itest == 2
    load essai.ext % ASCII file extracted from the file 'data_from_tn43_3.xls'
    titre_test = 'UAB reconstructed data from October 10th 1999 to June 30th 2000';
    [m,n] = size(essai);
    Xbs = zeros(m,2);
    % 1. Reading raw data from the file
    to = essai(:,1);
    nto = essai(:,2);
    dnto = diff(nton);
    Xbs(:,1) = essai(:,3)/14/(1+Kdis_h); % [NH3] (mol/l of molecular form) at end of
the column (for estimator 1 and 3)
    Xbs(:,2) = essai(:,5)/14; % [NO3] (mol/l) at end of the column (for estimator 1
and 3)
    Xis = essai(:,4)/14; % [NO2] (mol/l) measured at end of the column
    Fins = VL./to; % Liquid input flow rate
    % 2. Computation of absolute time 'Ts'. According to UAB experiment,
    % absolute time is runing when liquid flow rate is not null, only.
    Ts = zeros(m,1); % Absolute time (different from calendar time)
    Ts(1) = to(1) * nto(1);
    for ii = 2:m
        Ts(ii) = Ts(ii-1) + to(ii)*dnto(ii-1); % presumed algorithm used by UAB in TN
43.3
    end
    % 3. Reconstruction of [NH3] at input of the column, by investigation of TN 43.3
and 'xls' file
    dL_hs = zeros(m,1); % [NH3] (mol/l) at input of the column
    nto1 = 31.84; % number of residence times when step 0.37 --> 0.30 gN/l is assumed
to have been done
    nto2 =215.83; % number of residence times when step 0.30 --> 0.60 gN/l is assumed
to have been done
    nto3 =445.21; % number of residence times when step 0.60 --> 1.10 gN/l is assumed
to have been done
    ind = find(nton<nton1);
    dL_hs(ind) = .37*ones(size(ind)); % [NH4+] (g/l) at input of the column
    ind = find(nton>=nton1 & nton<nton2);
    dL_hs(ind) = .30*ones(size(ind)); % [NH4+] (g/l) at input of the column
    ind = find(nton>=nton2 & nton<nton3);
    dL_hs(ind) = .60*ones(size(ind)); % [NH4+] (g/l) at input of the column
    ind = find(nton>=nton3);
    dL_hs(ind) = 1.1*ones(size(ind)); % [NH4+] (g/l) at input of the column

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dL_hs = dL_hs/14/(1+Kdis_h); % [NH3] (mol/l of molecular form) at input of the
column
% 4. Reconstruction of Dissolved Oxygen in the column, by investigation of TN 43.3
and 'xls' file
DOs = zeros(m,1); % [DO] (%) in the column
nto1 = 521.61; % number of residence times when step DO 80 --> 40 % is done
nto2 = 532.78; % number of residence times when step DO 40 --> 20 % is done
nto3 = 563.90; % number of residence times when step DO 20 --> 40 % is done
nto4 = 575.77; % number of residence times when step DO 40 --> 80 % is done
ind = find(nto<nto1);
DOs(ind) = 80*ones(size(ind)); % [DO] (%)
ind = find(nto>=nto1 & nto<nto2);
DOs(ind) = 40*ones(size(ind)); % [DO] (%)
ind = find(nto>=nto2 & nto<nto3);
DOs(ind) = 20*ones(size(ind)); % [DO] (%)
ind = find(nto>=nto3 & nto<nto4);
DOs(ind) = 40*ones(size(ind)); % [DO] (%)
ind = find(nto>=nto4);
DOs(ind) = 80*ones(size(ind)); % [DO] (%)
% 5. Approximate time of accidents (in number of residence time)
ntoa = [455, 500.15, 516.00, 527.52, 556.72, 575.77];
Tsa = zeros(size(ntoa));
for jj = 1:max(size(ntoa))
    Tsa(1,jj) = Ts(find(nto==ntoa(jj)));
end
end

% Interpolated data for the estimators (constant sampling period)
Te = [min(Ts):dte:max(Ts)]; % constant discrete time of the estimators
Fin = interp1(Ts,Fins,Te); % Liquid input flow rate (l/h)
dL_h = interp1(Ts,dL_hs,Te); % [NH3] of the Liquid input flow
Xb = interp1(Ts,Xbs,Te); % NH3 and NO3 at end of the column (for estimator 1 and
3)
dL_a = zeros(size(dL_h)); % [NO3] of the Liquid input flow
dL_i = zeros(size(dL_h)); % [NO2] of the Liquid input flow
DO = interp1(Ts,DOs,Te); % DO in the column
%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)

% Choice of an interval for running the estimator
i_choice = 0;
if i_choice == 0, titre_test = 'UAB experiment from October 10th 1999 to June 30th
2000';
    Tel = min(Te); Te2 = max(Te);
elseif i_choice == 1, titre_test='Part of the experiment where temperature = 303
K';
    Tel = min(Te); Te2 = Ts(find(nto==400.22)); % from starting until April 10th 2000
elseif i_choice == 2, titre_test='Part of the experiment where Temp = 301 K';
    Tel = Ts(find(nto==438.87)); Te2 = max(Te); % from April 18th 2000 until the
end
elseif i_choice == 3, titre_test='Variation of the Dissolved Oxygen';
    Tel = Ts(find(nto==500.15)); Te2 = max(Te); % from May 23rd 2000 until the end
elseif i_choice == 4, titre_test='First increasing steps of input flow rate';
    Tel = min(Te); Te2 = Ts(find(nto==229.22)); % from starting until February 15th
1999
elseif i_choice == 5, titre_test = 'Variations of temperature';
    Tel = Ts(find(nto==337.00)); Te2 = Ts(find(nto==445.21)); % From March 28th to
April 19th 2000
elseif i_choice == 6, titre_test = 'Unusable for nitrite estimation';
    Tel = 3950; Te2 = 4600;
end
ind = find(Te >= Tel & Te <= Te2);
Te = Te(ind);
Fin = Fin(ind);
dL_h = dL_h(ind);
Xb = Xb(ind,:);
dL_a = dL_a(ind);
dL_i = dL_i(ind);

```

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DO = DO(ind);
ind = find(Ts >= Te1 & Ts <= Te2);
Ts = Ts(ind);
nto = nto(ind);
to = to(ind);
Xis = Xis(ind);
DOs = DOs(ind);
ind = find(Tsa >= Te1 & Tsa <= Te2);
Tsa = Tsa(ind);

if 0 % plotting the raw data
    dL_hs = dL_hs(ind);
    Xbs = Xbs(ind,:);
    Fins = Fins(ind);
    pou = 1;
    t_essai % plotting the raw data
    disp('Open a new figure and strike a key')
    pause
    pou = 2;
    t_essai % plotting the raw data
    disp('Open a new figure and strike a key')
    pause
end

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

% Plot
itrachbio = 1; % 1 --> biomass concentrations; 0 --> intermediate values of [NO2]
if i_choice == 0,
    pou = 3; % plot of the nitrite concentrations (process and estimation)
    pou = 6; % plot of the nitrite concentrations (process and estimation)
elseif i_choice == 3, titre_test='Variation of the Dissolved Oxygen';
else
    pou = 6; % plot of the nitrite concentrations (process and estimation)
end
t_est
nomfic = ['est1_',num2str(itest)];
eval(['save ',nomfic,' Te Xi Xi2 Cx itest titre_test'])
message = 'Open a new plotting window and strike a key'
pause

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

% Plot
pou = 4; % plot of the nitrite concentrations (process and estimation)
itrachbio = 1; % 1 --> biomass concentrations; 0 --> intermediate values of [NO2]
t_est
nomfic = ['est3_',num2str(itest)];
eval(['save ',nomfic,' Te Xi Xi2 Cx VL1 VL2 itest titre_test'])

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