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MELISSA

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Review of nitrite estimators

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0	0	August 2004	Draft
1	0	November 2004	Original version
2	0	November 2004	. Modification of Introduction and Conclusion . Addition of Annex 5

TABLE OF CONTENTS

Abbreviations or notations:
NH_3 : ammonia (gaseous or solvated) or ammonium ion
NO_2 : nitrite ion
NO_3 : nitrate ion
SO4 : sulphate ion
PO4 : phosphate ion
N_s : Nitrosomonas strain
N_b : Nitrobacter strain
CST: Completely Stirred Tank

1. INTRODUCTION

The nitrite is a poison for man and plants. Moreover a NO2 sensor is very expensive. So the idea is to replace the measurement by an estimator.
In the previous TN 77.1, an estimator based only on the Nitrogen element balance has been built and tested. Unfortunately, due to the necessity of very high accuracy on the measurement of the other Nitrogen compounds NH3 and NO3, this estimator is unable to work properly for the very low NO2 concentrations produced by the UAB Nitrifying column.
So two another methods of estimation have been studied: the first one based on a Kalman filter and the second one on the non linear optimisation.

For these 2 methods, it is necessary to dispose a model describing the main phenomena of the pilot plant. So the first step of the study is the checking of the existing First Principles model behaviour compared to the data obtained on the UAB pilot plant.
A sensitivity study has showed how sensitive are the model outputs to the chemical parameters. An attempt of modifying these parameters has been done in order to adjust the model. The checking has been done on behalf of existing data: two campaigns of tests on the pilot plant (one at the beginning of 2000 and one from March to May 2003).

Unfortunately the study has shown that the NO2 is not observable by means of the measurements of NH3 and NO3 at the column output.

New actions are proposed in conclusion.

Reminder of the present column model state
The present model is built from the LGCB TN's 27.1, 27.2 and 27.3, excepted that the biofilm described in TN27.3 is not modelled (the biomass is assumed to be homogenously dispersed in the liquid of each CST of the fixed bed). The inhibitory effects of NO2 and NO3 on the Nitrobacter growth is modelled like in TN 27.3 .
The KLa is computed according to TN 63.2 p.30 by LGCB.
The parameters values are set in TN 27.3 appendix A. These values are declared 'nominal' values from which the variations are done by multiplying them by a given factor.

2. CHECKING NOMINAL MODEL AGAINST UAB TESTS

2.1. Main features of the checking

The objective is to check the LGCB model against the tests done on the UAB pilot plant in 2000 (from October 1999 to June 2000, exactly) and 2003 (from March to May).
The LGCB model studied here is described in TN's 27.1 to 27.3, except that the biofilm is not modelled. Particularly the inhibition effect of NO2 and NO3 is taken into account. The Kla value is constant and computed at the starting of a simulation by the formula of TN 63.2 p.7.

Firstly the LGCB model has been checked against the tests of 2000.
Different values of N_B (number of CST used for the modelling of the fixed bed B) are tested in order to choose the optimal one that makes the model fit the process as far as possible.

The corresponding simulations are plotted in annex 1. It appears that N_B=7 is the optimal value for the test of 2000 (figure 2.1).

Secondly the LGCB model with N_B=7 is checked against the UAB tests of 2003. The model behaviour and the pilot plant behaviour are completely different (Annex 2).
A LGCB model with N_B=1 will fit the test in a better way (Annex 3).
In an attempt to make this last model with NB=1 to fit better the process, a sensitive study was done so that to propose a modification of the chemical parameters. Unfortunately the study showed that there is no interest to modify these parameters (Annex 4).

So a unique model cannot describe the pilot plant behaviour recorded on both 2000 and 2003 tests.

Then it has been decided to validate the method of the 'NO2 estimator' on an arbitrary model of the column: the LGCB model is retained with a number of tanks in the fixed bed B N_B equals 7.

This study follows in the next section 3 with 2 methods: one based on a Kalman filter and one on the non linear optimisation.

2.2. Checking the model against the tests done at UAB in 2000

In the concerned tests, the pilot plant is excited by steps of ammonia concentration and by steps of flow rate (2 first graphs at the top of the figure 2.1). The blue circles are the concentrations of NH3, NO3 and NO2 (graphs 3 to 5), measured at column output. These 3 variables are assumed characteristic of the process behaviour (the other variables are not measured). The green dotted lines represent the same characteristic variables of the model fed with the same inputs as the process.
The model is declared validated if the characteristic variables of the model are identical to those of the process.

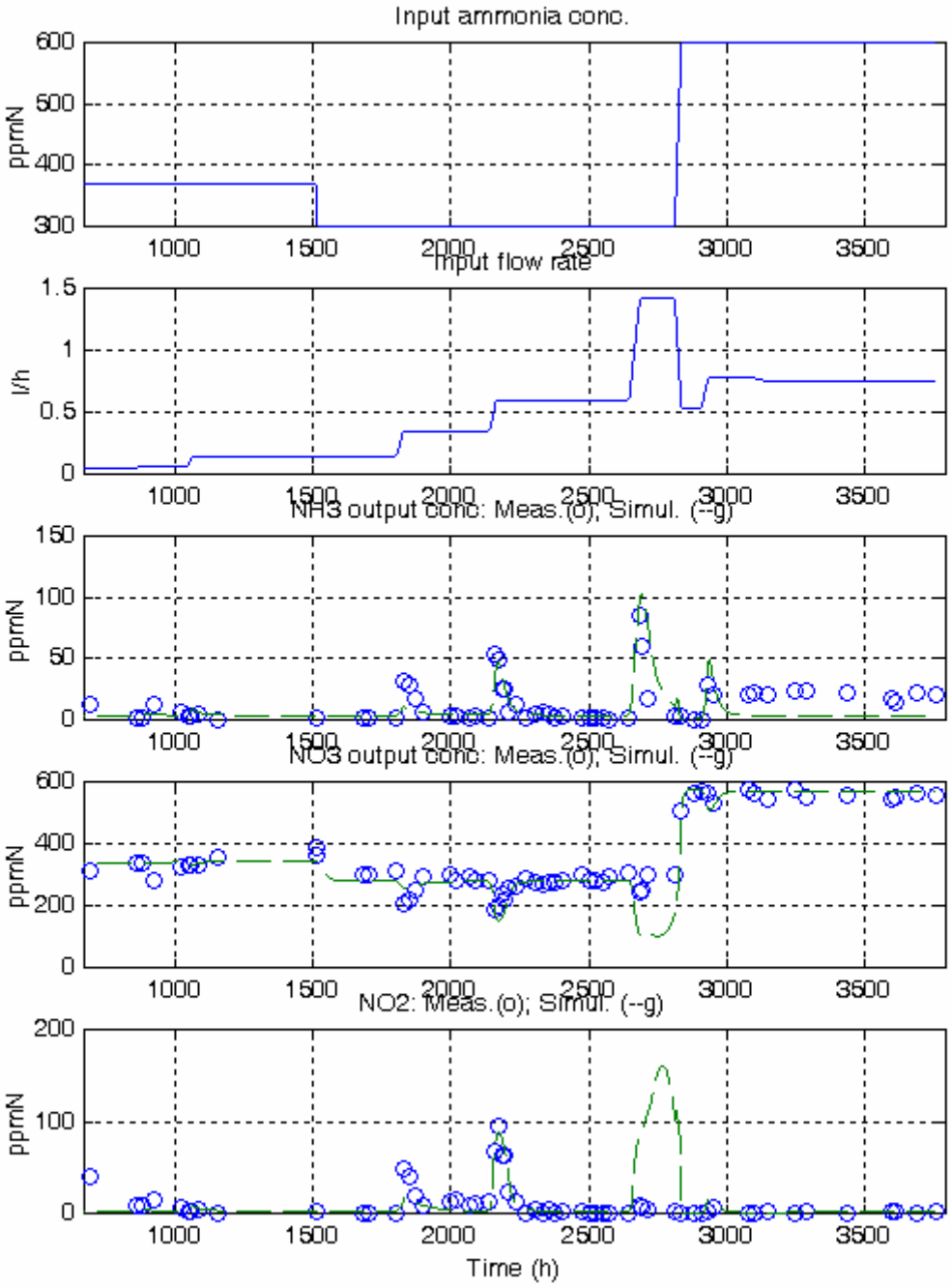


Figure 2.1: Test UAB 2000. Model and process behaviour.
Model: NB=7; KLa=175 h^{-1} .

Comparison of each process/model characteristic (graphs 3, 4 and 5 of figure 2.1 for NH3, NO3 and NO2 respectively) at each excitation of the process:

Positive flow rate step at about t=900h:

First it should be recalled that at this moment of the test, the column is restarting with new Ns and Nb strains of biomass. When the excitation occurs, the biomass concentrations are low. On the pilot plant it can be seen stronger peaks on NH3, NO3 and NO2 than the model predicts: the column is more sensitive to the load increasing as if the biomass growth kinetic were overestimated compared to the operating conditions.

Positive flow rate step at about t=1050h:

In the meantime, the biomasses have grown and seem to be more able to face a load increasing: the model is in good agreement with the process for the 3 characteristics (NH3, NO3 and NO2).

Negative input ammonia step at about t=1500 h:

Both process and model are in good agreement: no NH3 and NO2 peaks and a decreasing of NO3.

Positive flow rate step at about t=1700h:

On the pilot plant it can be seen stronger peaks on NH3, NO3 and NO2 than the model predicts. The difference of process/model behaviours is very similar to what has been observed in the first excitation at t=900 h: the column is more sensitive to the load increasing as if the biomass growth kinetic were overestimated.

Positive flow rate step at about t=2150h:

The model is in adequacy to the process perfectly: the 3 peaks on NH3, NO3 and NO2 have same amplitude and dynamic.

Positive flow rate step at about t=2650h:

To understand how the model works here, it is necessary to look at the evolution of O2 and biomasses along the fixed bed in the figure 2.2. The main graphs of this figure are the graph 2 (O2 L: O2 concentration in liquid of each of the 7 tanks B1 to B7 of the fixed bed B), graph 4 (O2 flux between Gas and Liquid phases), graphs 5 and 6 (active biomasses Ns and Nb).

When the flow rate step occurs, Ns increases in B1 and B2 (graph 5). Its increasing in B2 implies the O2 flux increasing that, unfortunately, comes to its maximum (graph 4). Due to competition between Ns and Nb, the increasing of Ns in B2 occurs at the expense of Nb that decreases consequently (green curve of graph 6). As the NO2 increases in B3 (because it is no more consumed in B2), Nb increases in B3. But it does at too small rate because of too low concentration there at that moment. The same phenomenon occurs in series in the following tanks B3 to B7 and, globally, the whole Nb of these tanks is unable to consume NO2 quickly enough. Then NO2 arrives in excess at column output, which gives the big peak that can be seen in graph 5 of figure 2.1. Consequently there is a lack of NO3 (graph 4 of fig 2.1).

So the NH3 peak is predicted very well. And the NO2 model appears here as very sensitive to O2 saturation and Nb repartition along the fixed bed: a little bigger Nb in B3 at load step would have changed the prediction of the model completely.

Simultaneous negative flow rate and positive concentration steps at about t=2800h:

The model predicts the process behaviour very well.

Positive flow rate step at about t=2900h:

The model predicts the process behaviour well: The amplitudes and dynamics are correct for NO3 and NO2 but NO2 does not come to its normal steady state point. Beyond t=3000 h till the end of the test, the NH3 process is higher than the model. As process and model are in

agreement for NO3 and NO2 on the same period of time (graphs 4 and 5 of fig2.1) and as the mass balance should apply, the process values are probably incorrect (NH3 is probably overestimated; may be a constituent is detected as ammonia by the sensor wrongly).

Conclusion of the test:
On this long duration test (nearly four months), the model predicts the pilot plant behaviour very well for NH3.
For NO2 and consequently for NO3, in particular operating condition the model becomes very highly non linear and this behaviour is not observed on the pilot plant (case of the ammonia step at t=2650h on the test).
May this non linearity be smoothed?

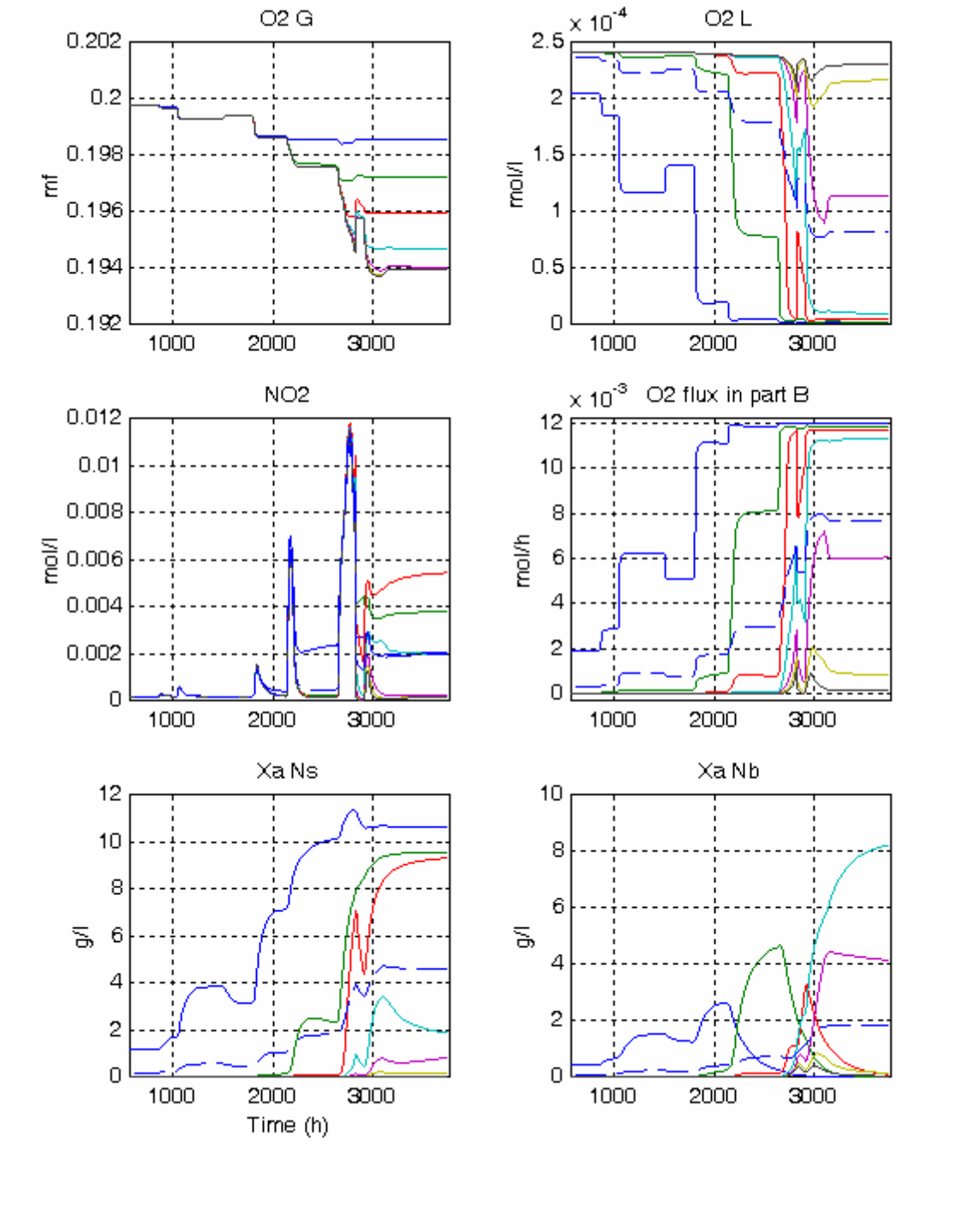


Figure 2.2: Test UAB 2000. Model behaviour in the CST B1 to B7 of the part B. Model: NB=7; KLa=175 h^{-1} .
B1: blue curve. B2: green curve. B3: red curve. B4: cyan curve. B5: magenta curve. Mean value on the whole fixed bed: dotted line.

2.3. Checking the model against the tests done at UAB in 2003

Four tests were done from March to May 2003 on the UAB pilot plant.
The LGCB model with NB=7 has been checked against these tests: the model has been fed with the same inputs as the pilot plant and the model outputs are compared to the process outputs.
It can be seen in the figures of Annex 2 (from A2.1 to A2.4) that the model behaviour and the pilot plant behaviour are completely different. The model with NB=7 cannot be validated on these tests.
Particularly in the case of the test on May 2003 '300-600 ppmN NH3 step', the NO3 at column output is decreasing instead of increasing. This can be explained by the evolution of biomasses Ns and Nb in the CST's B1 to B7 (fig A2.4 and A2.5).

2.4. Conclusion of the checking

A unique model cannot describe the pilot plant behaviour recorded on both 2000 and 2003 tests campaigns.

3. DIFFERENT PROCEDURES OF NO2 ESTIMATION

Two methods have been tested of the estimation of NO2 at column output.

3.1. Method (Working hypothesis)

Given a process, the method consists in testing the procedure through a robustness study.

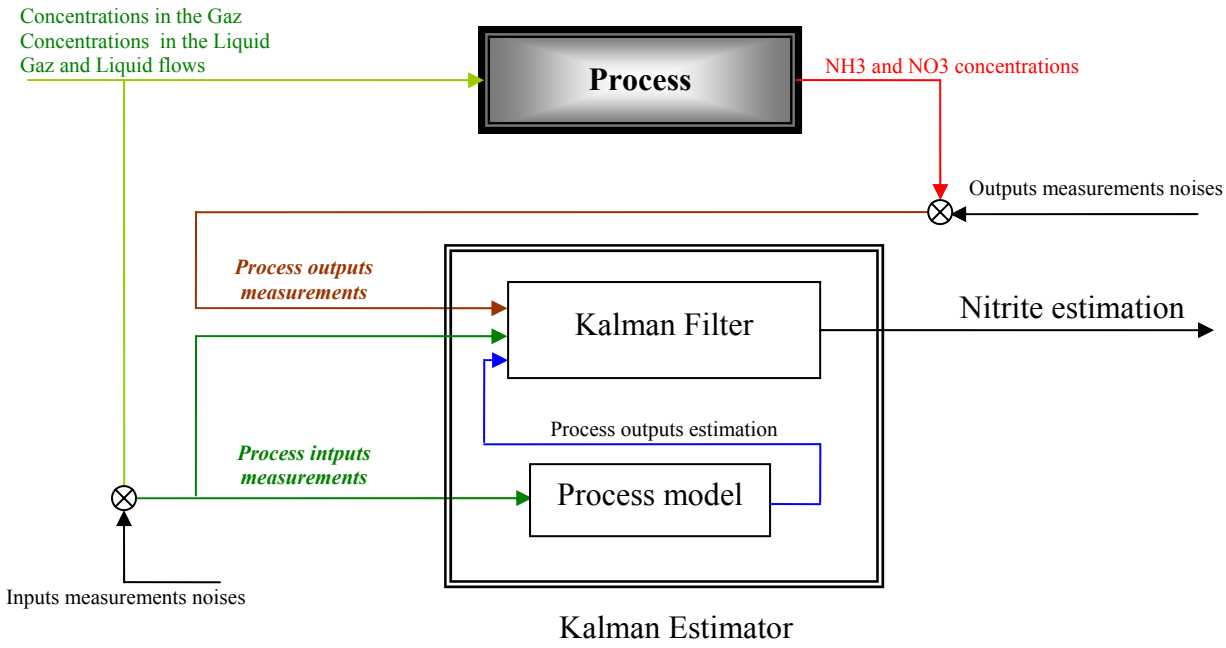
3.2. Procedure 1: Kalman filter

3.2.1. Approach

In TN77.1, NH3 and NO3 measurements are directly used as inputs for the nitrite estimator. The problem of this method is that the weight of measurements noise impacts directly the estimator precision.

The new proposed methodology consists in using a Kalman filter, which calibration is based on the noise characteristics (variances of the signals), to balance the weight of measurements at the input of the nitrite estimator.

The principle is illustrated by the following graph:



The Kalman filter balances the weight of the process outputs measurements and estimations for the calculation of nitrite concentration.

3.2.2. Preliminary study steps

To study the feasibility of this approach, we have tested in simulation the above scheme. The following different steps have been achieved :

1. Use of LGCB CIII model (with 44 states and 56 outputs) as the process.
2. Programming and linearization of a reduced model (with 9 states and 9 outputs) to use it as the process model.
3. Generation of the Kalman estimator based on the process reduced and linearized model.

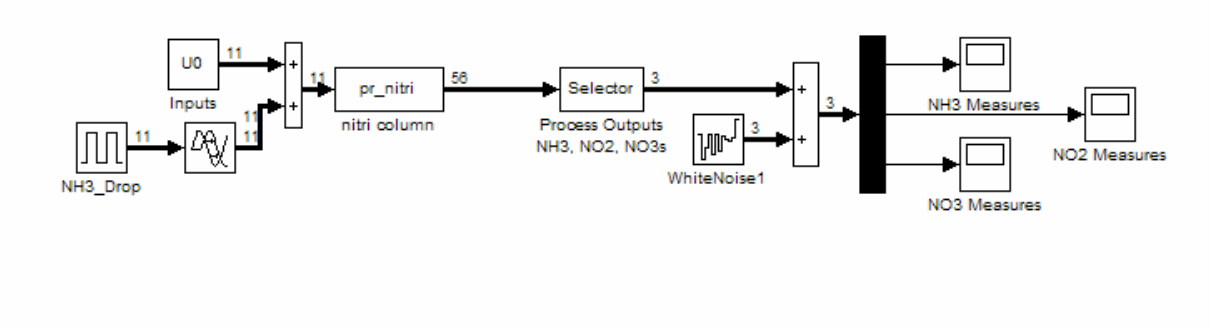
3.2.3. LGCB model

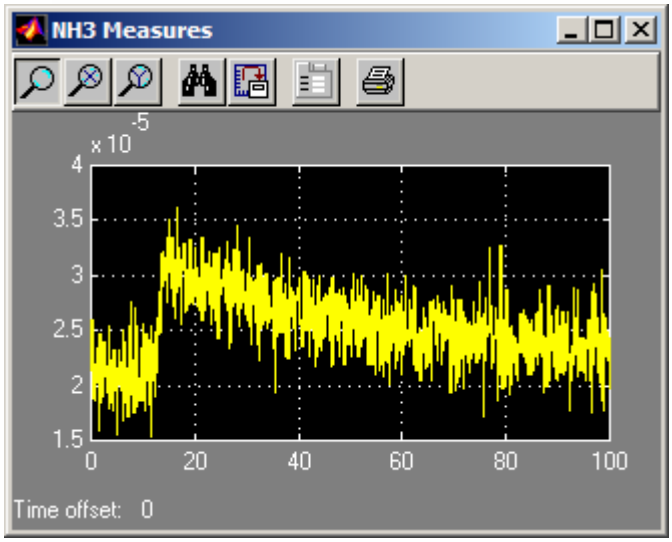
The LGCB model is considered in this study as the process.

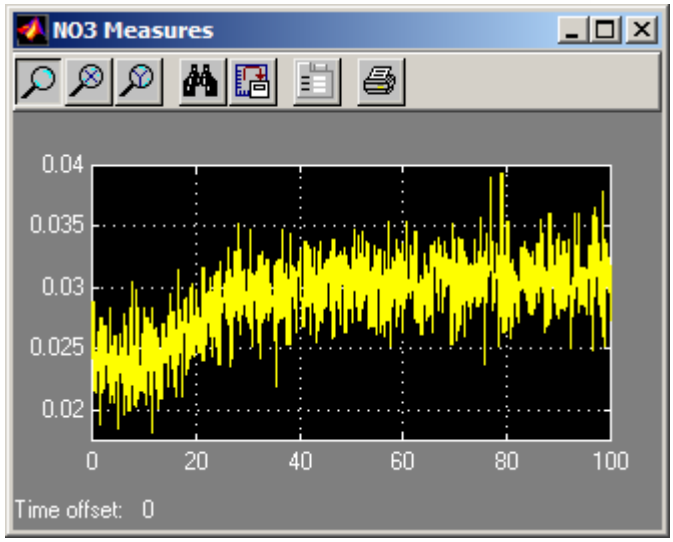
The three selected outputs, interesting for the study, are NH3, NO3 and NO2.

Noise on the NH3 and NO3 outputs of the model is added in order to characterize correctly a real process measurement. NO2 is not measured today.

The following example presents the obtained (simulated) measures on NH3 and NO3:







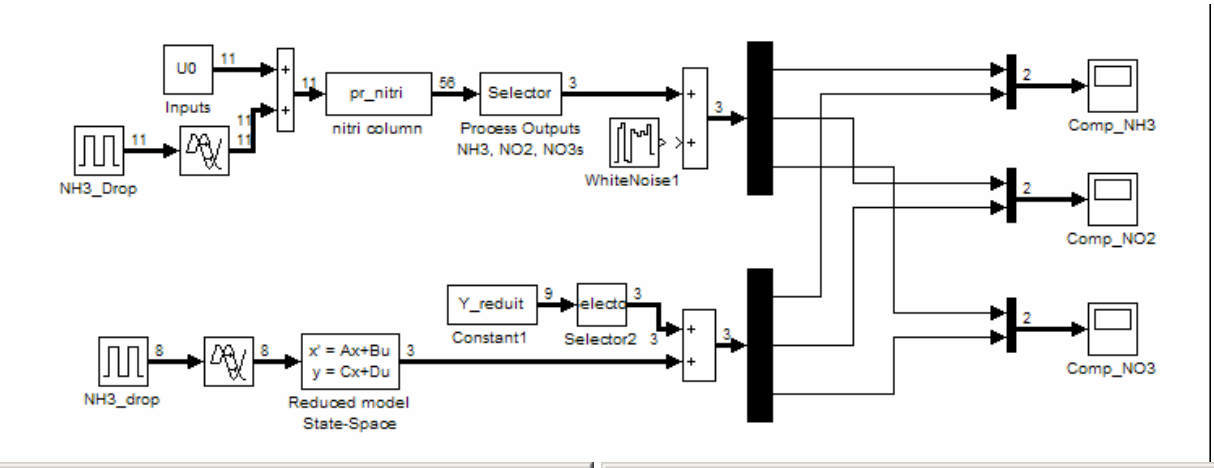
3.2.4. Reduced model and linearization

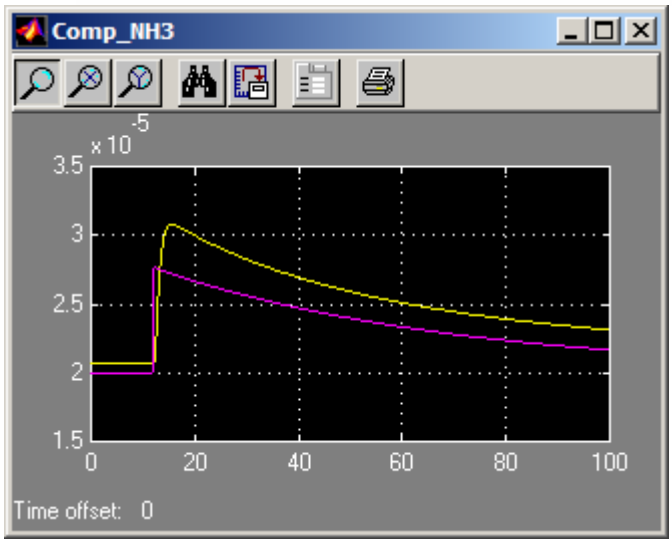
The aim of the reduced model is to be used to produce the Kalman estimator. Indeed, the LGCB model is not reversible because of dependant states.

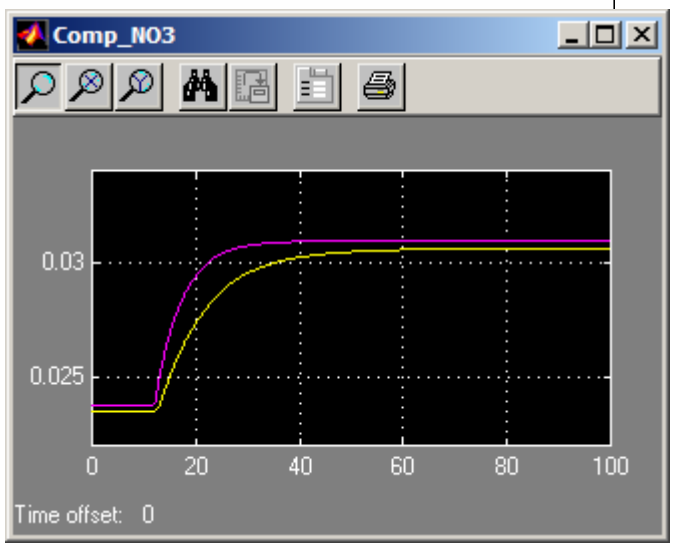
The linearization of the model permits to write it as a state space linear model and to generate the Kalman estimator.

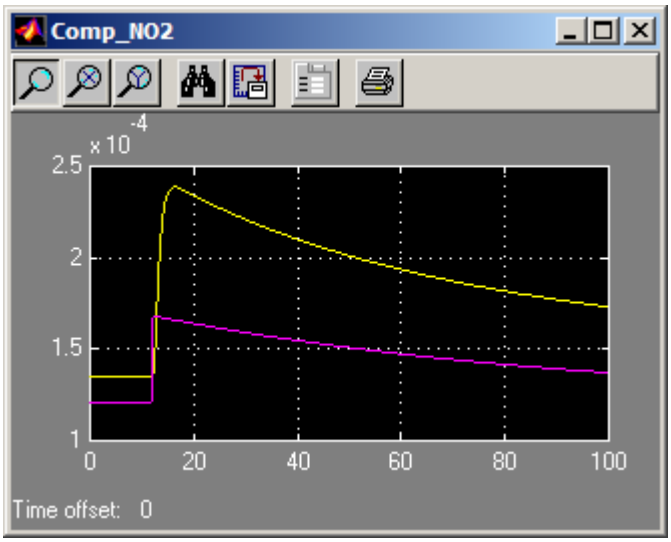
The non-correlation between the LGCB model and the reduced model is an issue for this study because it represents the future variance between the process measurements and the estimator. This difference is used to test the Kalman estimator.

The following example presents the results of the linearized model in parallel of the LGCB model:









We can observe the differences between the NH3, N02 and NO3 measures (yellow, without noise for the visibility) and estimations (pink).

The main aim of the Kalman filter is now to re-use the NH3 and NO3 noised measures to make a correction on the NO2 calculation and to move it closer to the NO2 measure.

3.2.5. Generation of the Kalman estimator

Based on the reduced state space model, the Kalman estimator uses in input the process measurements.

The Matlab Kalman function is described as follows :

[KEST,L,P] = KALMAN(SYS,QN,RN,NN) designs a Kalman estimator KEST for the continuous- or discrete-time plant with state-space model SYS. For a continuous-time model,

$x = Ax + Bu + Gw$ {State equation}
$y = Cx + Du + Hw + v$ {Measurements}

with known inputs u, process noise w, measurement noise v, and noise covariances

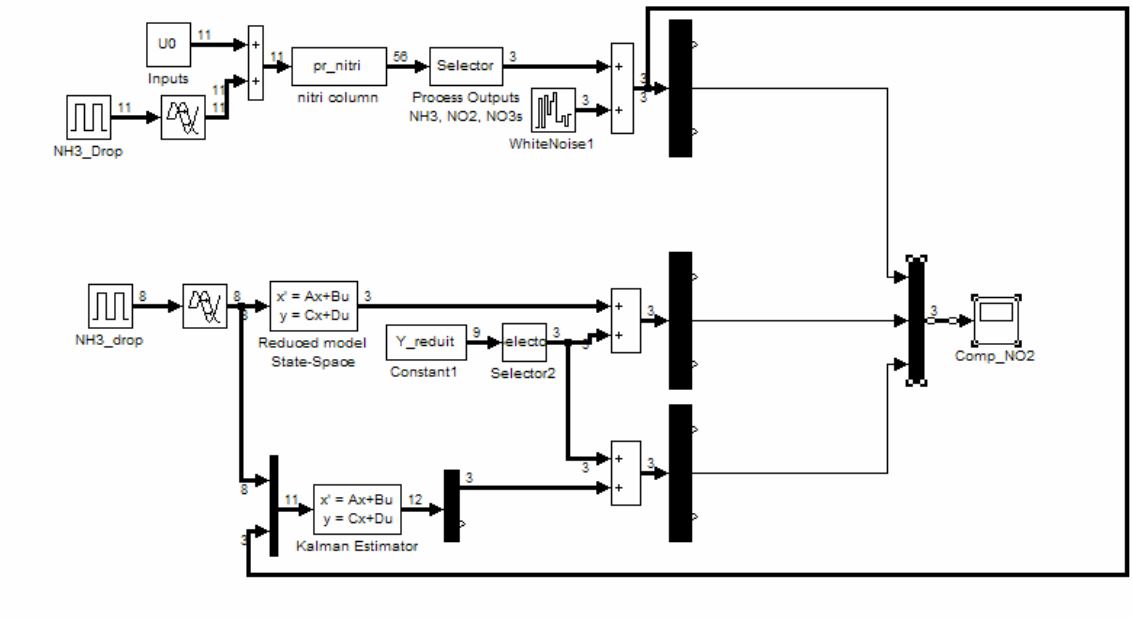
$E\{ww'\} = QN, \quad E\{vv'\} = RN, \quad E\{wv'\} = NN,$

the estimator KEST has input [u;y] and generates the optimal estimates y_e,x_e of y,x by:

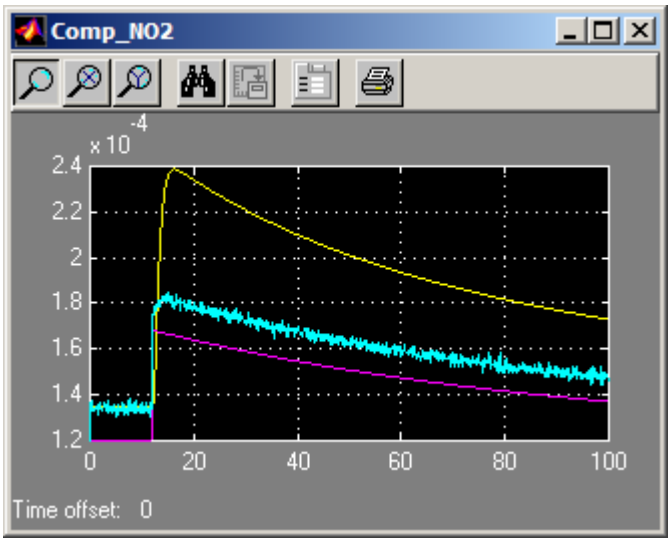
$x\_e = Ax\_e + Bu + L(y - Cx\_e - Du)$

$$\begin{vmatrix} y\_e \\ x\_e \end{vmatrix} = \begin{vmatrix} C \\ I \end{vmatrix} x\_e + \begin{vmatrix} D \\ 0 \end{vmatrix} u$$

Simulink program:



The Kalman estimation gives the following results :



We can see that, with a pre-parameterized Kalman filter (no optimisation study has been done at this step), the estimator (blue curve) gives a better result than the reduced model (pink curve).

3.2.6. Conclusion

The methodology of estimation of NO2 from a Kalman filter has been established and validated on a reduced model with a state vector of small dimension (the column is reduced to a only one tank for the fixed bed B, without parts A and C). Unfortunately, when the whole column is considered (parts A and C, and the fixed bed B composed of 7 CST's), the dimension of the state becomes huge (the state is composed of 99 components). Then, in that case, the Kalman filter is inefficient to compensate the state vector from only 2 measurements (NH3 and NO3 at column output).

3.3. Procedure 2: Non Linear Optimisation

3.3.1. Principle of the method

The process and the model are simulated under Simulink (figure 3.1) with different set of parameters (one set for the process; another one for the model). The inputs (designed 'dG' for the gas concentrations, 'dL' for the liquid concentrations, 'Fint' for the liquid flow rate and 'Gint' for the gas flow rate, on the figure 3.1) are identical for the process and the model.

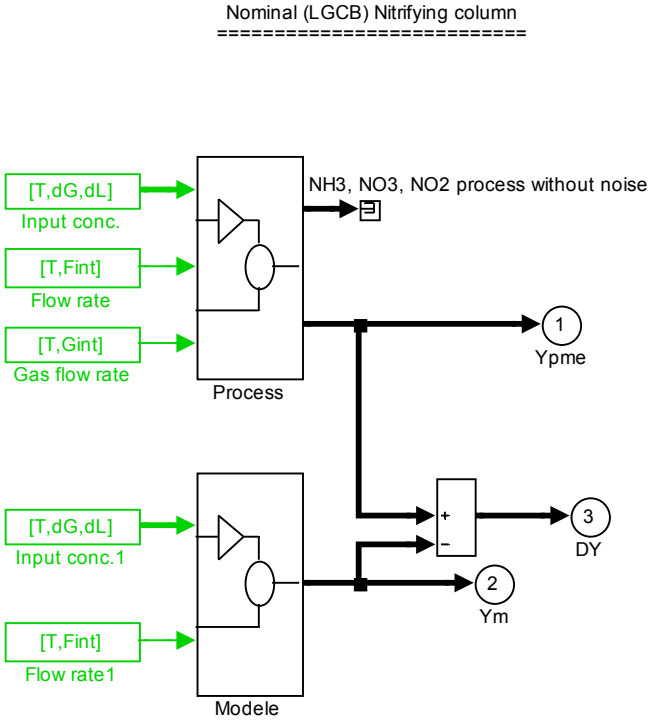


Figure 3.1

For each output NH3 and NO3, a criterion is computed. Here, for each output, the criterion is the distance between the process output (named 'Ypme' on the figure 3.1) and the model (named 'Ym' on the figure 3.1) output. The difference between these 2 signals is designed 'DY'.

The method consists in:

- Moving the parameters of the model so that the model output 'Ym' converges towards the process output 'Ypme'. This gives a 'recalibrated' model.
- Estimating the NO2 output by means of this 'recalibrated' model fed with the same inputs as the process. It is foreseen that the estimated NO2 is identical to the process NO2.

The algorithm is iterative. The optimisation work stops when the maximum iteration number is reached or when the distance criterion is lower than a given value, fixed by the operator.

3.3.2. Example of simulation

The optimisation is done offline (and not online): the algorithm moves the model parameters at each end of temporal simulation (10 hours) of a process (and a model) excited by a NH3 concentration step.
The figure 3.2 shows the differences of the process and model outputs at the starting of the iterative procedure. The differences are due to parameters mismatches.

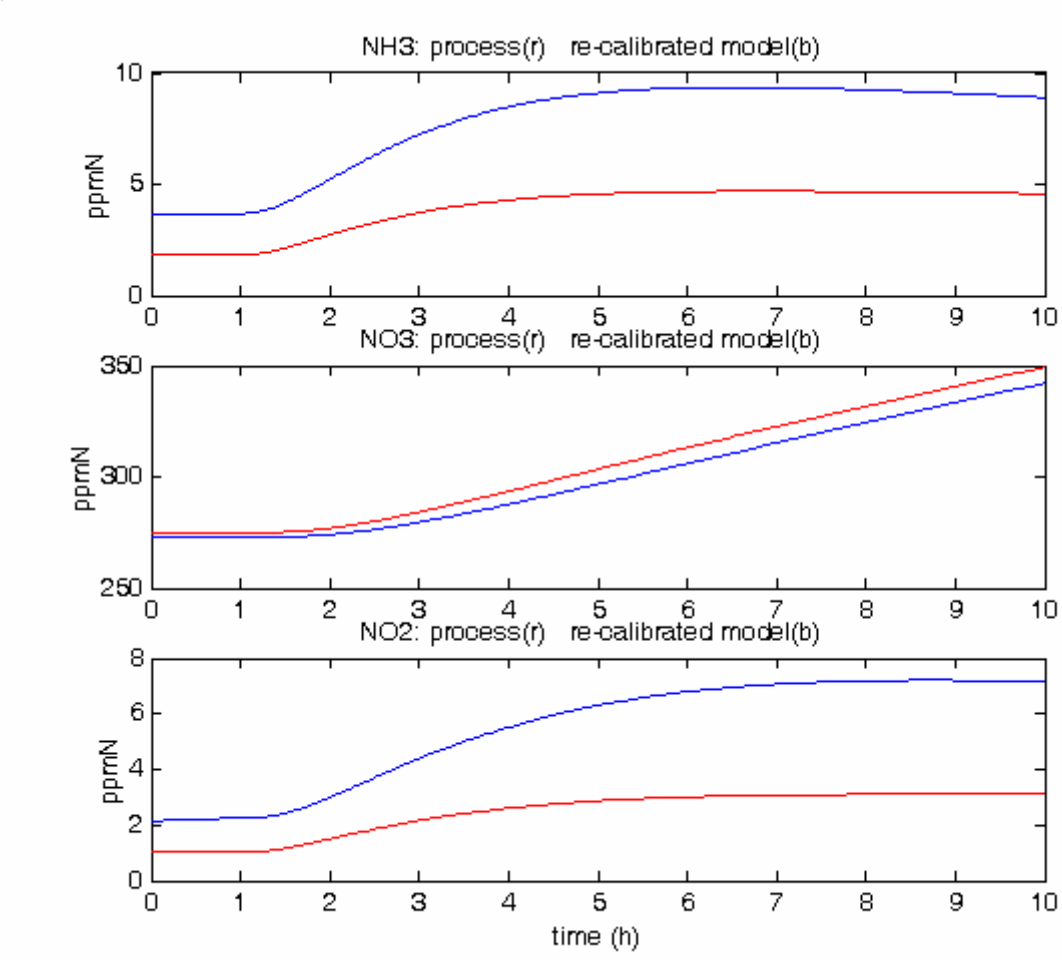


Figure 3.2: Starting of the offline optimisation simulation
The measured process ouputs are the NH3 and NO3 red curves; the model outputs are the NH3 and NO3 blue curves of the top graphs.
The process NO2 is the red curve; the estimated (or model) NO2 is the blue curve of the bottom graph.

The figure 3.3 shows the evolution of the optimisation simulation after 30 iterations. The model outputs NH3 and NO3 (blue curves of the top graphs) have converged towards the corresponding measured process outputs (red curves). BUT the NO2 estimation (blue curve of the bottom graph) has not converged towards the NO2 process output (red curve).

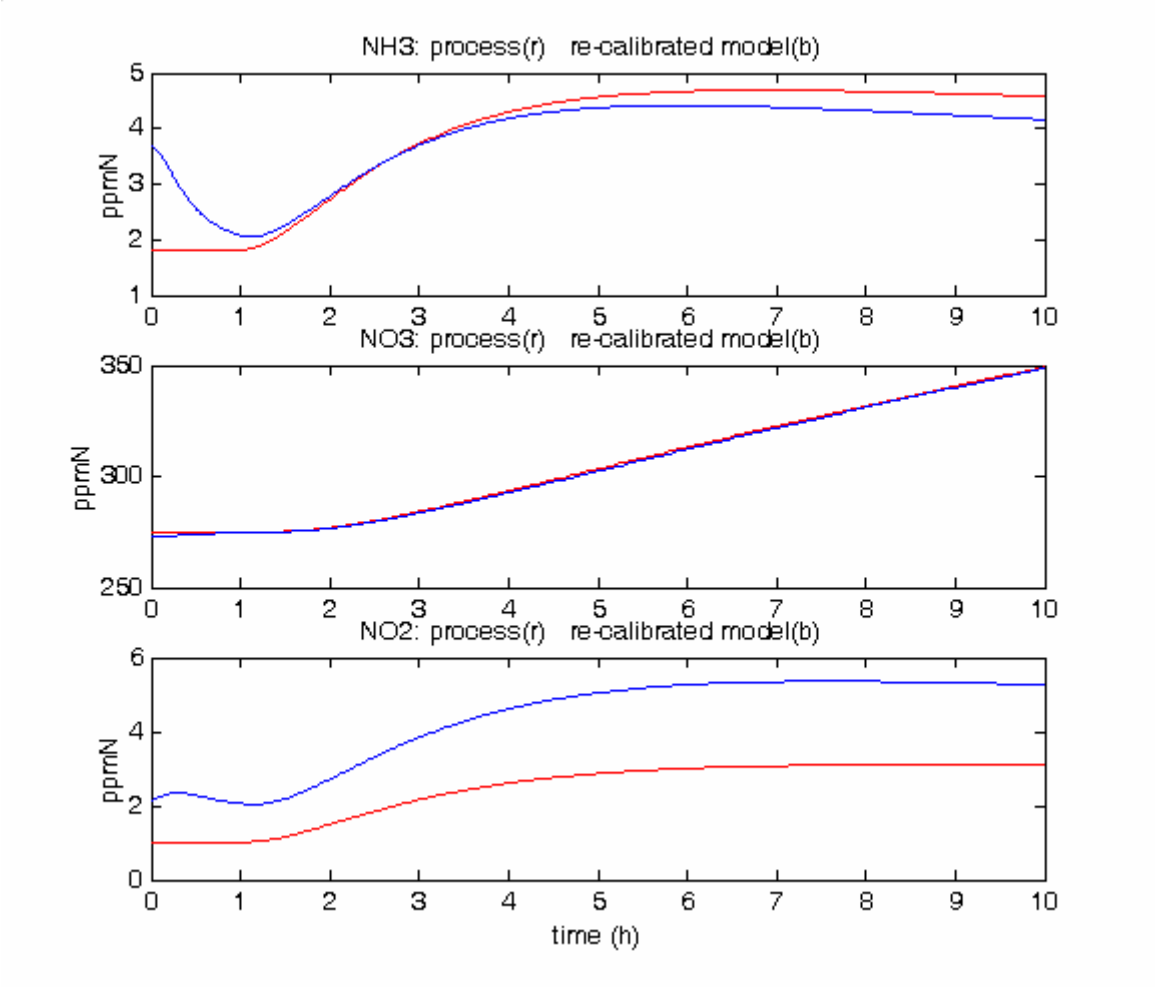


Figure 3.3: End of the offline optimisation simulation

3.3.3. Discussion

The parameters that have a big impact on NH3 or NO3 have a small impact on NO2. Then as the recalibrated parameters have a low impact on NO2 (only the parameter connected to NO2 has a big impact on NO2 and no impact on NH3 or NO3), it can be deduced that NO2 is nearly not observable by means of NH3 and NO3 measurements.

4. CONCLUSION

4.1. Analysis of the model and of the tests on 2000 and 2003

- Globally, the UAB tests realized in 2000 and those realized in 2003 are not consistent: the functioning point (in other words, the steady state) of NO2 is about 2 ppmN in 2000 and about 0.05 ppmN in 2003, for the same column inputs. During a test campaign, the NO2 functioning point is reproducible, but from a campaign to the another one it is not reproducible.

Proposed further work 1: the causes of these differences observed between 2000 and 2003 have to be explained.

- The nominal LGCB model is able to explain the NO2 behaviour of the tests on 2000. But it is unable to explain the one of the tests on 2003, particularly the very low level observed on 2003. The sensitivity study (annex 4) showed that the model is unable to explain the steady state and the peak height at the same time: it is impossible to move the chemical parameters (half saturation constants, specific growth rates and maintenance coefficients) in such a way that the NO2 steady state decreases while the peak height increases. Nevertheless the low level of NO2 of the tests on 2003 (particularly the 0.15-0.25 l/h flow rate step on March) could be reached by the model on condition that 3 parameters (liquid volume ratio and half saturation constants for Ns and Nb growth) were strongly modified (annex 5).

Proposed further work 2: one must check if the validity domain of the LGCB First Principle model may be extended to the low level of NO2 with the required accuracy.
If so, an action plan must be decided to obtain a representative model:

- Review of the current model (LGCB);
- Tests on the pilot plant (UAB);
- Validation and calibration of the model (LGCB, SHERPA).

4.2. NO2 control threshold

The toxicity level of NO2 has been specified to the value of 0.1 ppmN at the ESA meeting on 28 January 2004.
→ This required NO2 threshold (whose value is consistent with the tests on 2003) is outside the prediction domain of the current model.

Proposed further work 3: The NO2 toxicity level must be confirmed and the NO2 control setpoint must be specified clearly. Must NO2 be maintained under the toxicity level?

4.3. Analysis of the NO2 estimator

For the study of the NO2 estimation method, the LGCB model (the only one at our disposal) was used despite its lack of prediction for estimation.
Two methods were studied:

- The method with a Kalman filter: the state of the Kalman internal model is moved in function of the measurements. This method works only for a small dimension of the state and with a linear model.
- The method of Non Linear Optimisation that minimizes a distance criterion between the model outputs and the process outputs by moving the model parameters. This method is one of the parametrical non linear identification methods family. It is a generic one and applies to the present problem well. So the relevant model parameters are moved in function of the measurements and the NO2 is estimated from this calibrated model.

The study showed clearly that NO2 is very little observable by means of the NH3 and NO3 measurements applied to the LGCB model, whatever the method (the parameters that have a big impact on NH3 or NO3 have a small impact on NO2). So even if the LGCB model has a good relative prediction, it does not help in estimating NO2 with a good accuracy: this problem is connected to process itself and no mathematical method could compensate this lack of observability of NO2 by means of NH3 and NO3 measurements. The recalibrated parameters have a low impact on NO2 (only the parameter connected to NO2 has a big impact on NO2 and no impact on NH3 or NO3).
In conclusion, if a reviewed model cannot establish an exploitable relation between NH3, NO3 and NO2, the measurement of NO2 will be required.

Proposed further work 4: One of the following ways must be studied:

- Either measurement of NO2;
- Or building of a model (First Principle model or black box model) on the required functioning domain and checking if the estimation accuracy is good enough in open loop or after recalibration by a Sherpa method.

4.4. Control

The control strategy has already been elaborated (TN 73.1). This strategy needs first to have a model validated on the required functioning domain, which is not the case yet but seems possible at the end of the 'proposed further work 2'.

Proposed further work 5: If a First Principle model can be built, the following approach will be made:

- Offline or periodic recalibration of the parameters by a Non Linear Optimisation method or any other algorithm (for example, Ergun relation proposed by Forler for computation of the liquid volume ratio);
- Estimation of NO2 by means of the recalibrated model fed with the inputs of the column (concentrations in the gas and liquid flows, gas and liquid flow rates);
- Control of NO2 by means of the internal model extracted from the First Principle model.

Proposed further work 6: A backup method must be foreseen to compensate for the First Principle method. This backup method consists in:

- Measurement of NO2;
- Control of the NO2 by means of a black box model obtained directly from the column by identification tests.

4.5. What Sherpa Engineering has done

- Analysis and proposal of an action plan;
- Building of generic methods for estimation and control. These methods need a valid model to be applied; up to now they have been tested with a theoretical model.

5. 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

POUGHON L. "Modelling of the Nitrifying compartment of MELISSA". ESTEC contract PRF 151739, October 1996, TN27.3

6. ANNEX 1: CHECKING THE MODEL AGAINST THE UAB TESTS OF 2000

In this annex, different values of NB and KLa of the LGCB model are tested.
As it can be seen, the model behaviour is very sensitive to these 2 parameters. The differences can be appreciated by simply looking at the simulation plotting.
For KLa=175 h^{-1}, the optimum value of NB is 7 as reported in the previous section.

The tested values of NB and KLa are gathered in the following table:

Figure	NB	KLa	Comments
A1.1	1	175	Value of NB unacceptable: the steady states (of NH3, NO3 and NO2) are correct but the amplitude of all the peaks are too small compared to those of the process.
A1.2	4	175	Value of NB unacceptable: only 2 peaks of NH3 are predicted with the right amplitude and dynamic.
A1.3	5	175	Value of NB unacceptable: only 2 peaks of NH3 and 1 peak of NO3 are predicted with the right amplitude and dynamic.
A1.4	6	175	Value of NB possible but not optimum.
A1.5	7	175	Value of NB optimum (for KLa=175 h^{-1}).
A1.6	8	175	Value of NB possible but not optimum.
A1.7	10	175	Value of NB unacceptable: 2 peaks of NO3 and 2 peaks of NO2 are predicted with too high amplitude.
A1.8	7	150	An important NO2 peak (at t=2200 h) has disappeared.
A1.10	7	200	An important NO2 peak (at t=1800 h) has disappeared.
A1.12	1	50	Too much NO2 when the load is greater than 0.15 gN/h .

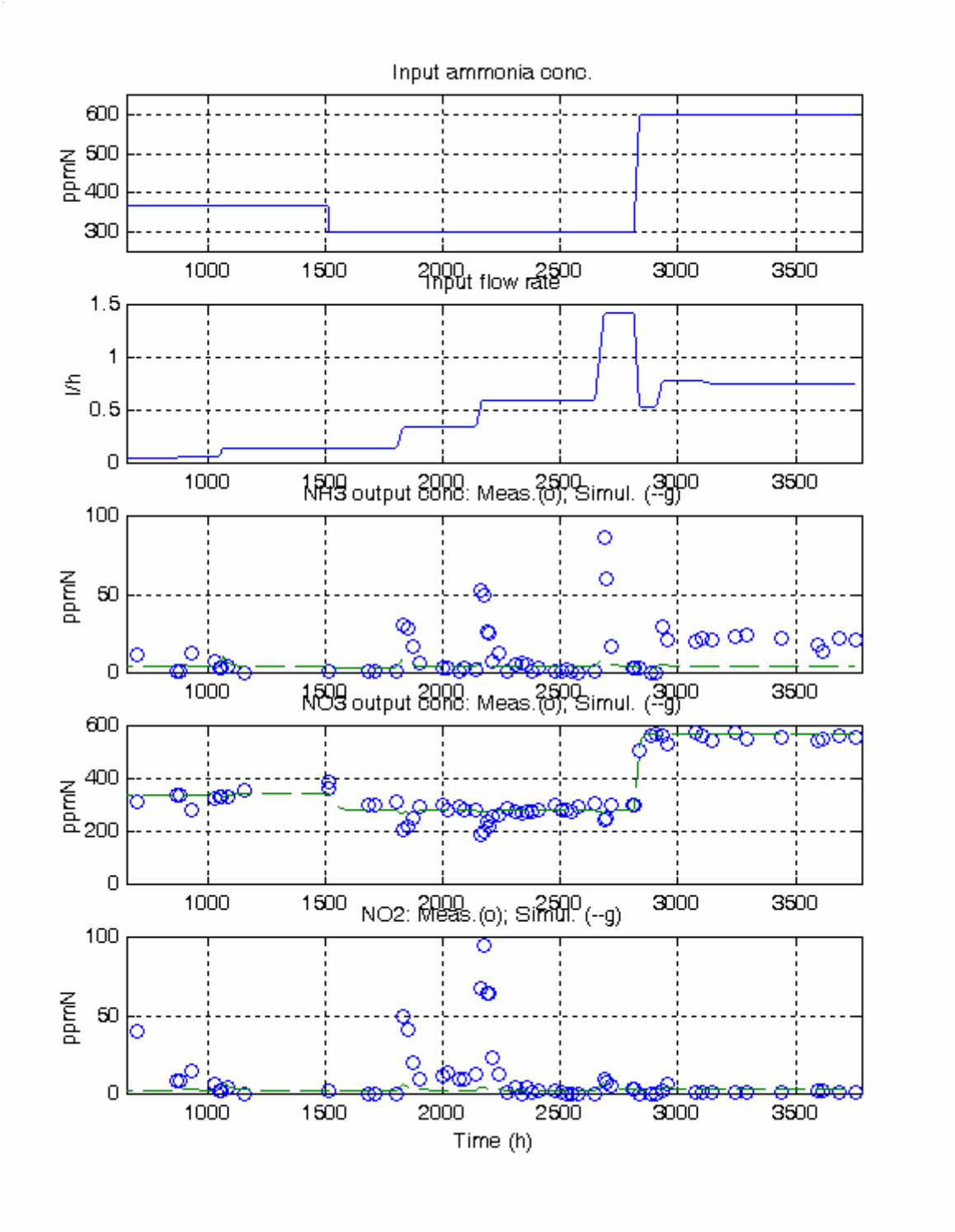


Fig A1.1 : NB=1; KLa=175 h-1 ; Test UAB 2000

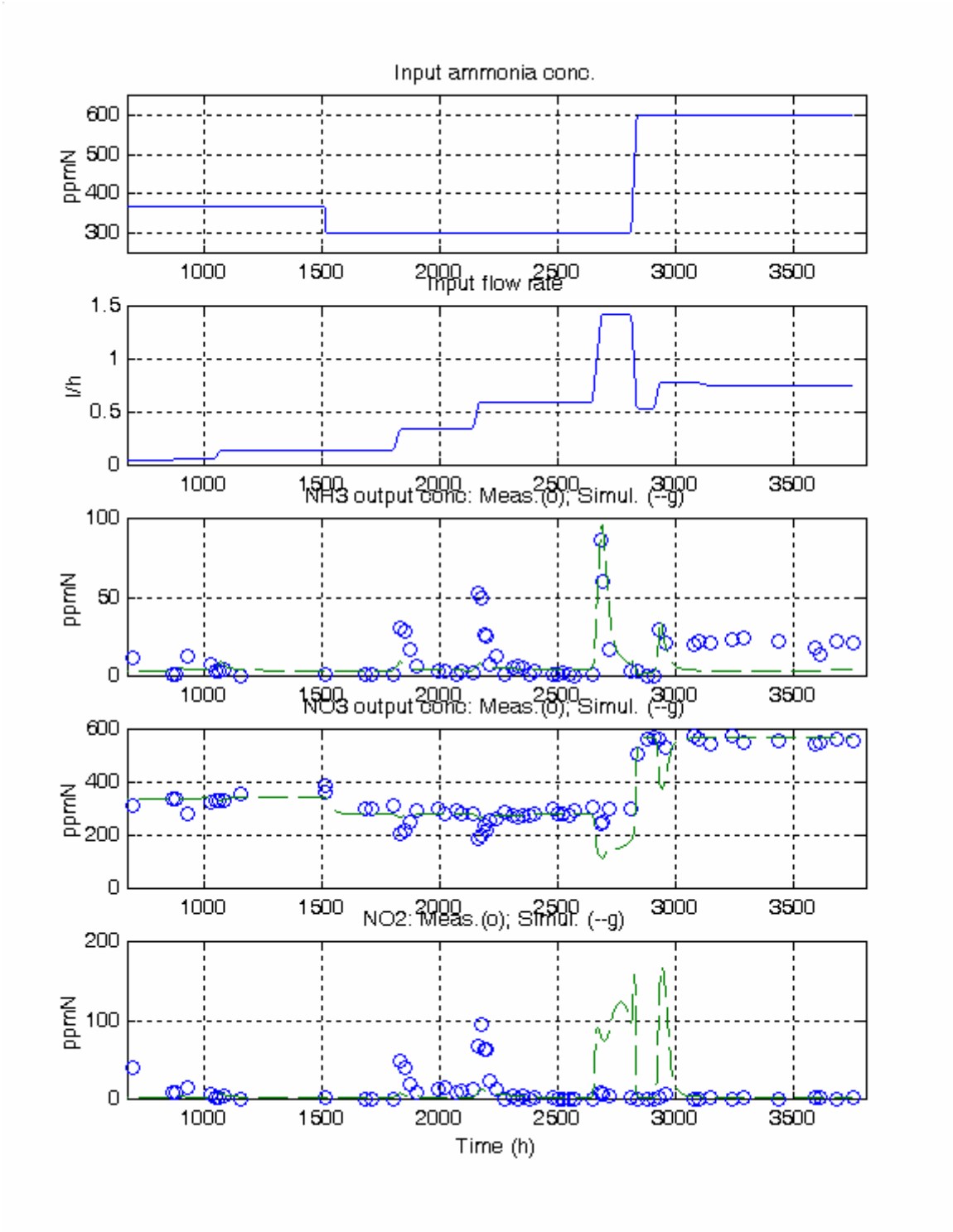


Fig A1.2: NB=4; KLa=175 h-1 ; Test UAB 2000

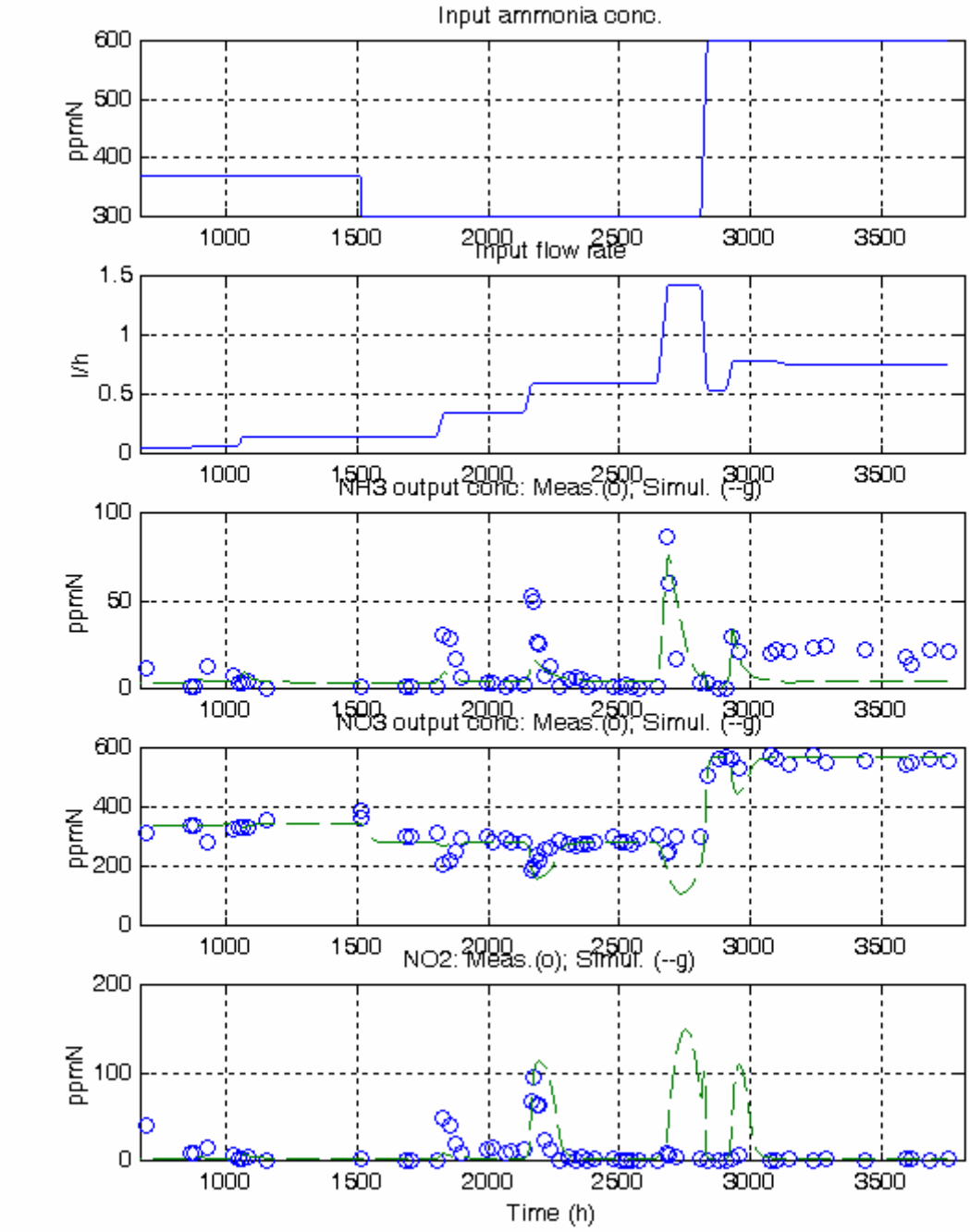

Input ammonia conc.
ppmN
Input flow rate
l/h
NH3 output conc: Meas.(o); Simul. (--g)
ppmN
NO3 output conc: Meas.(o); Simul. (--g)
ppmN
NO2: Meas.(o); Simul. (--g)
ppmN
Time (h)

Fig A1.3: NB=5; KLa=175 h-1 ; Test UAB 2000

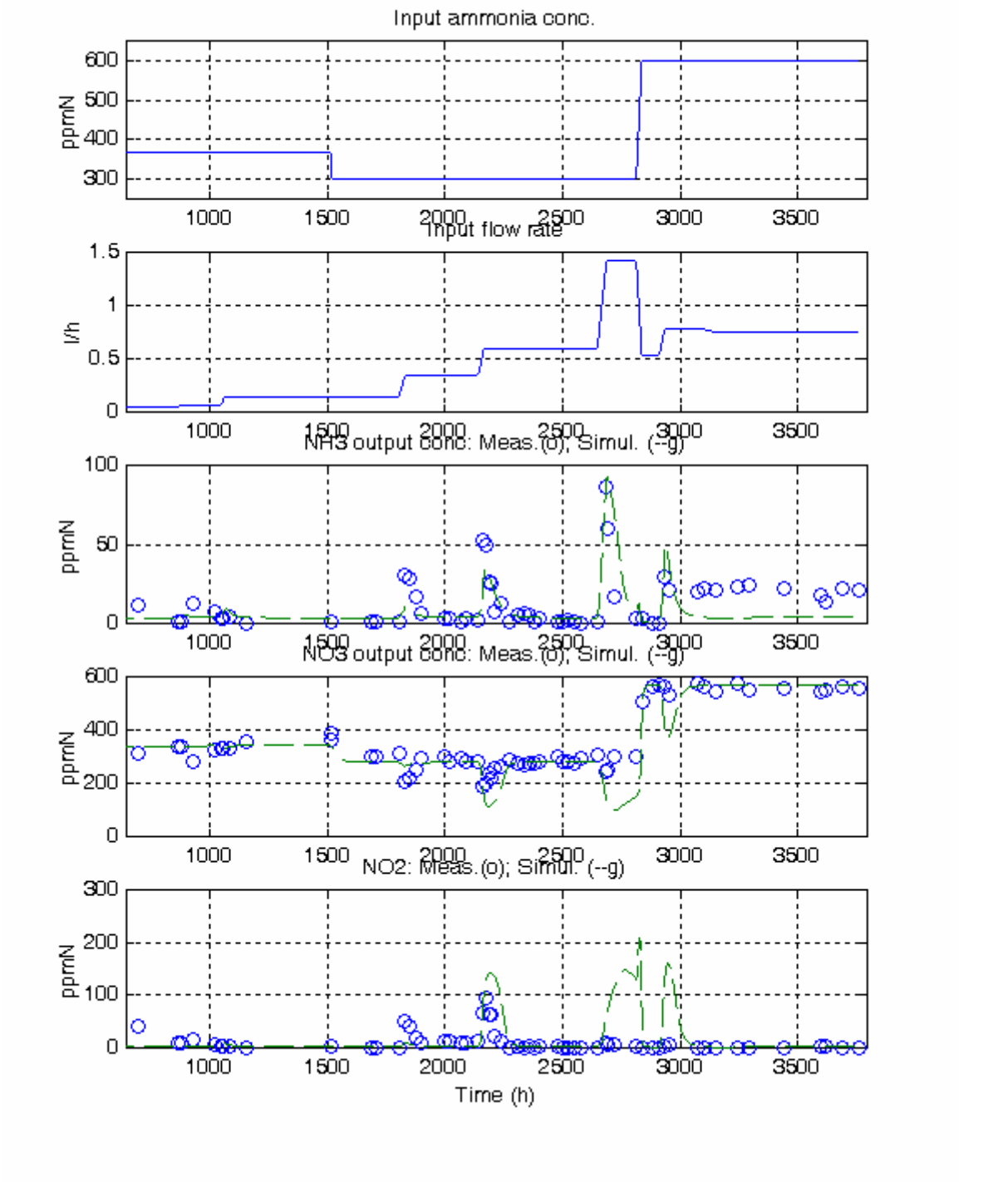


Fig A1.4: NB=6; KLa=175 h-1 ; Test UAB 2000

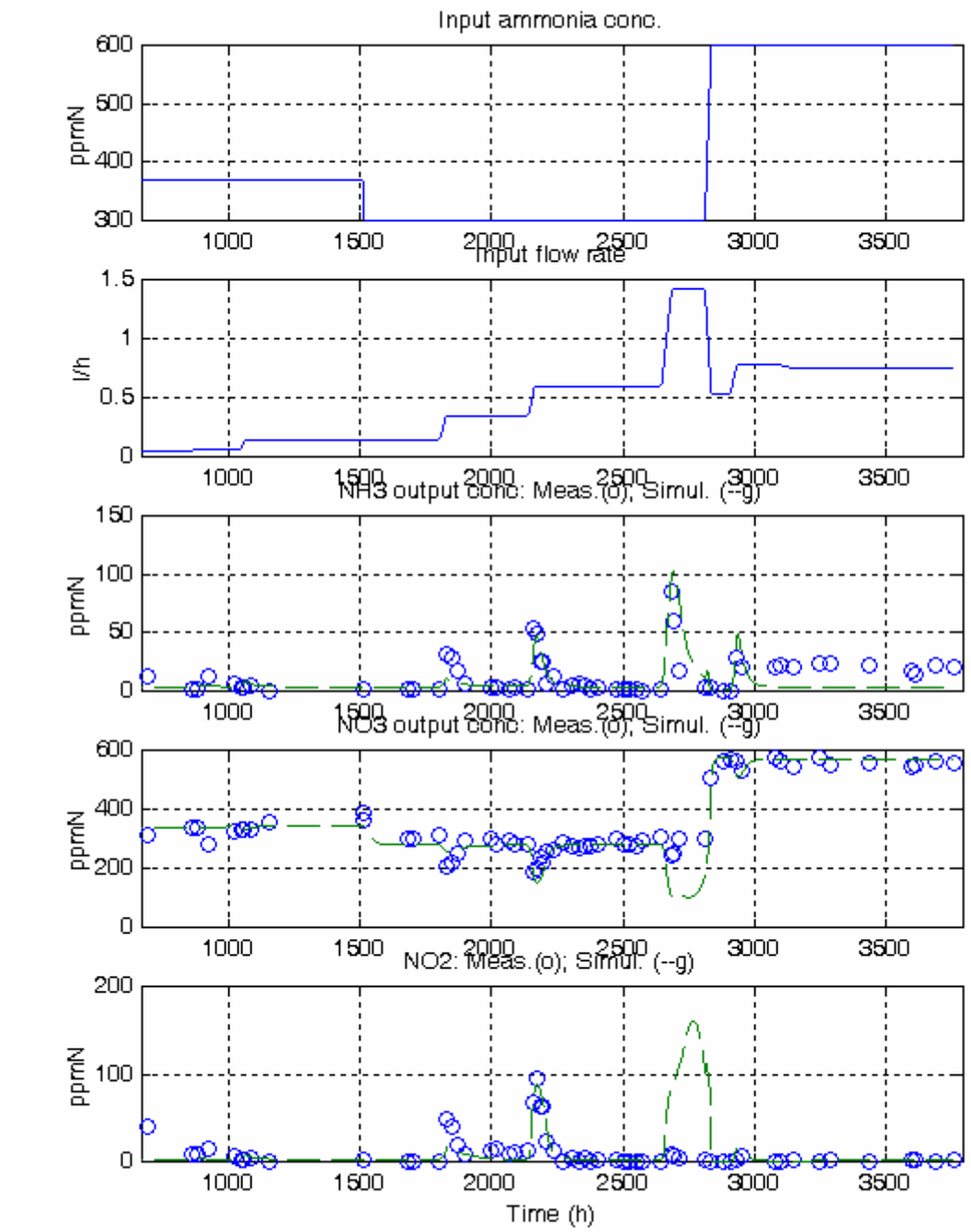


Fig A1.5: NB=7; KLa=175 h-1 ; Test UAB 2000

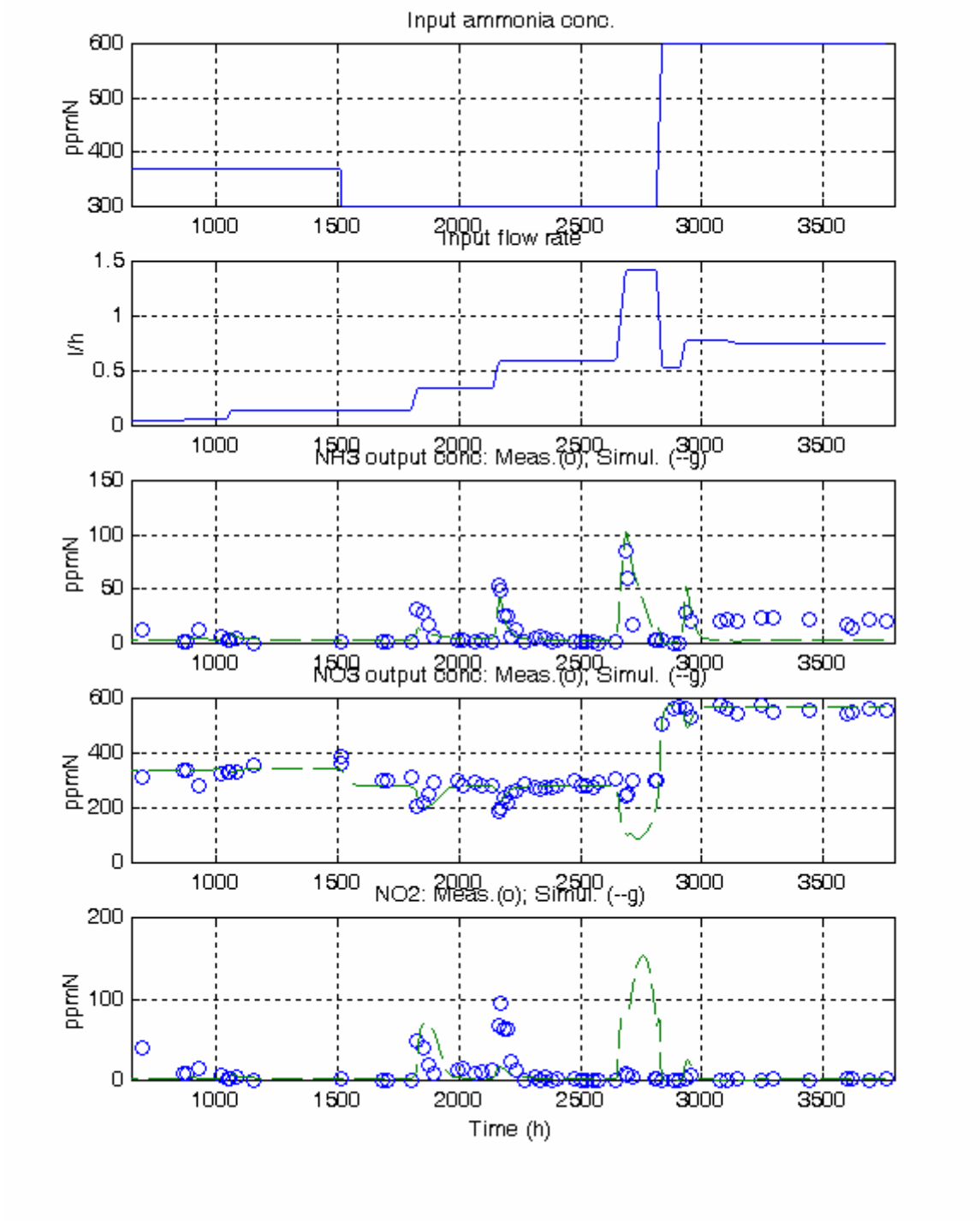


Fig A1.6: NB=8; KLa=175 h-1 ; Test UAB 2000

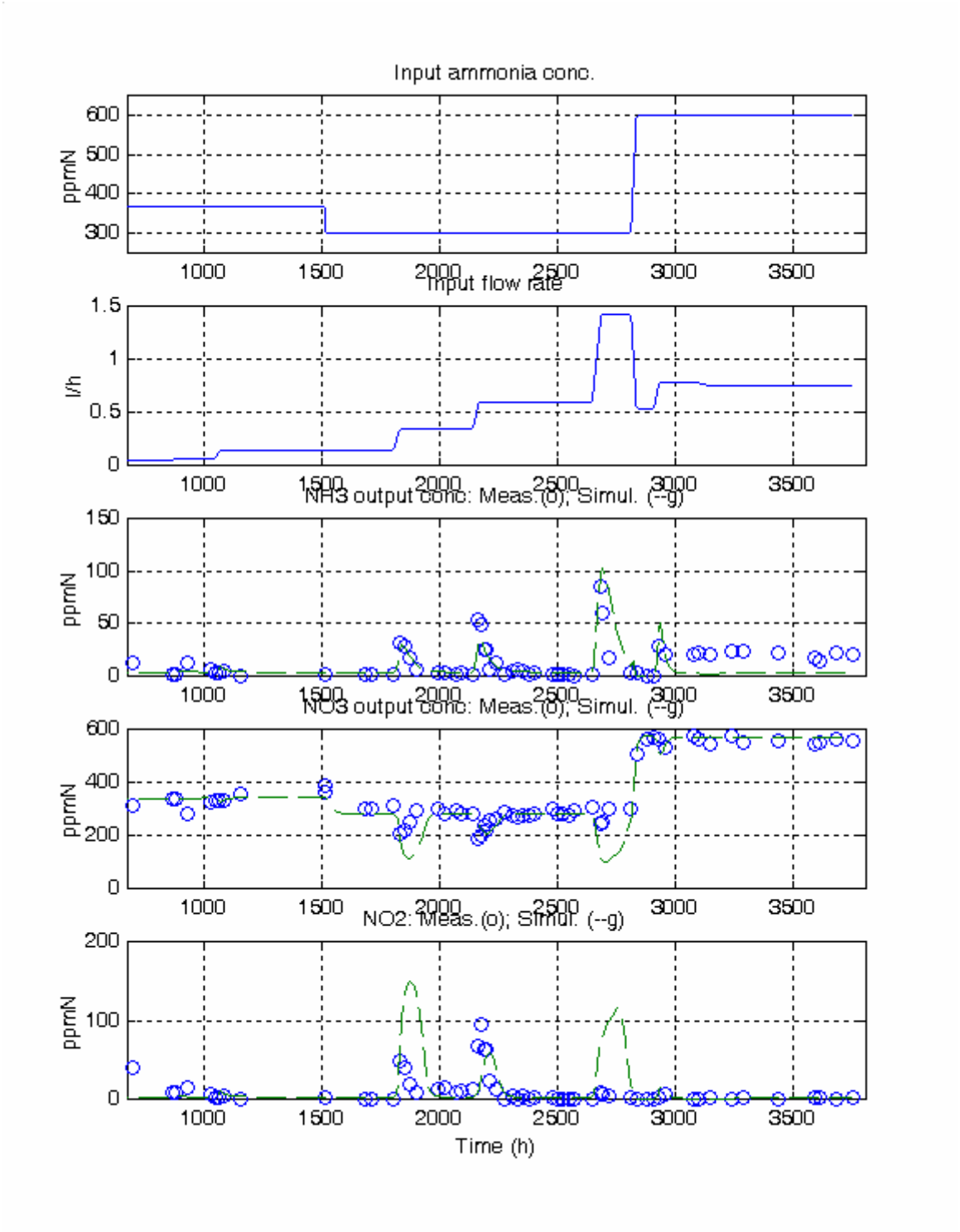


Fig A1.7: NB=10; KLa=175 h-1 ; Test UAB 2000

Particular case: NB=7; KLa=150 h-1

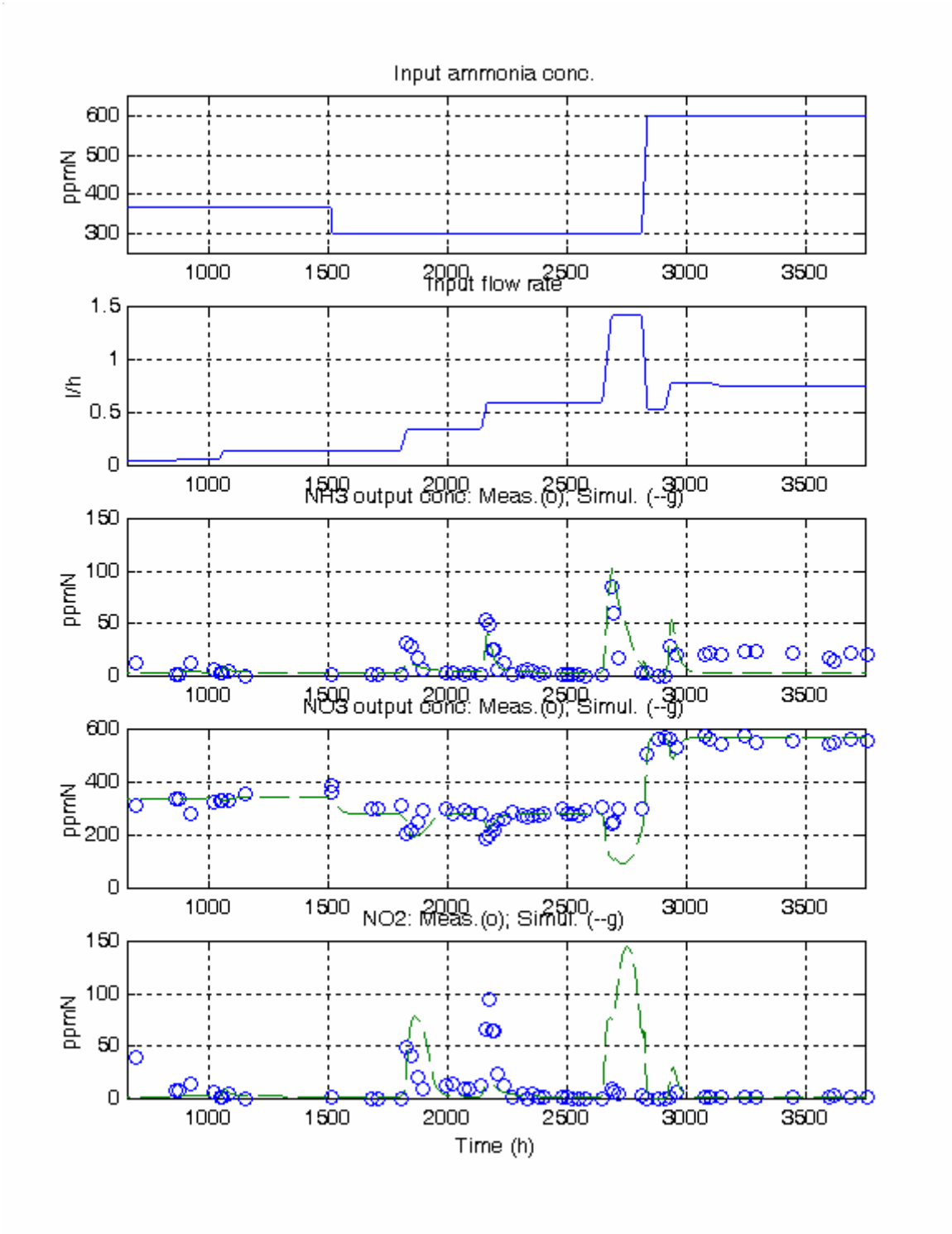


Fig A1.8: NB=7; KLa=150 h-1 ; Test UAB 2000

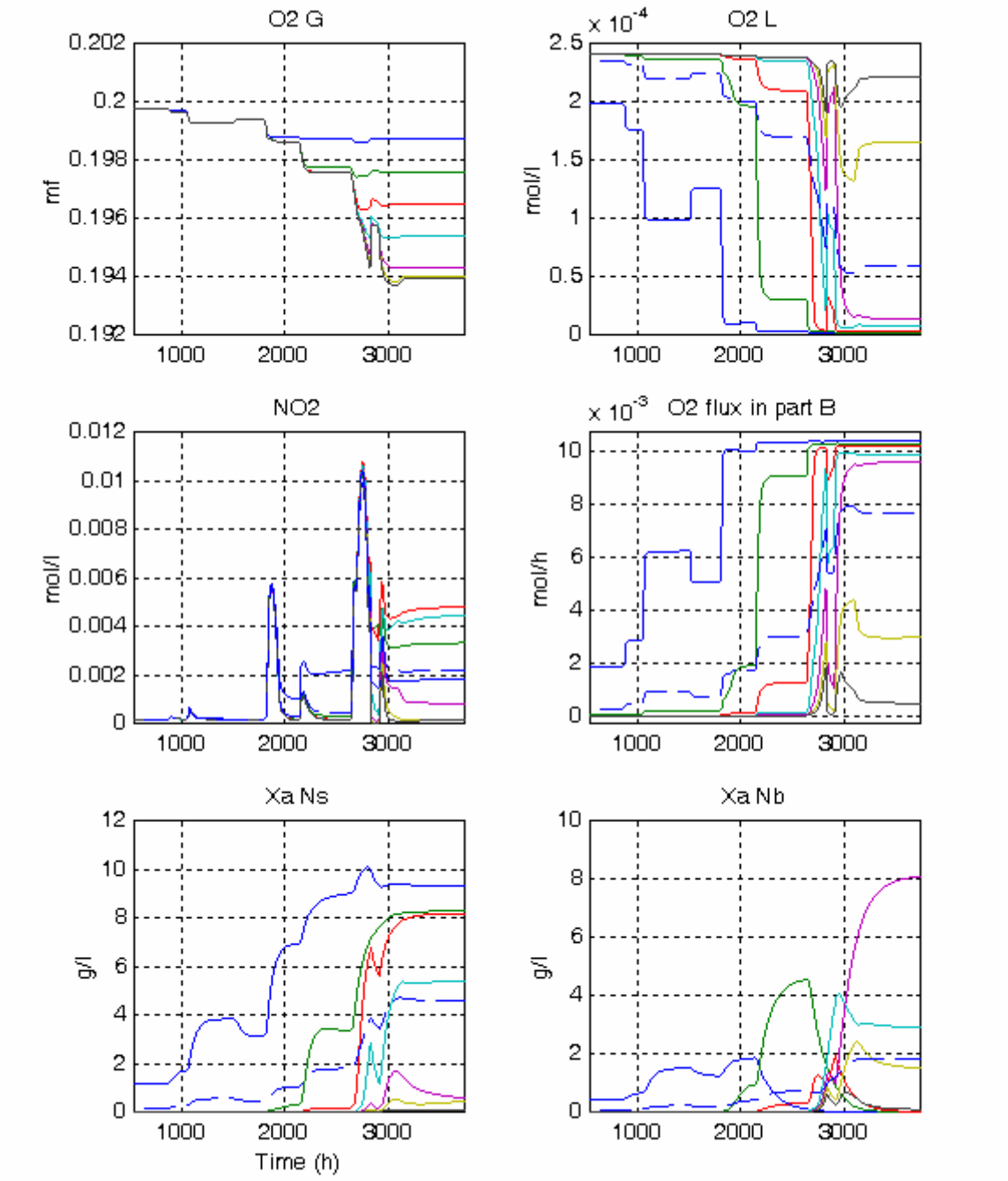


Fig A1.9: NB=7; KLa=150 h-1 ; Test UAB 2000

Evolution along the fixed bed

Particular case: NB=7; KLa=200 h-1

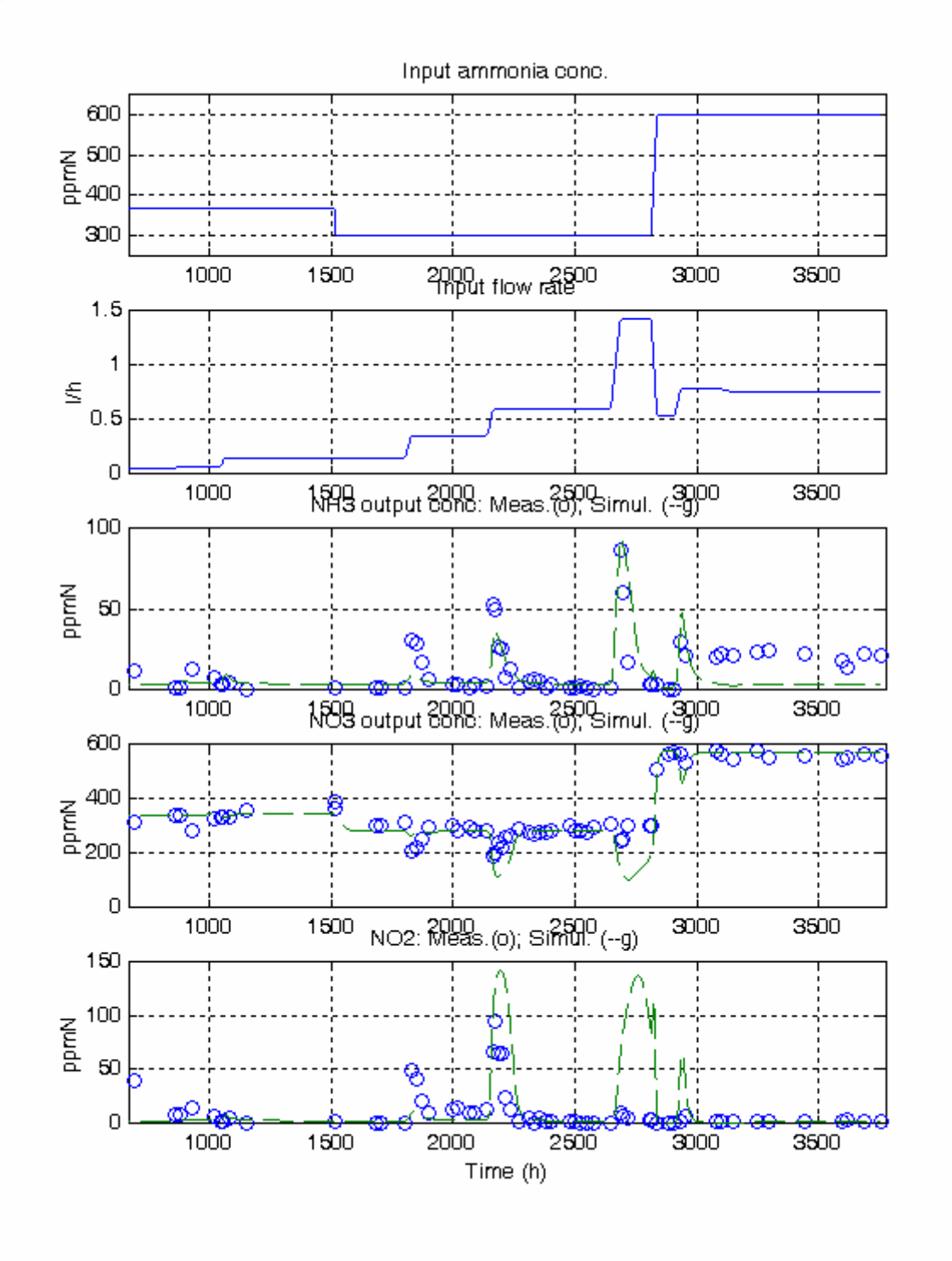


Fig A1.10: NB=7; KLa=200 h-1 ; Test UAB 2000

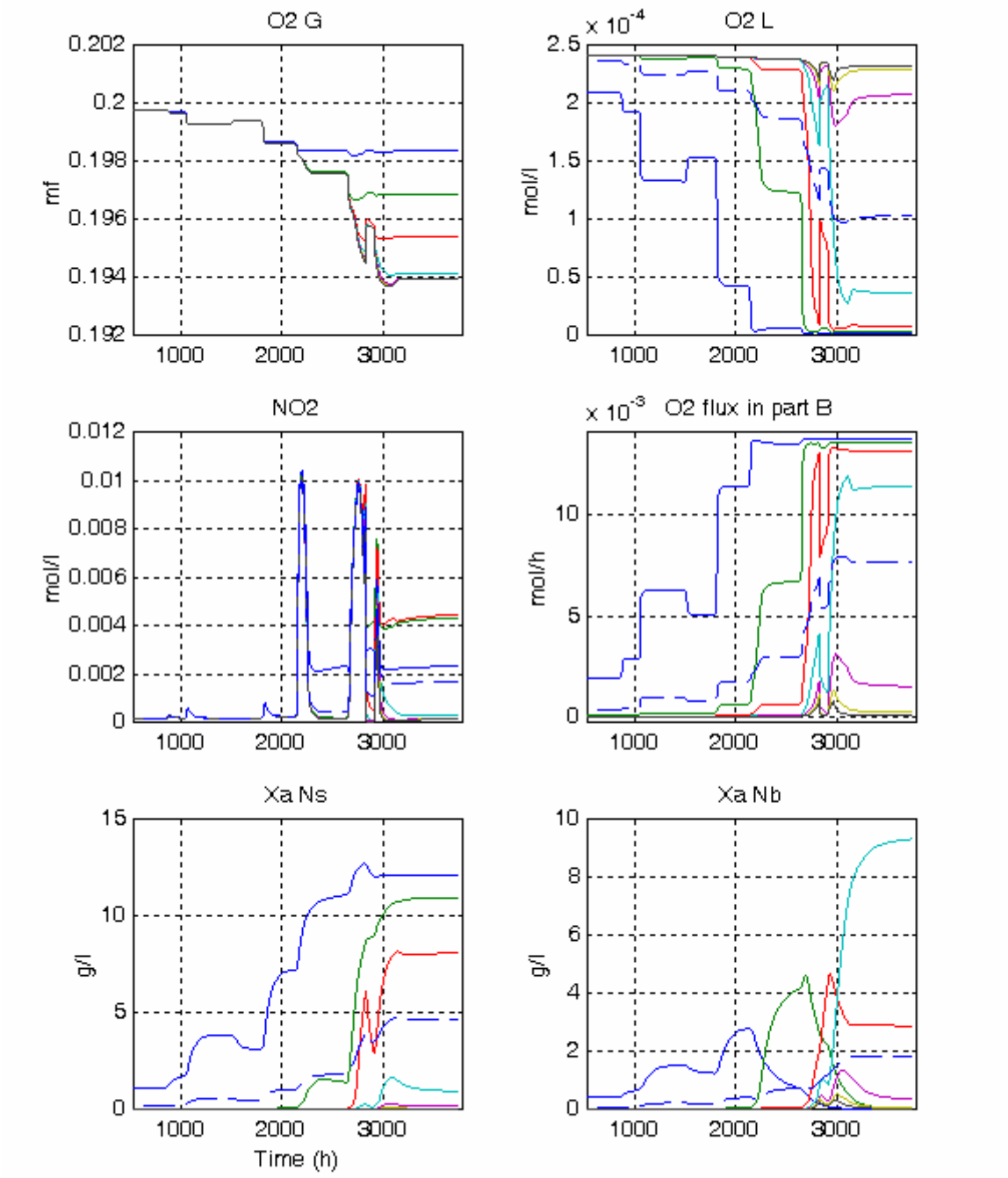


Fig A1.11: NB=7; KLa=200 h-1 ; Test UAB 2000
Evolution along the fixed bed

Particular case: NB=1; KLa=50 h-1

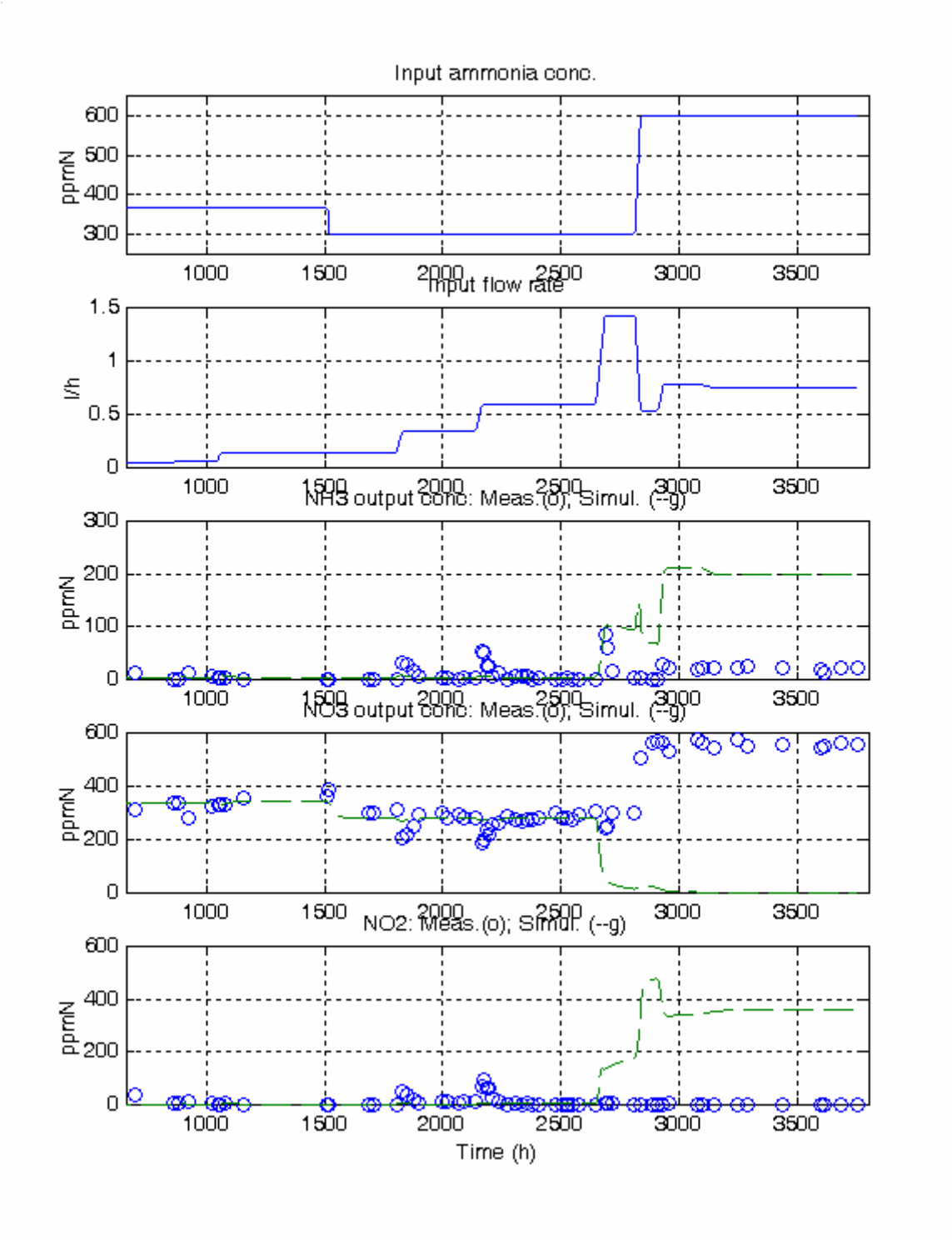


Fig A1.12: NB=1; KLa=50 h-1 ; Test UAB 2000

7. ANNEX 2: CHECKING THE MODEL AGAINST THE UAB TESTS OF 2003

Four tests were done from March to May 2003 on the UAB pilot plant.
The LGCB model with NB=7 has been checked against these tests: the model has been fed with the same inputs as the pilot plant and the model outputs are compared to the process outputs.
It can be seen in the following figures (from A2.1 to A2.4) that the model behaviour and the pilot plant behaviour are completely different. The model with NB=7 cannot be validated on these tests.
Particularly in the case of the test on May 2003 '300-600 ppmN NH3 step', the NO3 at column output is decreasing instead of increasing. This can be explained by the evolution of biomasses Ns and Nb in the CST's B1 to B7 (fig A2.4 and A2.5).

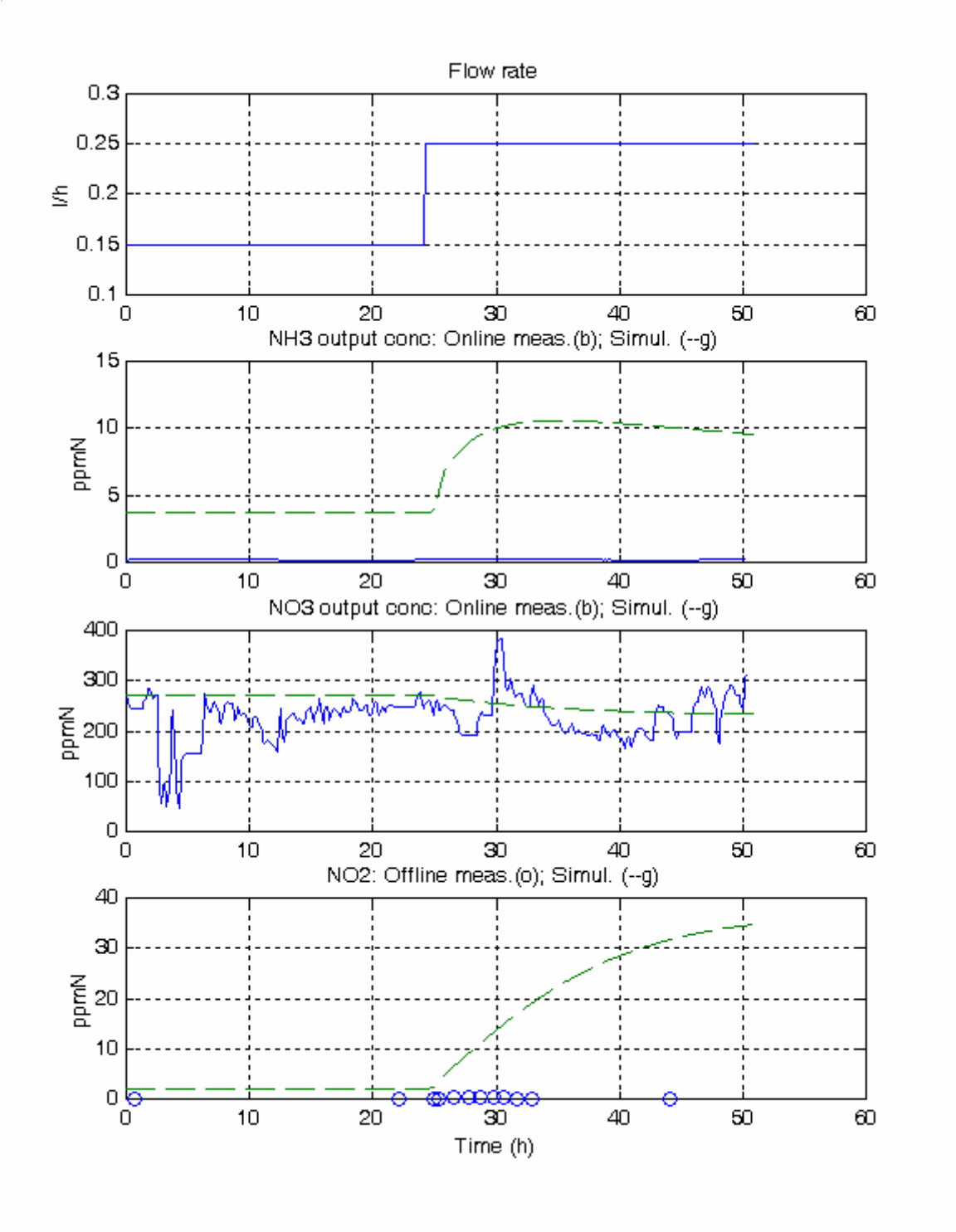


Fig A2.1: NB=7; KLa=115 h^{-1} ; Test UAB March 2003; 0.15 - 0.25 l/h step.
Process output: continuous blue line; Model output: dotted green line (graphs 2 to 4)

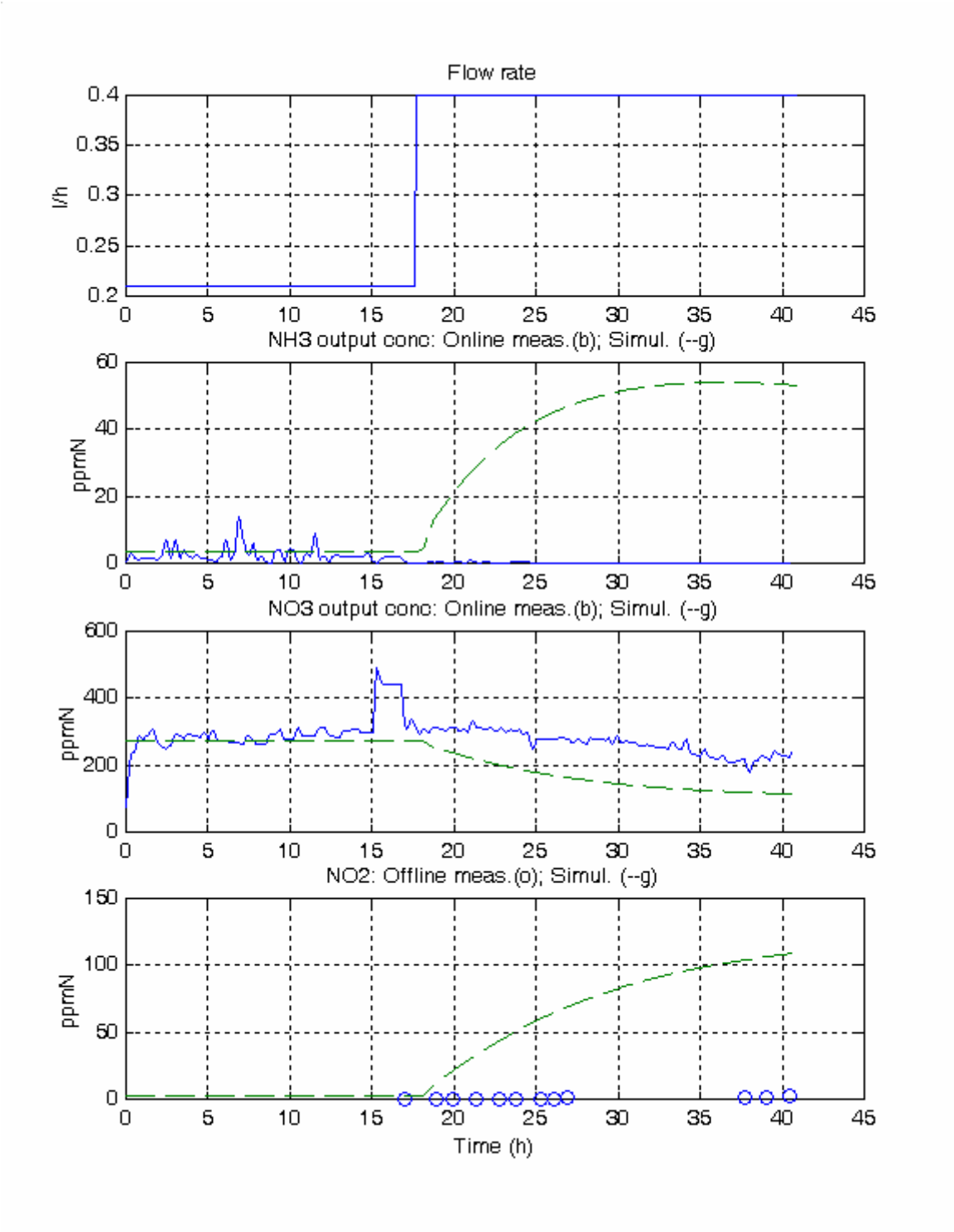


Fig A2.2: NB=7; KLa=115 h^{-1} ; Test UAB April 2003; 0.21 - 0.40 l/h step.
Process output: continuous blue line; Model output: dotted green line (graphs 2 to 4)

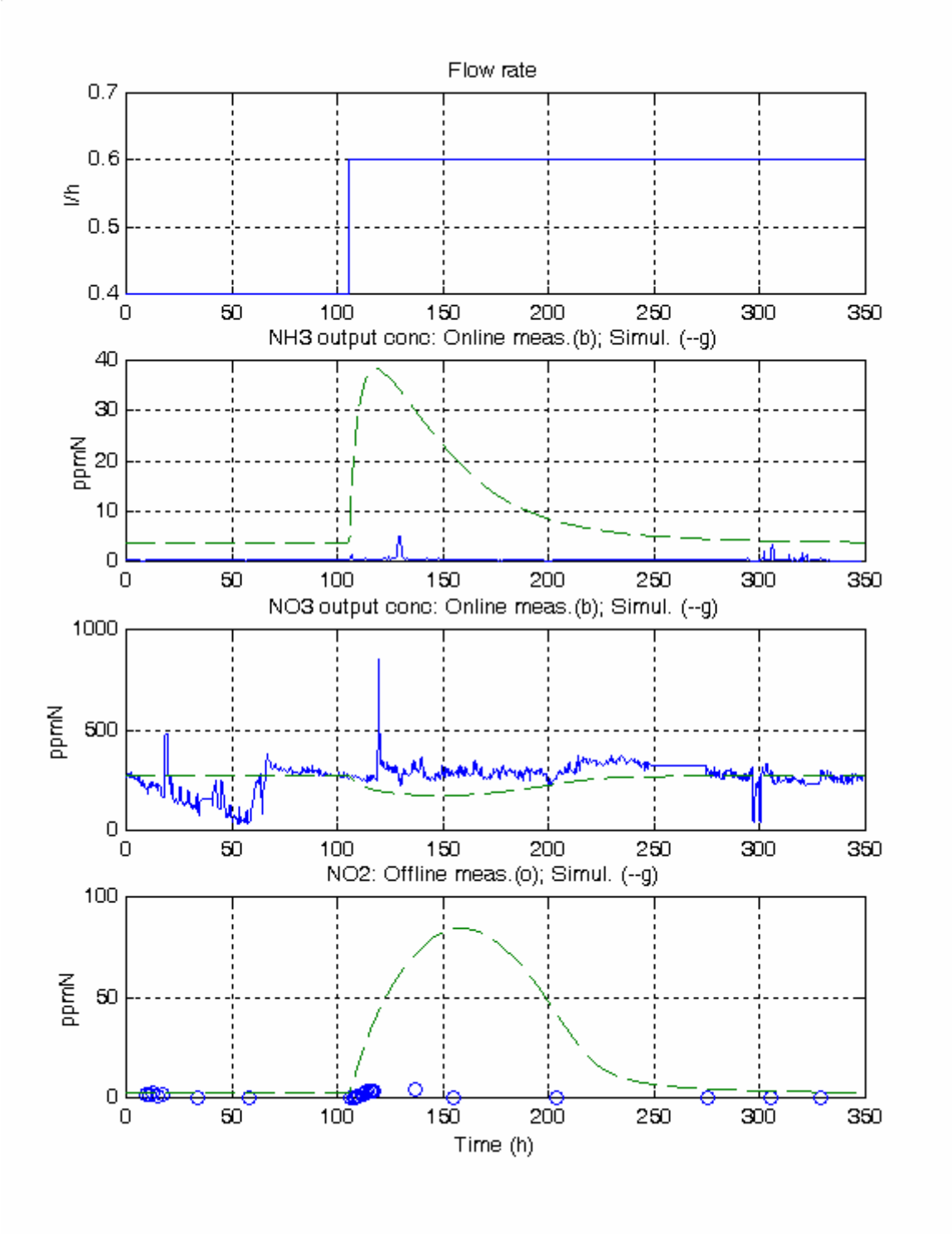


Fig A2.3: NB=7; KLa=115 h^{-1} ; Test UAB April-May 2003; 0.40 - 0.60 l/h step. Process output: continuous blue line; Model output: dotted green line (graphs 2 to 4)

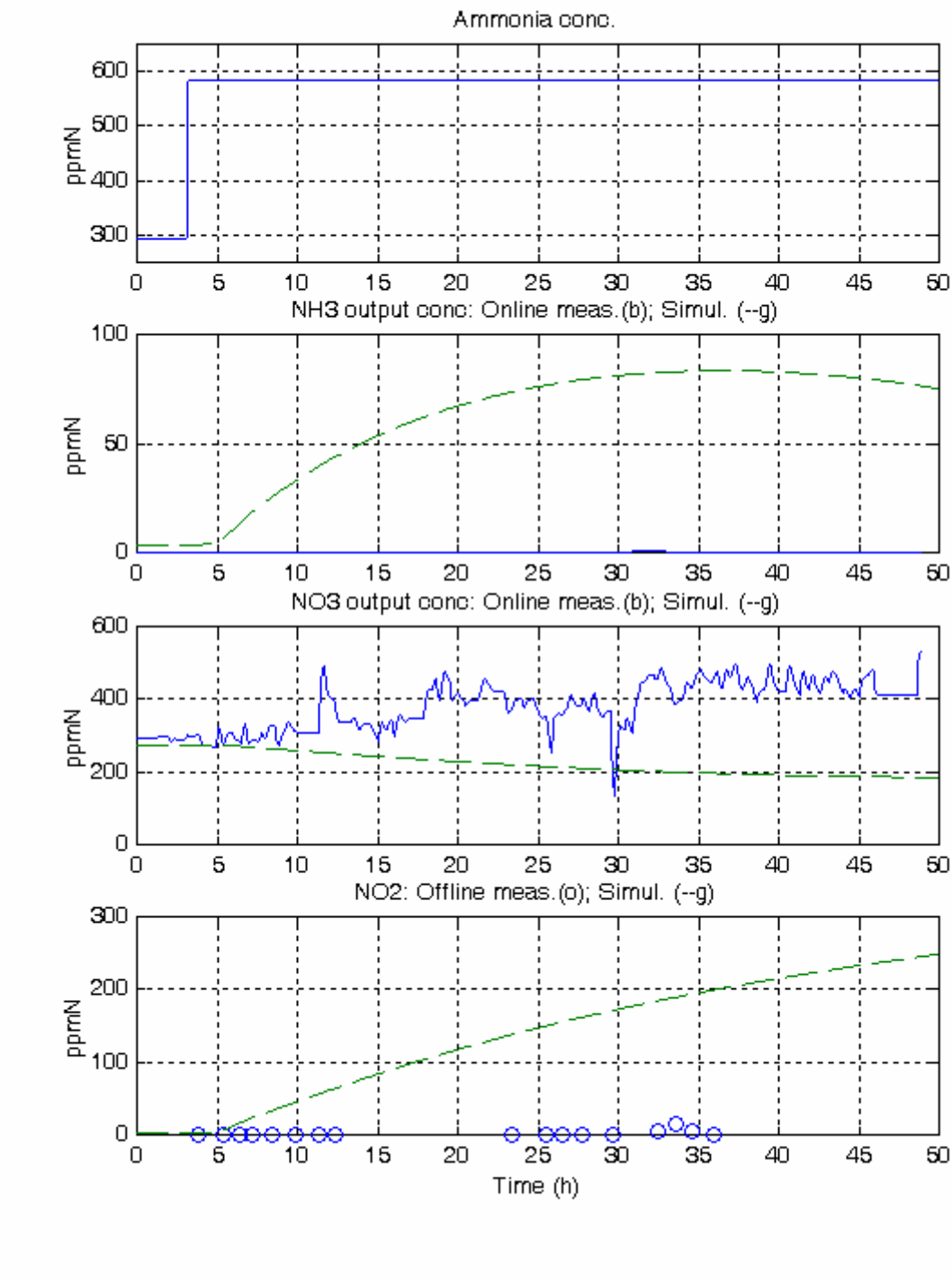


Fig A2.4: NB=7; KLa=90 h^{-1} ; Test UAB May 2003; 300-600 ppmN NH3 step

The NO3 model is decreasing instead of increasing. All the biomass Ns and Nb is in B1 and B1 is already saturated (Fig A2.5) before the load step. When the ammonia step occurs there is not enough Ns and Nb biomass in B2. In B1 Ns increases but not quickly enough to transform all the NH3 that is not transformed in B2 because of low Ns. The Ns increasing in

B1 is done at the expense of Nb (because the O2 flux in B1 is at its maximum). So NO2 increases in B1. Unfortunately Nb is too low in B2 to quickly grow and to oxidise it into NO3. Then NO3 decreases at column output (graph 3 of fig A2.4).

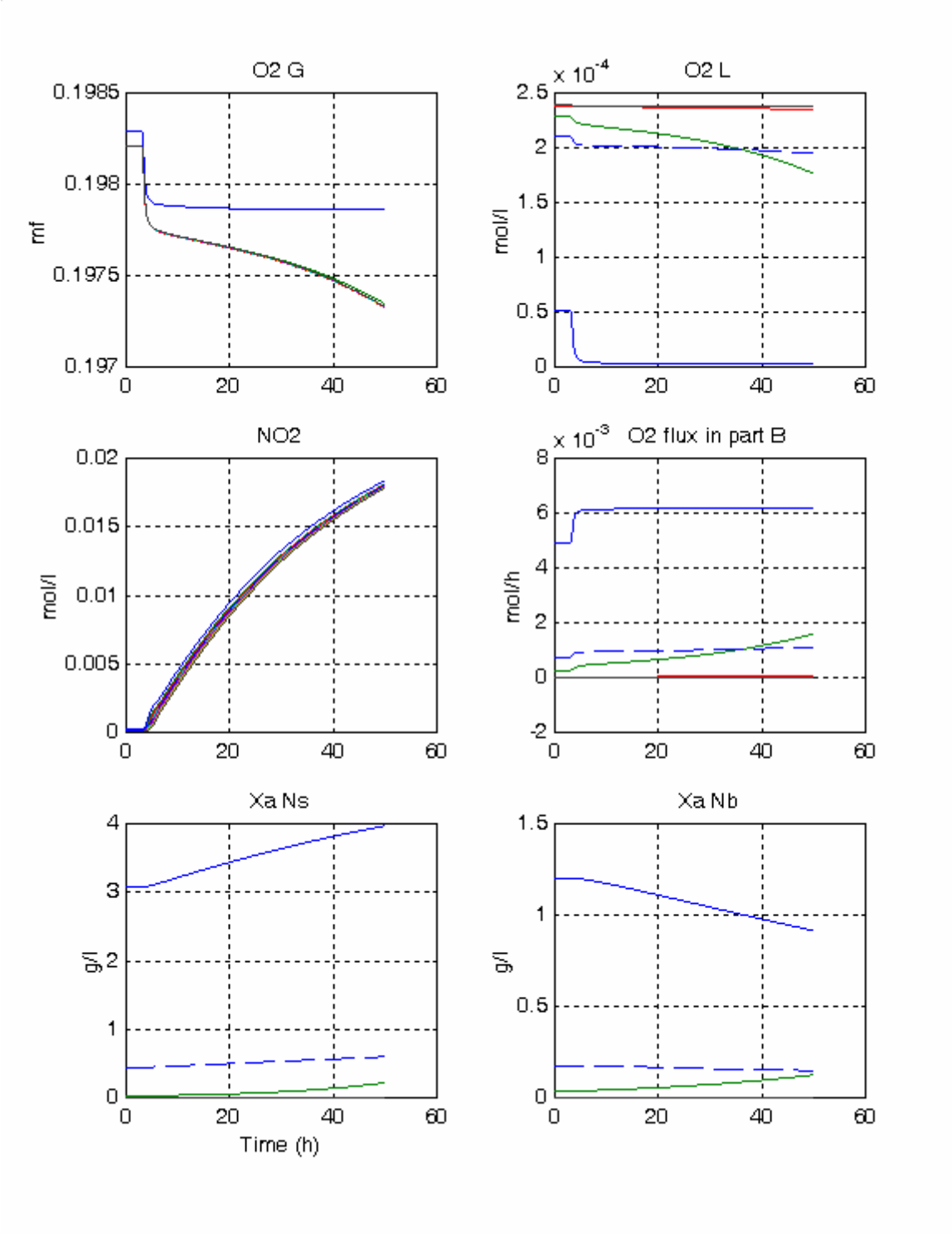


Fig A2.5: NB=7; KLa=90 h^{-1} ; Test UAB May 2003; 300-600 ppmN NH3 step.
Evolution of O2, NO2, Ns and Nb along the 7 tanks of the fixed bed.
B1: blue curves.
B2: green curves.
Average of the 7 tanks: dotted line.

8. ANNEX 3: MODEL WITH NB=1 CHECKED AGAINST THE TESTS OF 2003

The number of tanks (NB) of the LGCB model has been modified and set to 1. Then it has been checked against the four tests one from March to May 2003 on the UAB pilot plant: the model has been fed with the same inputs as the pilot plant and the model outputs are compared to the process outputs.
It can be seen in the following figures (from A3.1 to A3.4) that the model behaviour and the pilot plant behaviour are different but closer than with NB=7.

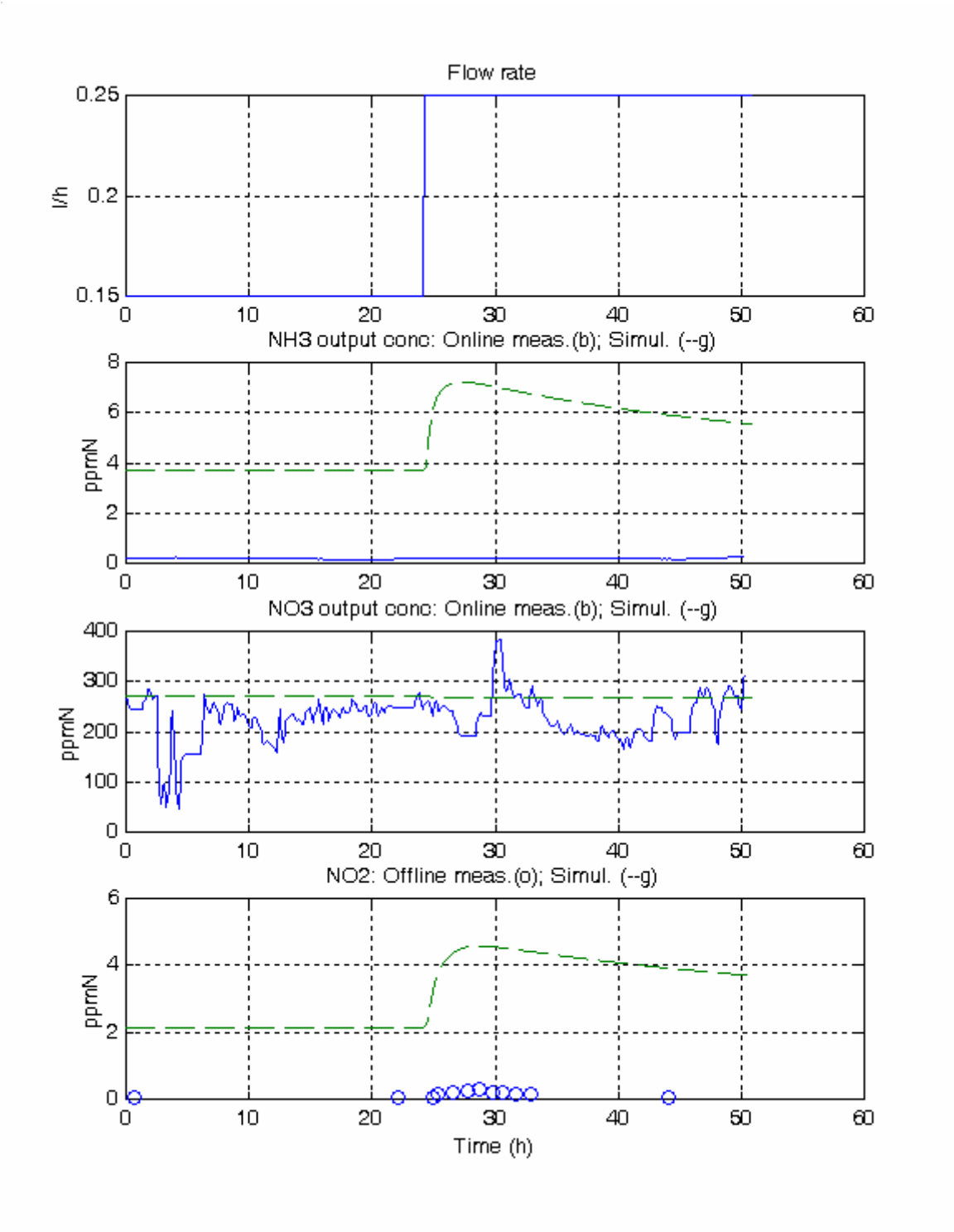


Fig A3.1: NB=1; KLa=115 h^{-1} ; Test UAB March 2003; 0.15 - 0.25 l/h step. Process output: continuous blue line; Model output: dotted green line (graphs 2 to 4).

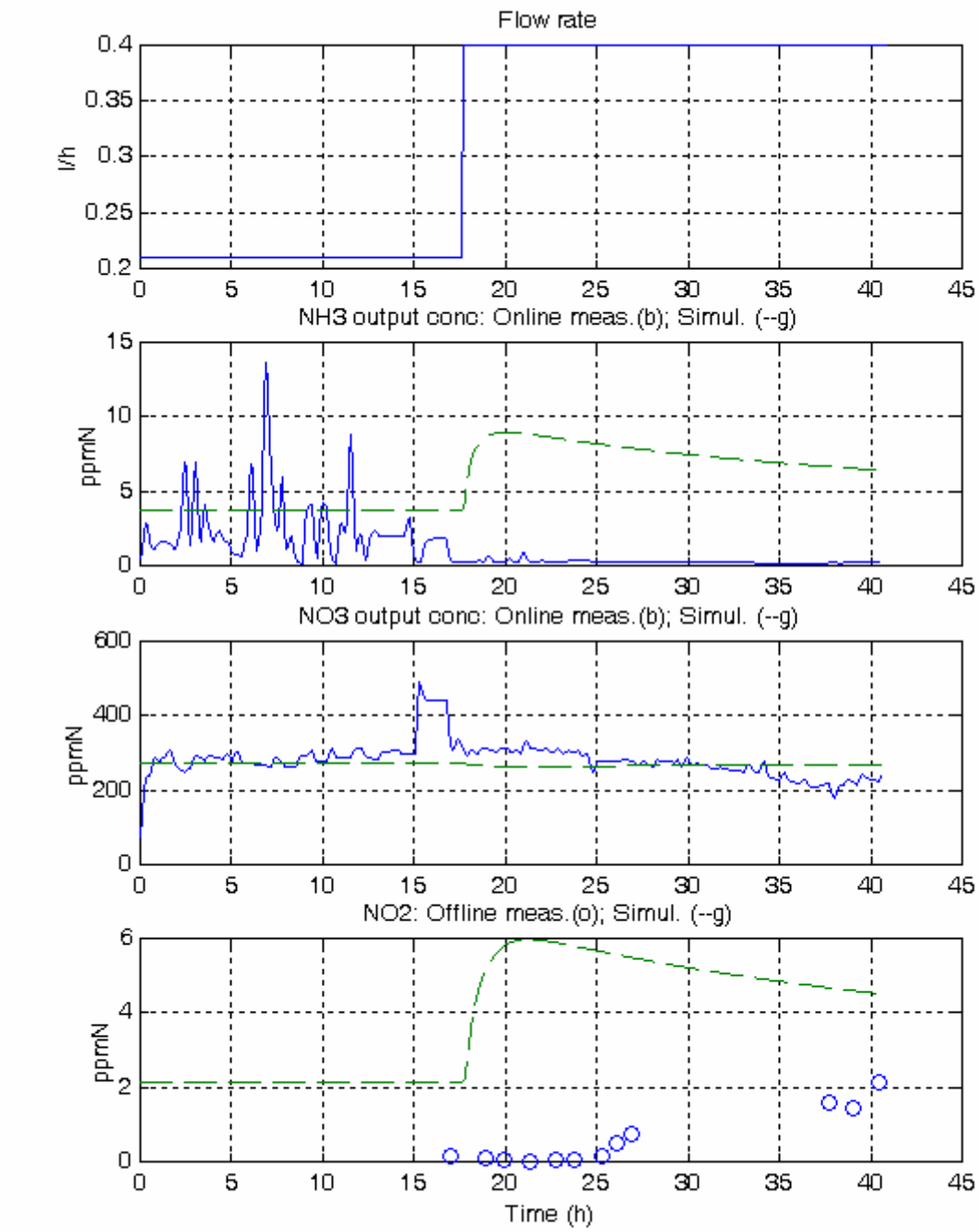


Fig A3.2: NB=1; KLa=115 h^{-1} ; Test UAB April 2003; 0.21 - 0.40 l/h step.
Process output: continuous blue line; Model output: dotted green line (graphs 2 to 4).

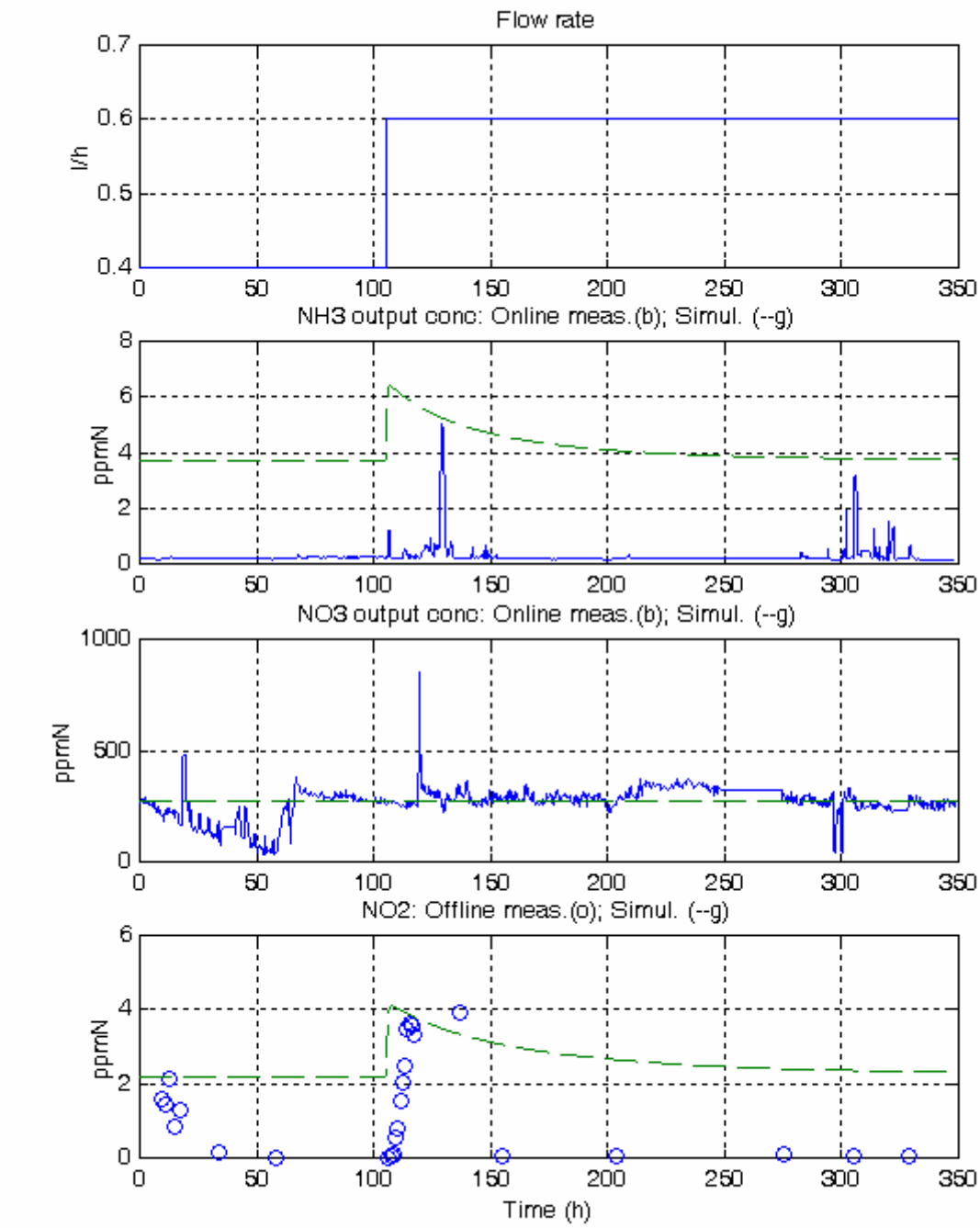


Fig A3.3: NB=1; KLa=115 h-1 ; Test UAB April-May 2003; 0.40 - 0.60 l/h step

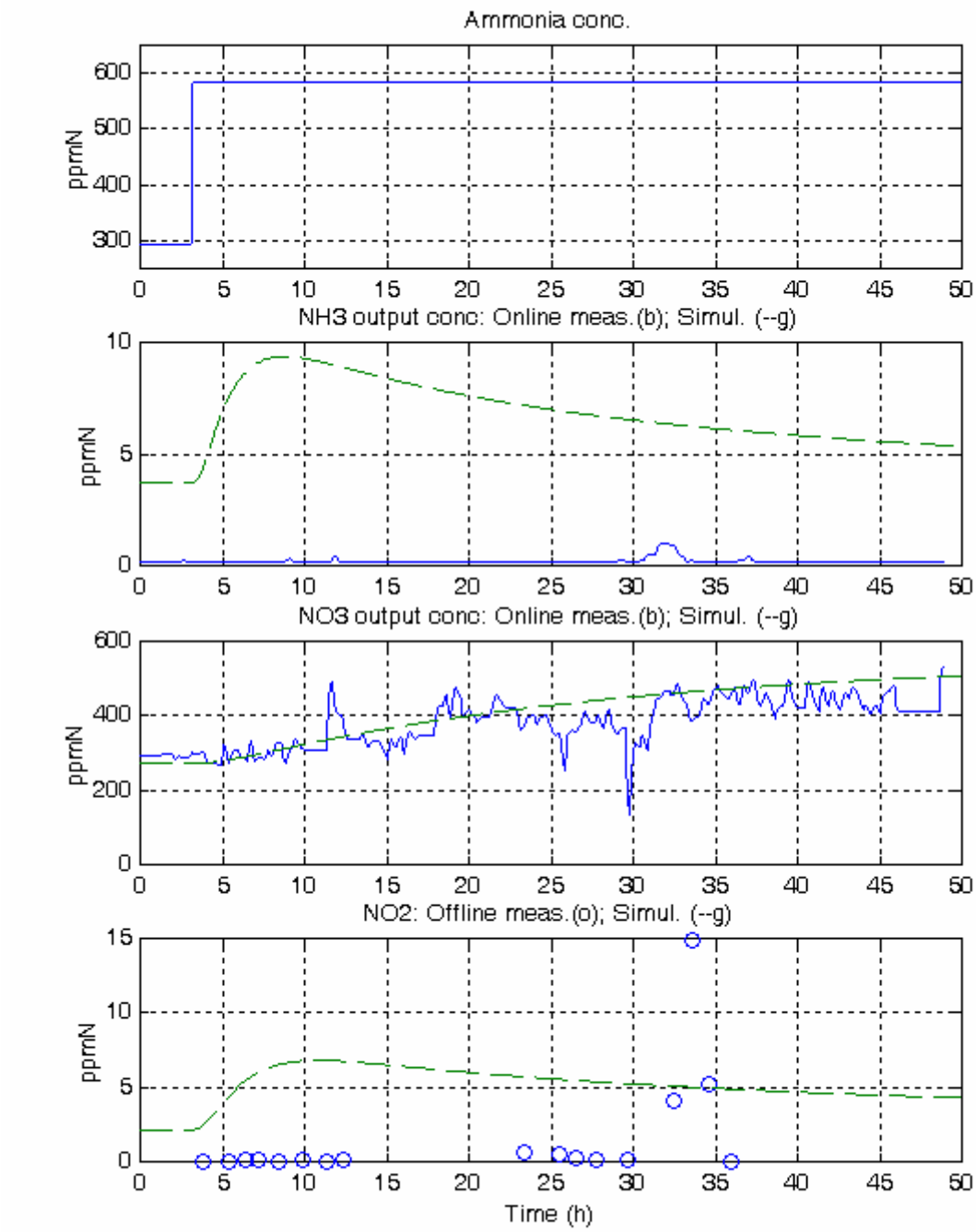


Fig A3.4: NB=1; KLa=90 h^{-1} ; Test UAB May 2003; 300-600 ppmN NH3 step. Process output: continuous blue line; Model output: dotted green line (graphs 2 to 4).

9. ANNEX 4: SENSITIVITY ANALYSIS

9.1. Introduction

The objective is to evaluate the sensitivity of the main outputs (NO2, NH3 and NO3 at column output) to the chemical parameters (half saturation constants, specific growth rates and maintenance coefficients).
The process is excited by a step of flow rate from 0.15 to 0.25 l/h.

9.2. Model state

The present model is built from the LGCB TN's 27.1, 27.2 and 27.3, excepted that the biofilm described in TN27.3 is not modelled (the biomass is assumed to be homogenously dispersed in the liquid of each CST of the fixed bed). The inhibitory effects of NO2 and NO3 on the Nitrobacter growth is modelled like in TN 27.3 .
The KLa is computed according to TN 63.2 p.30 by LGCB.
The parameters values are set in TN 27.3 appendix A. These values are declared 'nominal' values from which the variations are done by multiplying them by a given factor.

9.3. Results

A preliminary observation is that NO3 is nearly not sensitive to the studied parameters.

For the other process outputs (NO2 and NH3), the results are expressed on the figures A4.1 to A4.3:
. figure A4.1 shows the variation of the functioning point in function of the variation of the chemical parameters;
. figure A4.2 shows the variation of the peak height;
. figure A4.3 shows the ratio 'peak height' on 'functioning point'. This ratio is constant for a given parameter and depends only on the amplitude of the process excitation step.

It is recalled that the following results in figures A4.1 to A4.3 concern a process excited by a flow rate step.

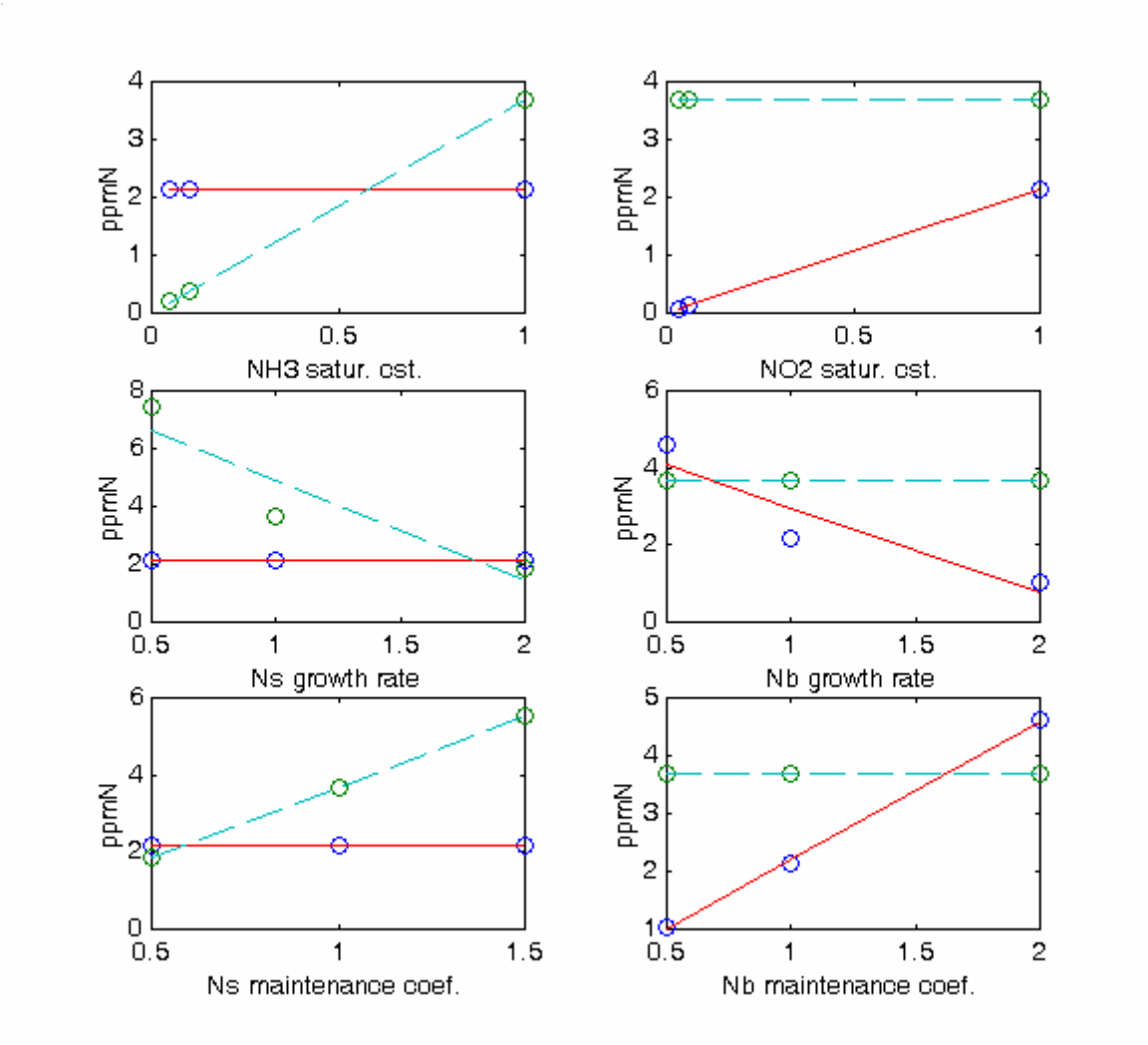


Figure A4.1: Variation of the functioning point in function of variation of the parameters.

Parameters are: NH3 and NO2 half saturation constants, Ns and Nb specific growth rates, Ns and Nb specific maintenance coefficients.
The x-coordinate of each graph is the multiplicative factor of the 'nominal' parameter value.
The y-coordinate of each graph is the functioning point value expressed in ppmN.
The circles are for the simulated points and the lines are for their linear regression.
The green circles and green dotted lines are for NH3.
The blue circles and red continuous lines are for NO2.
The left hand side graphs show that the NO2 functioning point is not sensitive to NH3 half saturation constant or to Ns growth rate and maintenance coefficient.
The right hand side graphs show that the NH3 functioning point is not sensitive to NO2 half saturation constant or to Nb growth rate and maintenance coefficient.

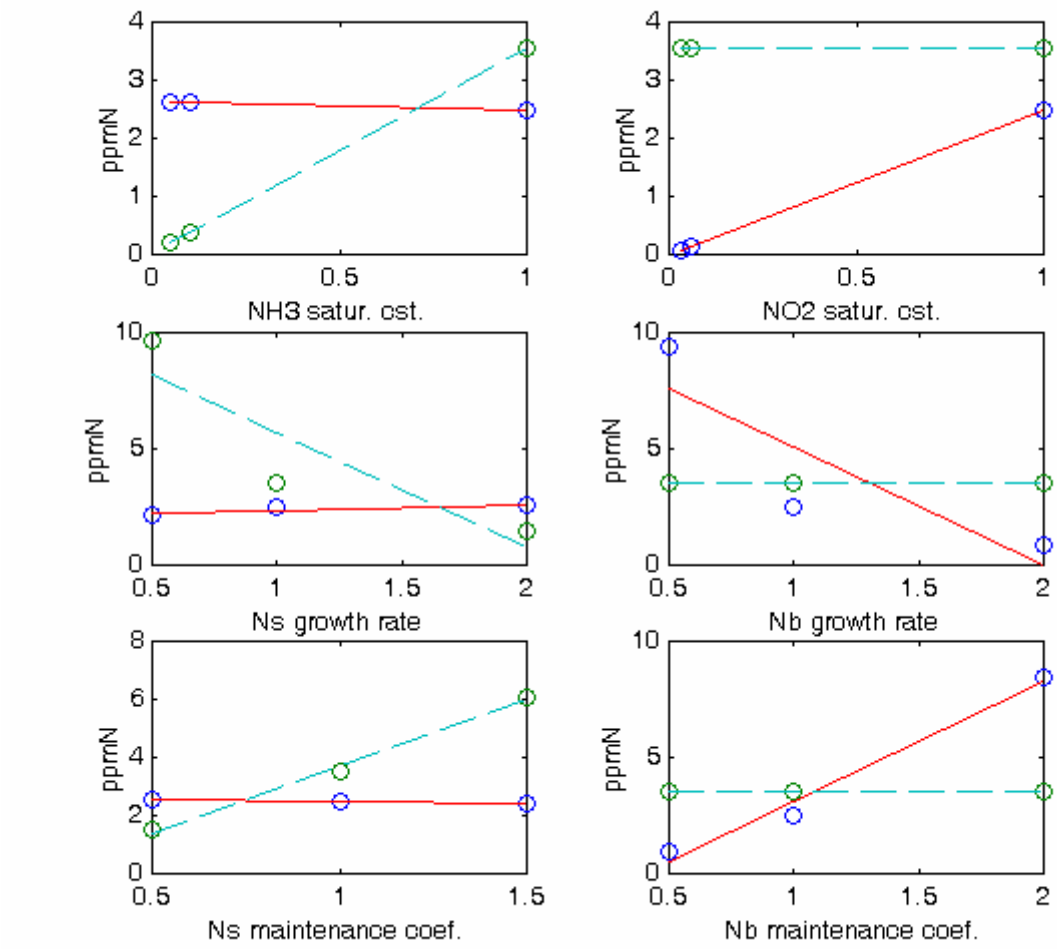


Figure A4.2: Variation of the peak height in function of variation of the parameters.
Parameters are the same as in figure A4.1(NH3 and NO2 half saturation constants, Ns and Nb specific growth rates, Ns and Nb specific maintenance coefficients).
The x-coordinate of each graph is the multiplicative factor of the 'nominal' parameter value.
The y-coordinate of each graph is the peak height value expressed in ppmN.
The circles are for the simulated points and the lines are for their linear regression.
The green circles and green dotted lines are for NH3.
The blue circles and red continuous lines are for NO2.
The left hand side graphs show that the NO2 peak height is not sensitive to NH3 half saturation constant or to Ns growth rate and maintenance coefficient.
The right hand side graphs show that the NH3 peak height is not sensitive to NO2 half saturation constant or to Nb growth rate and maintenance coefficient.

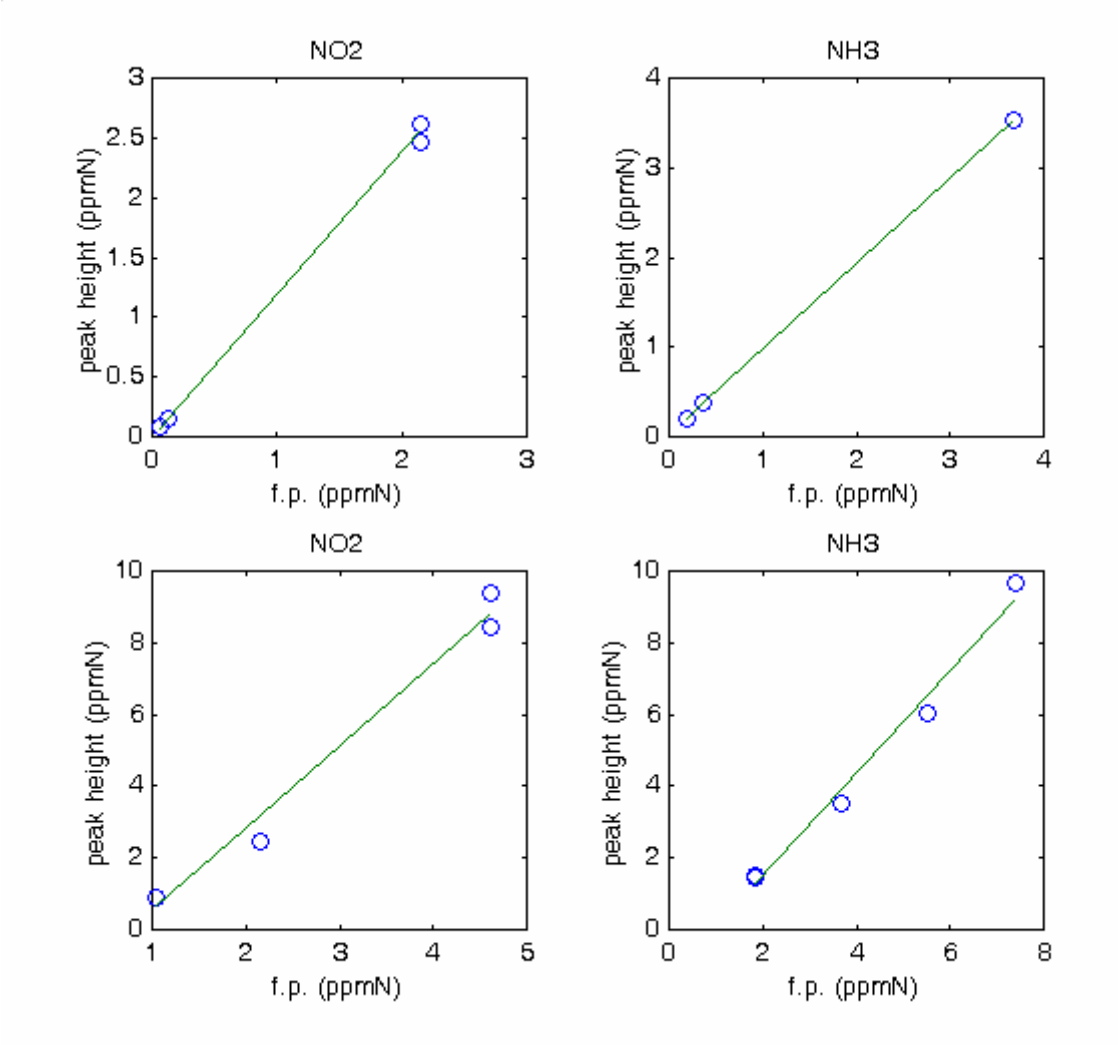


Figure A4.3: Ratio 'peak height' on 'functioning point' in function of the parameters variations.

The 2 upper graphs are for NH3 and NO2 half saturation constants.
The 2 lower graphs are for Ns (left hand side graph) and Nb (right hand side graph) specific growth rate and maintenance coefficient.
These graphs show that the peak height is directly proportional to the functioning point (and is not independent). The correlative slope depends on the amplitude of the excitation step. For low value of the functioning point (lower than 2 ppmN), this slope is nearly about 1 for all the parameters variations.

9.4. Recall of the UAB test: liquid flow rate step from 0.15 to 0.25 l/h

The present simulation can be compared to the UAB test: liquid flow rate step from 0.15 to 0.25 l/h done from 25 to 27 March 2003.

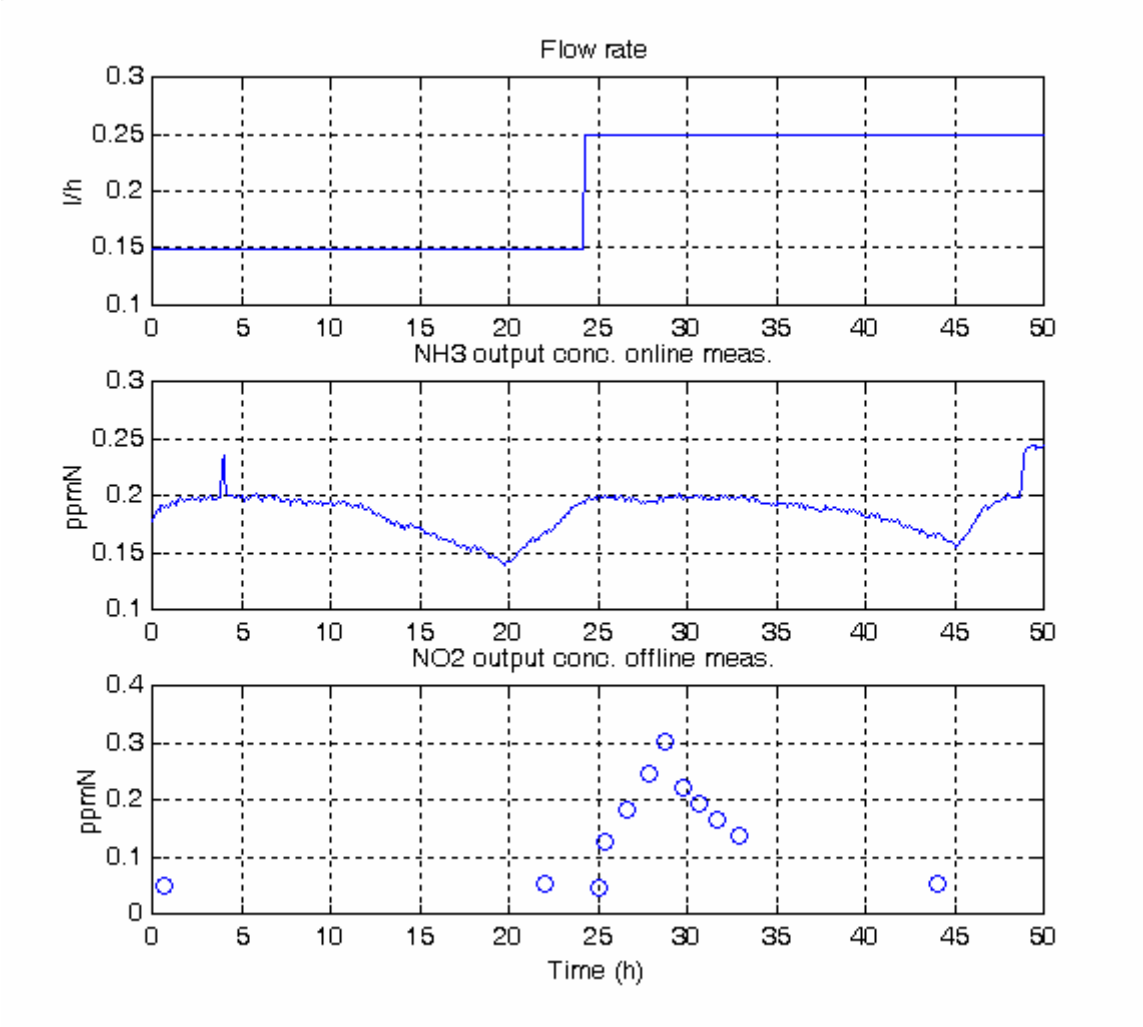


Figure A4.4: UAB liquid flow rate step (from 25 to 27 March 2003)

In the UAB test (figure A4.4) where the excitation is the same as in the simulation, the results are:

	Functioning point (ppmN)	Peak height (ppmN)
NH3	0.2	0
NO2	0.05	0.25

9.5. Conclusion

According to figure A4.3 where the ratio 'peak height' on 'functioning point' is nearly the same for all the parameters variations and equal to about 1, a functioning point of 0.05 ppmN implies that the expected NO2 peak height is also of 0.05 ppmN.

Now on the UAB test the measured NO2 peak height is six times as high.
So there is no interest to modify the model parameters: any change of the parameters will not be able to make the model closer to the process.

9.6. Further study

The same kind of work has been done with another process excitation: a NH3 concentration step. Nevertheless it is not exploitable because the ‘ammonium concentration step’ test done by UAB produced NO2 and NH3 peaks at unexpected moments after the step.

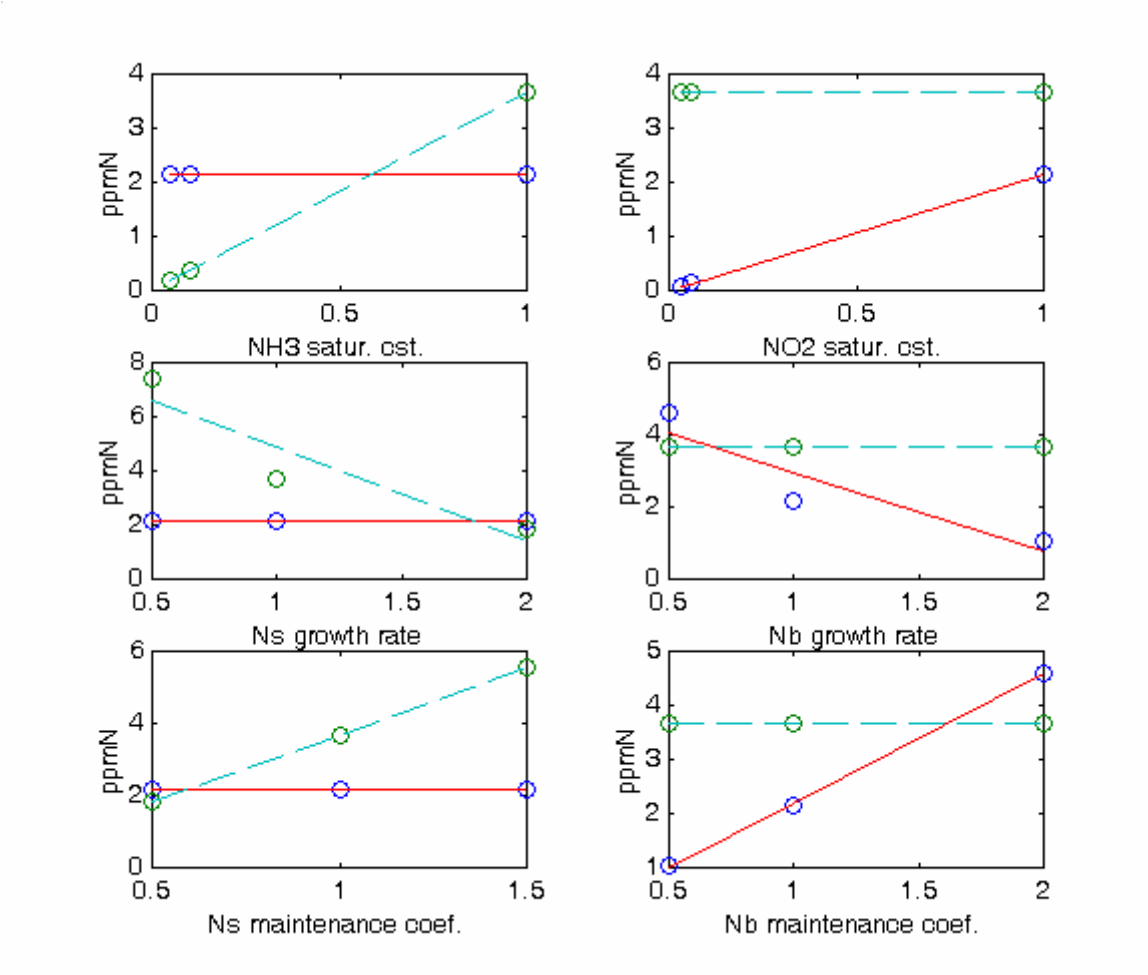


Figure A4.5: Variation of the functioning point in function of variation of the parameters.

Parameters are: NH3 and NO2 half saturation constants, Ns and Nb specific growth rates, Ns and Nb specific maintenance coefficients.
The x-coordinate of each graph is the multiplicative factor of the 'nominal' parameter value.
The y-coordinate of each graph is the functioning point value expressed in ppmN.
The circles are for the simulated points and the lines are for their linear regression.
The green circles and green dotted lines are for NH3.
The blue circles and red continuous lines are for NO2.
The left hand side graphs show that the NO2 functioning point is not sensitive to NH3 half saturation constant or to Ns growth rate and maintenance coefficient.
The right hand side graphs show that the NH3 functioning point is not sensitive to NO2 half saturation constant or to Nb growth rate and maintenance coefficient.

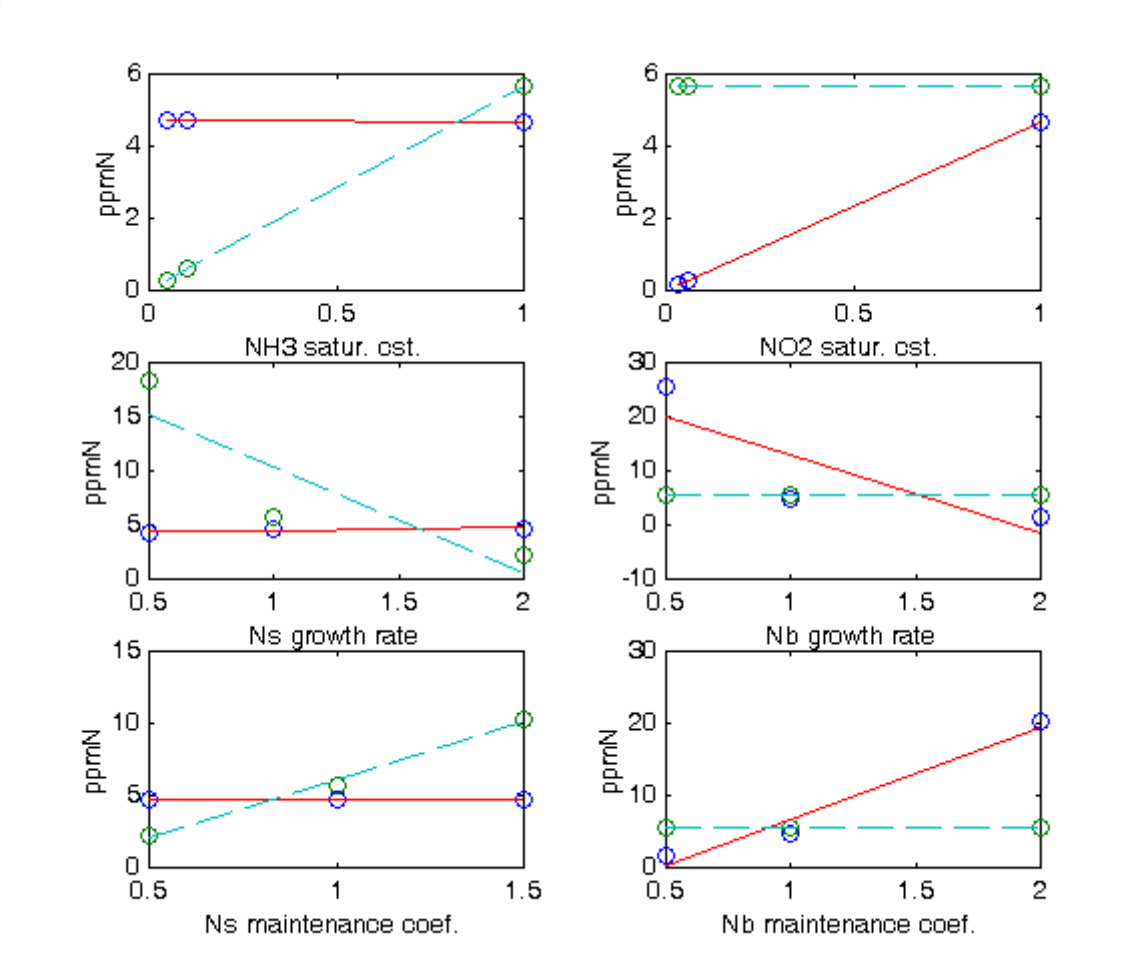


Figure A4.6: Variation of the peak height in function of variation of the parameters.
Parameters are the same as in figure A4.1(NH3 and NO2 half saturation constants, Ns and Nb specific growth rates, Ns and Nb specific maintenance coefficients).
The x-coordinate of each graph is the multiplicative factor of the 'nominal' parameter value.
The y-coordinate of each graph is the peak height value expressed in ppmN.
The circles are for the simulated points and the lines are for their linear regression.
The green circles and green dotted lines are for NH3.
The blue circles and red continuous lines are for NO2.
The left hand side graphs show that the NO2 peak height is not sensitive to NH3 half saturation constant or to Ns growth rate and maintenance coefficient.
The right hand side graphs show that the NH3 peak height is not sensitive to NO2 half saturation constant or to Nb growth rate and maintenance coefficient.

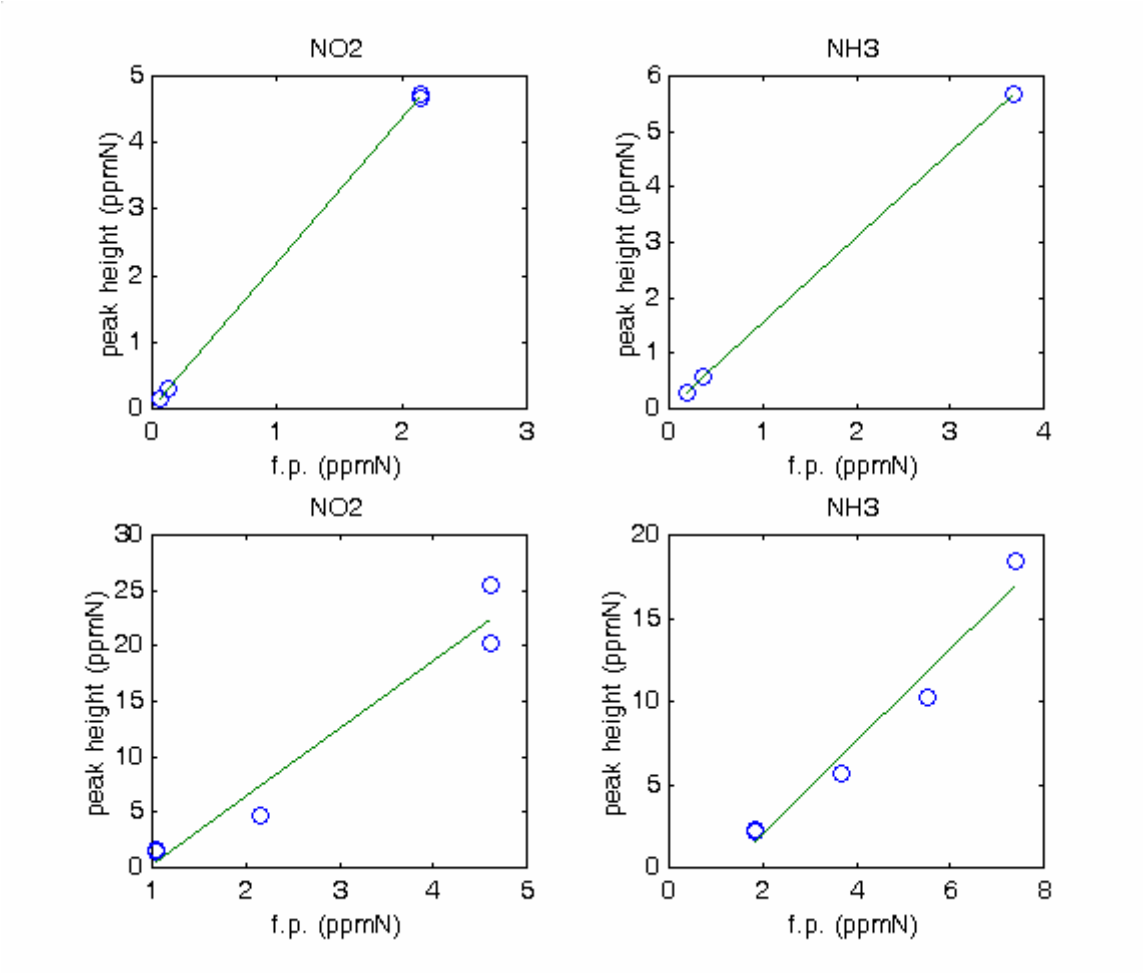


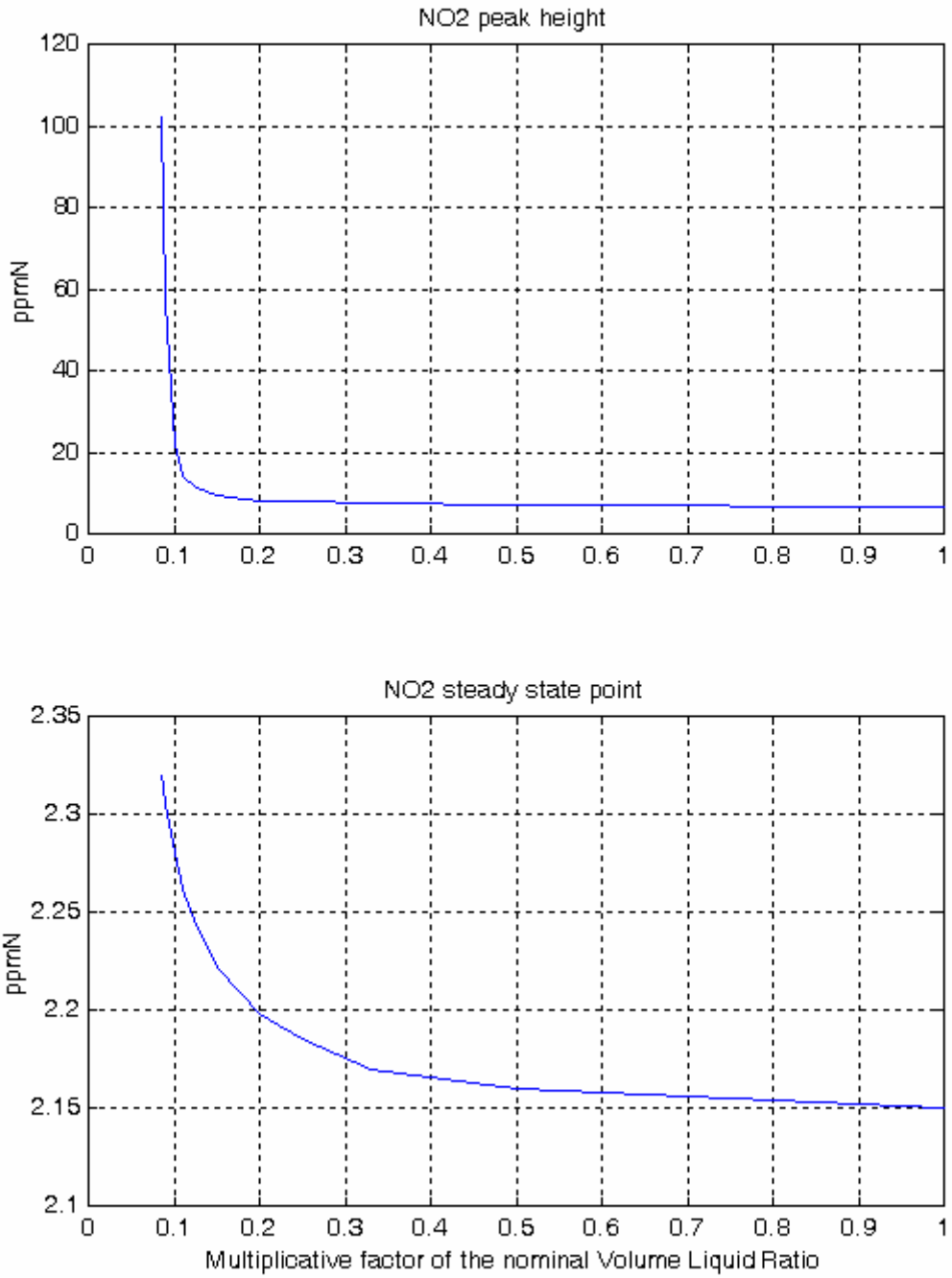
Figure A4.7: Ratio 'peak height' on 'functioning point' in function of the parameters variations.

The 2 upper graphs are for NH3 and NO2 half saturation constants.
The 2 lower graphs are for Ns (left hand side graph) and Nb (right hand side graph) specific growth rate and maintenance coefficient.
These graphs show that the peak height is directly proportional to the functioning point (and is not independent). The slope of the correlation straight line depends on the amplitude of the excitation step.

10. ANNEX 5: COMPLEMENTARY SENSITIVITY ANALYSIS

10.1. Sensitivity of the NO2 against the liquid volume ratio

The sensitivity of output NO2 against the clogging of the column has been studied by modifying the liquid volume ratio ε_L .
The evolution of the NO2 peak height and of the NO2 steady state point in function of the liquid volume ratio is shown in figure A5.1.
The nominal value of the volume liquid ratio (ε_L=33%) is multiplied by a factor lower than 1 in order to simulate a clogging (the volume of liquid is decreased). In the figure 1, this factor varies from 1 to 0.09. On that range, the impact of the volume liquid ratio mismatch is very important on the NO2 peak height but not on the NO2 steady state point : the NO2 peak height moves strongly from 2 to 100 ppmN although the NO2 steady state point moves lightly from 2.15 to 2.32 ppmN.



Peak Height and Steady State Point = function(Volume Liquid Ratio)

Figure A5.1

The NO2 peak height moves strongly from 2 to 100 ppmN although the NO2 steady state point moves lightly from 2.15 to 2.32 ppmN.

10.2. Proposal of parameters modification

The sensitivity study (section 9 above) has shown that the chemical parameters (half saturation constants, specific growth rates and maintenance coefficients) could not be modified in such a way that the values of steady state point and peak height of 2003 UAB test (particularly the flow rate step on March, plotted in figure A5.2) can be reached.

In fact, changing simultaneously the parameters 'liquid volume ratio' and 'half saturation constants for Ns and Nb growth' (associated to substrates NH3 and NO2) allow to obtain simulated results near ones of the previous UAB test.

A simulation of the UAB test (flow rate step from 0.15 to 0.25 l/h at NH3 conc. of 300 ppmN) has been done with modified parameters (results in fig A5.3 and A5.4).
These modified parameters are :
. half saturation constant for Ns growth (substrate NO2) = nominal value multiplied by 0.03;
. half saturation constant for Nb growth (substrate NH3) = nominal value multiplied by 0.05;
. liquid volume ratio = nominal value multiplied by 0.22 .
As it can be seen, these parameters are strongly modified against their nominal values. Such modifications must be validated by complementary tests and the evolution of these parameters must be connected to the history of the column (clogging, …). The liquid volume ratio could be computed from the pressure drop Ergun relation proposed by Forler (1992).

The simulation gives results similar to those of the UAB test of fig.A5.2 :
Figure A5.3:
NO2 steady state point = 0.07 ppmN (to be compared to 0.05 ppmN in UAB test fig. A5.2)
NO2 peak height = 0.38 ppmN (to be compared to 0.30 ppmN in UAB test fig.A5.2)

Figure A5.4:
NH3 steady state point = 0.2 ppmN (to be compared to 0.2 ppmN in UAB test fig. A5.2)
NH3 peak height = 0.48 ppmN (to be compared to no peak in UAB test fig. A5.2)

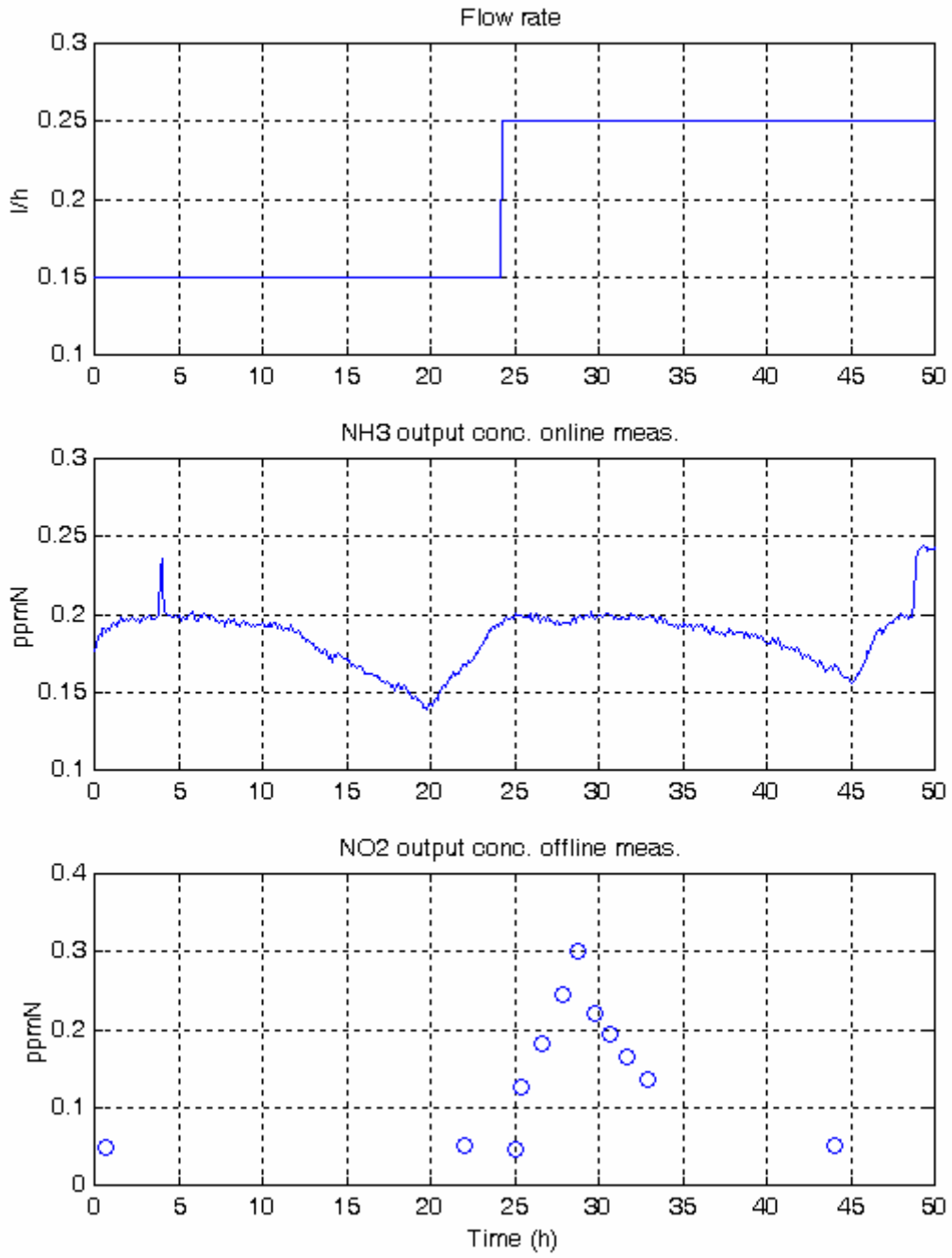
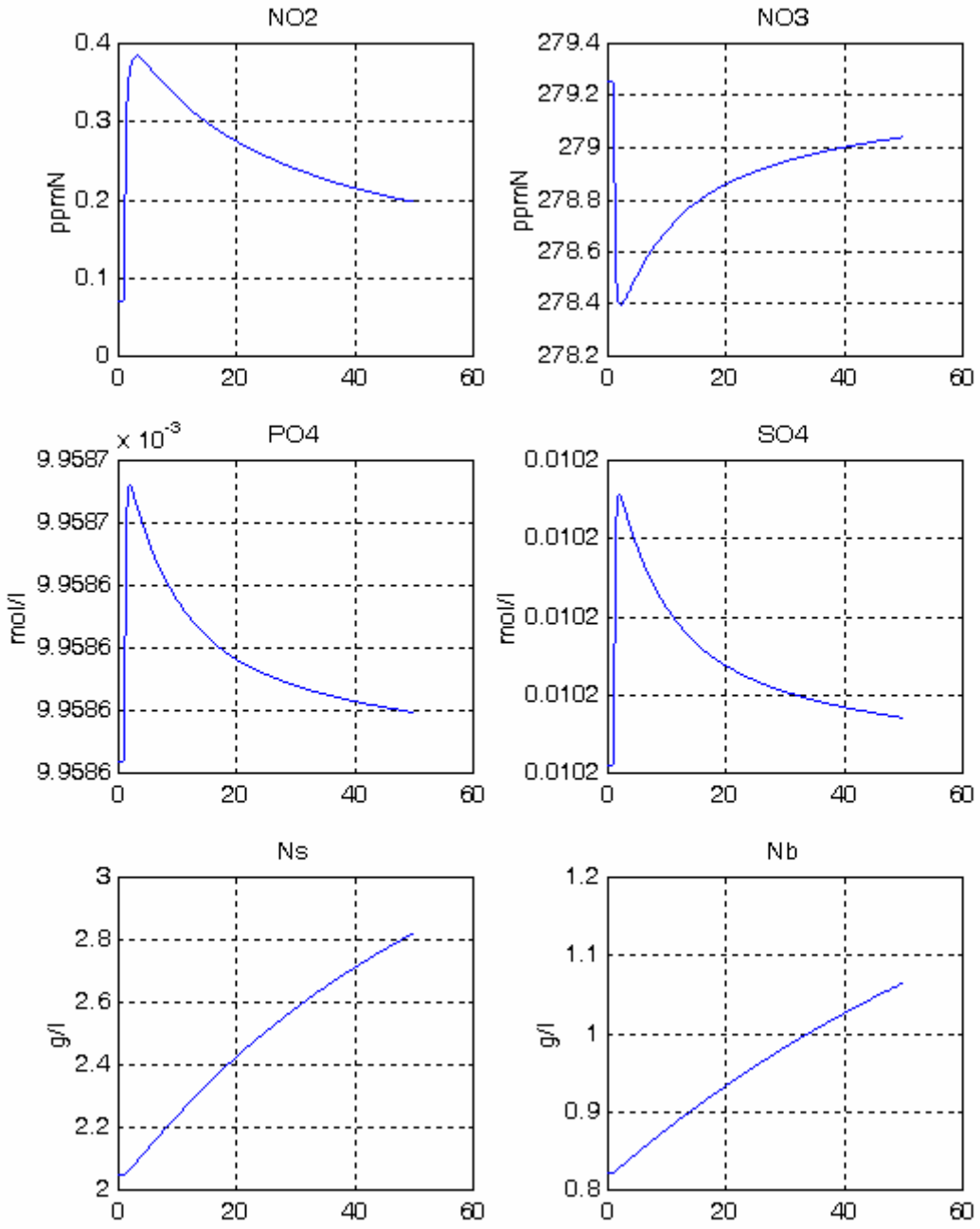
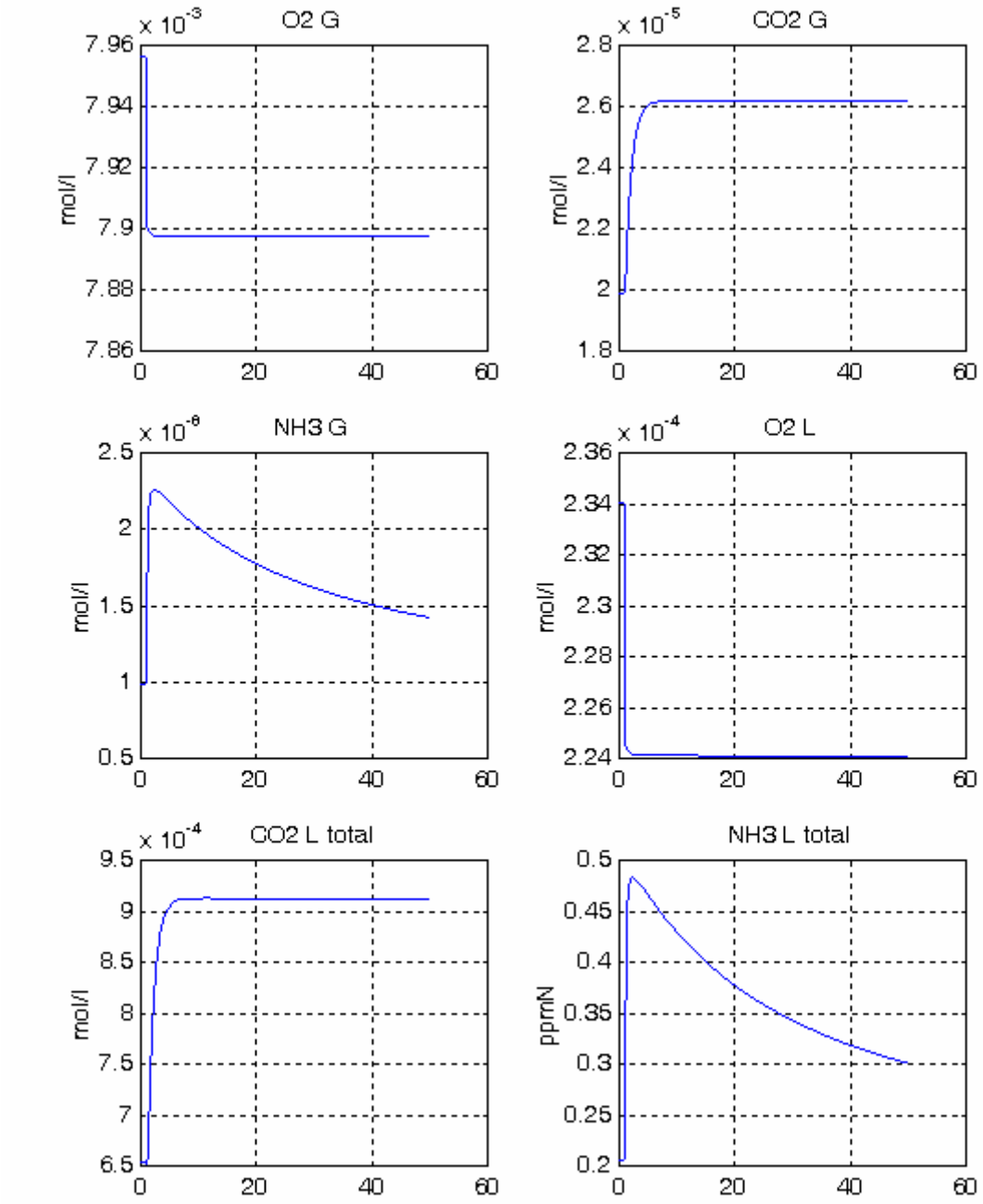


Figure A5.2 : UAB test (flow rate step) March 2003 from 25th to 27th.



Test 16; NO2 half saturation constant and Volume liquid ratio mismatches

Figure A5.3 : Flow rate step from 0.15 to 0.25 l/h at NH3 conc. of 300 ppmN.
NO2 at column output appears on the graph at top left hand side.
the steady state point = 0.07 ppmN (to be compared to 0.05 ppmN in UAB test fig. A5.2)
peak height = 0.38 ppmN (to be compared to 0.30 ppmN in UAB test fig. A5.2)



Test 16; NO2 half saturation constant and Volume liquid ratio mismatches

Figure A5.4 : Flow rate step from 0.15 to 0.25 l/h at NH3 conc. of 300 ppmN. total NH3 at column output appears on the graph at bottom right hand side. the steady state point = 0.2 ppmN (to be compared to 0.2 ppmN in UAB test fig. A5.2) peak height = 0.48 ppmN (to be compared to no peak in UAB test fig. A5.2)