EPAS n.v.
Eco Process Assistance
De Prijkels • Venecoweg 19 • B-9810 Nazareth
Tel. +32 9 381.51.30
Fax +32 9 221.82.18
www.epas.be • epas@epas.be

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	Name		Signature
Prepared by:	Jean Joseph Leclercq		
Checked by:	PM	Noëlle Michel	
Approved by:	BUM	Dries Demey	

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1. Simplified model

1.1 Introduction

The objective was to build a simplified model from the First Principles model elaborated by LGCB on 30 July 2004. It is extracted from the Technical Notes quoted in the section 'Reference' and from direct exchange with the author of the FP model. The simplified model will be used for the optimisation study of the working conditions of the Liquefying compartment.

1.2 Description of the model

1.2.1 Stoechiometry

The global chemical reactions of the process are expressed in the LGCB file 'equations_model.doc' on 16 July 2004. This document is attached in annex 1 and contains the set of equations named '[E1]' to '[E16]' that have been chosen to describe the bio-chemical aspect of the process.
The compounds involved in the process are listed in the following table.

Table 1. Compounds (under their molecular form) involved in the simulated process.

Compound	Meaning
Faeces	Faeces
Wheat	Wheat
Salad	Salad
Potato	Potato
AA	Acetic Acid (CH_3COOH)
PA	Propionic Acid (C_2H_5COOH)
BA	Butyric Acid (C_3H_7COOH)
VA	Valeric Acid (C_4H_9COOH)
CA	Caproic Acid ($C_5H_{11}COOH$)
NH3	ammonia
CO2	Carbon dioxide
SolubleInert	Soluble inert
SolidInert	Solid inert
MonoSacch	Monosaccharide $C_6H_{12}O_6$
AminoA	Amino_A or poolAA $CH_{1.98}O_{0.5122}N_{0.2693}S_{0.00635}$
OMFibre	OM_Fibre
BioDead	Dead biomass
OMCarb	OM_Carb $CH_{1.6667}O_{0.8333}$
OMProt	OM_Proteins $CH_{1.56828}O_{0.3063}N_{0.2693}S_{0.00635}$
OMLip	OM_Lipids $CH_2O_{0.125}$
BioSugar	Bio_Sugar
BioAA	Bio_AA
BioLCFA	Bio_LCFA
BioSugar2	Bio_Sugar2

1.2.2 Biochemical kinetics

The simulator 'awc_ms' on 30 July 2004 introduces 3 types of biochemical kinetics :

- N order reactions;
- Monod/Pirt + non-competitive inhibition + pH effect;
- Lethality reaction..

1.2.2.1 N order reactions

For a N order reaction, the expression of the chemical kinetics is :

$$r = \frac{k}{\alpha} \cdot [S]^n$$

where $[S]$ is the concentration of the substrate S and α its stoechiometric coefficient .

In agreement with the document 'equations_model.doc' and the simulator 'awc_ms', the N order reactions are recapitulated in Table 2.

[E 1] Hydrolysis	$FAECES \longrightarrow 0.00869\ [CHONSP]_{Mono\_sacche} + 0.7654\ [CHONSP]_{OM\_Prot} + 0.1956\ [CHONSP]_{OM\_lipe} + 0.7828\ Inert soluble$
[E 2] OM Carbohydrate hydrolysis	$6\ [CHONS]_{carbohydrates} + 1.5\ H_2O \longrightarrow [CHONP]_{oses}$
[E 3] OM proteins hydrolysis	$[CHONS]_{proteins} + 0.2057\ H_2O \longrightarrow [CHONP]_{poolAA}$
[E 8] Wheat hydrolysis	$WHEAT \longrightarrow 0.24574166[CHONSP]_{OM\_Prot} + 0.05824135[CHONSP]_{OM\_Lip} + 1.95915864[CHONSP]_{OM\_Carb} + 0.04799087[CHONSP]_{Fibre} + 0.60395883\ Inert solide$
[E 9] Potatoe hydrolysis	$POTATOE \longrightarrow 0.3049197[CHONSP]_{OM\_Prot} + 0.02285434[CHONSP]_{OM\_Lip} + 3.53060129[CHONSP]_{OM\_Carb} + 0.08343911[CHONSP]_{Fibre} + 0.33315195\ Inert solide$
[E 10] Salad hydrolysis	$SALAD \longrightarrow 0.74076846[CHONSP]_{OM\_Prot} + 0.18122404[CHONSP]_{OM\_Lip} + 0.99985678[CHONSP]_{OM\_Carb} + 0.20033494[CHONSP]_{Fibre} + 0.46094085\ Inert solide$
[E 16] Fiber hydrolysis	$[CHONSP]_{OM\_Fibre} \longrightarrow 3.9216[CHONSP]_{OM\_Carb}$

Table 2. List and characteristics of the N order reactions

Reaction	k (h^{-1})	S	n
E1	0.2	Faeces	1
E2	0.2	OM_Carb	1
E3	0.2	OM_Prot	1
E8	0.2	Wheat	1
E9	0.2	Potatoe	1
E10	0.2	Salad	1
E16	0.01	OM_Fibre	1

Considering the general expression of the N order reactions :

$\alpha A + \beta B \rightarrow \gamma C + \delta D.$

the variation rates (consumption or production rates) of compounds A, B, C and D are bound to 'r' according to :

$$r = \frac{1}{\alpha'} \cdot \frac{d[A]}{dt} = \frac{1}{\beta'} \cdot \frac{d[B]}{dt} = \frac{1}{\gamma'} \cdot \frac{d[C]}{dt} = \frac{1}{\delta'} \cdot \frac{d[D]}{dt}$$

where α', β' are negative values of α, β and γ', δ' are equal to γ, δ

Particularly in reaction [E2], the consumption of OM_Carb is :

$$\frac{d[OM\_Carb]}{dt} = \alpha' \cdot \frac{k}{\alpha} \cdot [OM\_Carb]^n \quad \text{with } \alpha' = -6 \ , \ \alpha = 6 \quad \text{and } k = 0.2\ h^{-1}$$

1.2.2.2 Monod/Pirt + non-competitive inhibition + pH effect reactions

For these reactions, the general expression of the chemical kinetics 'r' (expressed in g/l/h) is :

$$r = \mu_M \cdot \frac{[S_1]}{k_{S1} + [S_1]} \cdot \frac{[S_2]}{k_{S2} + [S_2]} \cdot \frac{1}{1 + \frac{[S_I]}{k_I}} \cdot [Biomass]$$

In agreement with the document 'equations_model.doc' and the simulator 'awc_ms', the Monod/Pirt reactions are recapitulated in

Table 3. There is no maintenance term.

[E 4] acidogenesis	$1.091\ [CHONSP]ose + 0.1091 NH_3 \longrightarrow 0.1091 [CHONSP]_{Bio\_sugar} + 0.6667 Acetate + 1.3333 Propionate + 0.6667 CO_2 + 0.9939 H_2O$
[E 5] acidogensis	$1.0833\ \ [CHO]_{oses} + 0.1\, NH_3 \longrightarrow 0.1 [CHONSP]_{Bio\_sugar2} + + C3H7COOH + 2\, CO_2 + 0.3\, H_2O$
[E 6] acidogenesis (amino-acids)	$[CHONS]_{poolAA} + 0.3482\ H_2O \Downarrow 0.0241\ [CHONSP]_{Bio\_AA} + 0.16373\ CH_3COOH + 0.0612\ C_2H_5COOH + 0.019\ C_3H_7COOH + 0.0177\ C_4H_9COOH + 0.01734\ C_5H_{11}COOH + 0.11816\ CO_2 + 0.2489 NH_3$
[E 7] acidogenesis (lipids)	$0.95\ [CHON]_{lipids} + 0.05\, NH_3 + 0.68125\, H_2O \longrightarrow 0.05 [CHONSP]_{Bio\_LCFA} + 0.35\, CH_3COOH$

Table 3. List and characteristics of the Monod/Pirt reactions

Reaction	Biomass (g/l)	μ_M (h^{-1})	S_1		S_2		S_I	
				k_S (g/l)		k_S (g/l)		k_I (g/l)
E4	Bio_Sugar	$\frac{0.4}{0.1091}$	NH3	10^{-4}	Mono_Sacch	10^{-2}		
E5	Bio_Sugar2	$\frac{0.1}{0.1}$	NH3	10^{-4}	Mono_Sacch	10^{-4}		
E6	Bio_AA	$\frac{0.21}{0.0241}$			Amino_A	0.01	NH3	0.9
E7	Bio_LCFA	$\frac{0.4}{0.05}$	NH3	10^{-3}	OM_Lip	10^{-3}		

1.2.2.3 Lethality reactions

For these reactions, according to TN74.1 p.11 :
Given the decay reaction : a_1 Biomass → a_2 OM
The biomass decay rate is $r_{Biomass} = -k_D \cdot [Biomass]$

and the OM production is $r_{OM} = \frac{a_2'}{a_1'} \cdot r_{Biomass}$ where a_1' and a_2' are signed $(a_1' < 0 \ , a_2' > 0)$

According to 'awc_ms', there are 4 biomasses involved in the process :

[E 11] Decay biomass	$[CHONSP]_{Bio\_sugar} \longrightarrow [CHONSP]_{Bio\_dead}$
[E 12] Decay biomass	$[CHONSP]_{Bio\_AA} \longrightarrow [CHONSP]_{Bio\_dead}$
[E 13] Decay biomass	$[CHONSP]_{Bio\_LCFA} \longrightarrow [CHONSP]_{Bio\_dead}$
[E 15] Decay Biomass	$[CHONSP]_{Bio\_sugar2} \longrightarrow [CHONSP]_{Bio\_dead}$

Table 4. List and characteristics of the lethality reactions

Reaction	k_D (h^{-1})	Biomass
E11	0.01	Bio_Sugar
E12	0.01	Bio_AA
E13	0.01	Bio_LCFA
E14		non produced
E15	0.01	Bio_Sugar2

1.2.3 Acid-Base dissociation

The acid/base dissociation is taken into account for all the concerned compounds : CO2, NH3 and VFA's.
According to TN 23.1 by LGCB, the acidity constants K_A at 55 °C is reminded in Table 5.

Table 5. Acidity constants

Equilibrium	K_A at 55 °C
CO_2 / HCO_3^-	5.2468e-007
HCO_3^- / CO_3^{2-}	7.0061e-011
NH_4^+ / NH_3	4.0625e-009
AA / AA^-	1.5919e-005
PA / PA^-	1.1718e-005
BA / BA^-	1.2358e-005
VA / VA^-	1.5100e-005
CA / CA^-	1.4300e-005

In the conditions of temperature (55 °C) and pH (pH=5.6), the proportion K of ionic form against molecular one is :

$$K = \frac{[\text{IonicForm}]}{[\text{MolecularF orm}]} = \frac{K_A}{10^{-pH}}$$

K is given in Table 6.

Table 6. Proportion K of ionic form against molecular one

ionic form	molecular form	K
$HCO_3^- + CO_3^{2-}$	CO_2	0.209
NH_4^+	NH_3	618
AA^-	AA	6.34
PA^-	PA	4.67
BA^-	BA	4.92
VA^-	VA	6.01
CA^-	CA	5.69

1.2.4 Gas-Liquid equilibrium

The numerical value of the partition coefficients, k_i, are computed from TN 23.1 by LGCB (p.5 & 10) and gathered in Table 7 for the concerned compounds : NH3, CO2 and VFA's.

Table 7. Partition coefficients k_i

Compound	k_i
CO_2	3082
NH_3	22.7
AA	$9\ 10^{-2}$
PA	$3\ 10^{-2}$
BA	$9\ 10^{-3}$
VA	$3\ 10^{-3}$
CA	$2\ 10^{-4}$

The partition coefficient of CO2 is far bigger than the others. So only CO2 is considered in the gaseous phase, the other compounds (NH3 and VFA's) being not present in the gaseous phase. Measurements on the prototype confirmed that CO2 is the major compound of the gas phase.

1.2.5 Dilution or hydrodynamic behaviour

Given the reactor (of liquid volume V assumed constant) with the filter unit (Figure 1).
Given a compound A whose concentrations at the different places are named :
. 'a_i' at reactor input;
. 'a' at reactor output (and inside the reactor);
. 'a_f' in the filtrate flow;
. 'a_d' in the drain flow (a_d=a because the drain is connected directly to the reactor);
. 'a_r' in the flow off the FU coming back to the reactor.
Given the different flow rates :
. 'q_i' at reactor input;
. 'q' at reactor output;
. 'q_f' at filtrate outlet of the filter unit;
. 'q_d' : drain flow rate.
The variation rate (production or consumption rate) of the compound A inside the reactor due to the biochemical reaction is named 'r_A'. It is function of the kinetics.

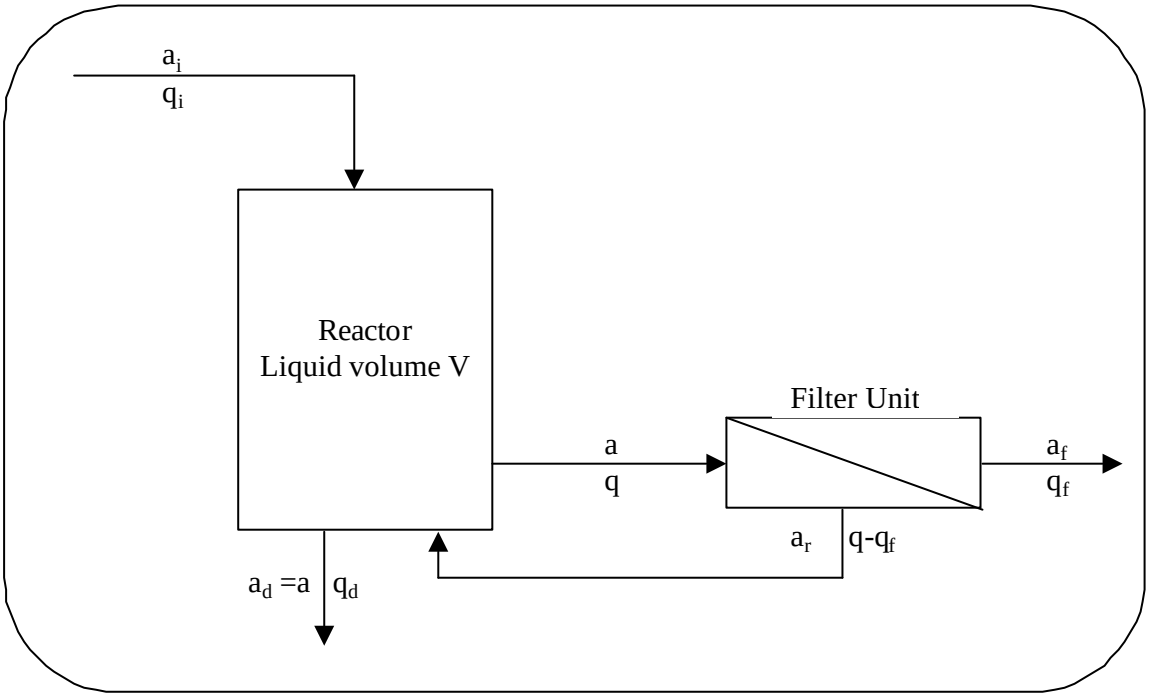


Figure 1. Scheme of the reactor and its filter unit

Equations of the system :
Variation of concentration of A in the reactor :

$$V \cdot \dot{a} = q_i \cdot a_i + (q - q_f) \cdot a_r - (q + q_d) \cdot a + V \cdot r_A \qquad (2.1)$$

The volume is constant $\Rightarrow$

$$q_i = q_f + q_d \qquad (2.2)$$

The mass is balanced instantaneously between inlet and outlets of FU $\Rightarrow$

$$a \cdot q = a_r \cdot (q - q_f) + a_f \cdot q_f \qquad (2.3)$$

Condition on the flow rates :

$$q \geq q_f \qquad (2.4)$$

The 2 types of A are now considered.
In the present study, one makes the simplifying assumption that the effect of the FU on the 'liquid' and 'solid' compounds (that are defined in section 3) is :

- no effect on the concentrations for 'liquid' compounds;
- no solid can go through the membrane.

The compound A is soluble (or 'liquid') in the liquid phase :

$\Rightarrow$ The FU has no effect on the concentrations $\Rightarrow$ $a_r = a$ and $a_f = a$
(and equation (2.3) is trivial).

(2.1) becomes :

$$V \cdot \dot{a} = -a \cdot q_i + a_i \cdot q_i + V \cdot r_A \qquad (2.5)$$

The compound A is insoluble (or solid) :

$\Rightarrow$ The FU is assumed to be fully efficient $\Rightarrow$ $a_f = 0$

(2.3) $\Rightarrow a \cdot q = a_r \cdot (q - q_f)$

(2.1) becomes :

$$V \cdot \dot{a} = -a \cdot q_d + a_i \cdot q_i + V \cdot r_A \qquad (2.6)$$

1.2.6 Dilution and acid/base dissociation

When a soluble compound exists on the 2 forms : ionic and molecular because of acid/base dissociation, equation (2.5) must be modified, considering that r_A is the production or consumption rate of the molecular form only (and not of the molecular form plus ionic form).

Given a' : the concentration of the molecular form of A.

Given K : the proportional factor such that the total of the 2 forms is $K \cdot a'$.

(2.5) becomes :

$$V \cdot K \cdot \dot{a}' = -K \cdot a' \cdot q_i + K \cdot a_i' \cdot q_i + V \cdot r_A$$

$\Leftrightarrow$

$$\dot{a}' = -\frac{q_i}{V} \cdot a' + \frac{q_i}{V} \cdot a_i' + \frac{1}{K} \cdot r_A \qquad (2.7)$$

The concentration of the ionic form of A is $(K-1) \cdot a'$.

A solid compound is not concerned by acid/base dissociation. So (2.6) remains unchanged.

1.2.7 Dilution, acid/base dissociation and gas/liquid equilibrium

The temperature and pressure of gas are assumed constant.

The gas/liquid equilibrium is defined by the law (TN 23.1 p.4 by LGCB) :

$$k_i = \frac{y_i}{x_i} \qquad (2.8)$$

where

k_i is the partition coefficient (constant at given temperature and pressure)

x_i is the molar concentration of the compound i in the liquid phase

y_i is the molar concentration of the compound i in the gas phase

In the present case, according to section 2.4, the gas phase is composed of the CO2 going out of the liquid and of the inert gas (N2) that is used for flushing and can be present, totally or partly, at initialization of a simulation.

Given :

n_{CO2} : number of mole of CO2 in the volume of gas;

n_{N2} : number of mole of N2 in the volume of gas.

As no N2 is produced or consumed by the reactor, n_{N2} is constant all along a simulation and equal to its initial value fixed by the operator (it is assumed that the gas is ideally stirred).
Given c the molar concentration of the molecular form of the concerned gas (CO2) in the reactor at gas/liquid equilibrium.
Its molar fraction in the liquid phase is (assuming the concentrations of all the involved compounds negligible against the concentration of water):

$$x = \frac{c}{n_0}$$

$$\text{with } n_0 = \frac{1000}{18} = 55.55 \text{ mol/l}$$

So relation (2.8) becomes :

$$k_p = \frac{n_{CO2}}{n_{CO2} + n_{N2}} \cdot \frac{n_0}{c} \quad \Leftrightarrow \quad c = \frac{n_{CO2}}{n_{CO2} + n_{N2}} \cdot \frac{n_0}{k_p} \tag{2.9}$$

where k_p is the partition coefficient of CO2 at reactor temperature.

Given b the molar concentration of the dissolved gas (CO2) in the bulk of the reactor.
The flux of gas entering into the liquid is :

$$\Phi = K_{La} \cdot (c - b) \tag{2.10}$$

where K_{La} is the volumetric transfer coefficient of CO2 in liquid phase.
Note : the flux is positive when c>b. When b > c, then CO2 is leaving the liquid phase (degassing).

Taking into account this flux, the mass balance law (2.7), applied to CO2, becomes :

$$V \cdot K \cdot \dot{b} = -K \cdot b \cdot q_i + K \cdot b_i \cdot q_i + V \cdot \Phi + V \cdot r_B$$

where r_B is the variation rate of dissolved CO2.

$\Leftrightarrow$

$$\dot{b} = -\frac{q_i}{V} \cdot b + \frac{q_i}{V} \cdot b_i + \frac{1}{K} \cdot \Phi + \frac{1}{K} \cdot r_B$$

$$\text{with } \Phi = K_{La} \cdot (c - b) \tag{2.11}$$

$$\text{and } c = \frac{n_{CO2}}{n_{CO2} + n_{N2}} \cdot \frac{n_0}{k_p}$$

The molar variation rate of CO2 towards the gas phase is opposite to $V \cdot \Phi$:

$$\dot{n}_{CO2} = -\Phi \cdot V \tag{2.12}$$

where

n_{CO2} is the number of mole of CO2 in the volume of gas.

<u>Remark regarding relations (2.11) and (2.12) :</u>

The condition $n_{CO2} \geq 0$ must be checked when integrating (2.12). That has consequence on relation (2.11) as it follows.

When n_{CO2} is equal to 0, the derivative $\dot{n}_{CO2}$ cannot be negative (otherwise n_{CO2} would become negative after integration).

Or, which is equivalent, when n_{CO2} is equal to 0, the flux Φ cannot be positive; which simply means that, when the CO2 gas volume is null, no CO2 gas can go into the liquid.

So in the relation (2.11) the flux Φ computed by (2.10) must be set to 0 when :

$$n_{CO2} \leq 0 \quad \text{and} \quad c - b > 0$$

$\Leftrightarrow$

$$n_{CO2} \leq 0 \quad \text{and} \quad b < \frac{n_0}{k_p} \qquad (2.13)$$

1.3 Comparison of the simulators

In order to check the simplified simulator, its results have been compared to the results given by the simulator 'awc_ms V2.0.0b' and its associated data delivered on 30 July 2004 by LGCB.

For that purpose, the following modifications have been done on the simulator 'awc_ms' in order to run the simulators in the same conditions (to have the same process parameters on both simulators).

Modification 1 :

As NH3 (and not NH_4^+) is implied in the chemical reactions, it has been added to the previous 46 compounds. The stoechiometry of NH3, instead of NH_4^+, has been introduced accordingly in the reactions E4, E5, E6 and E7.

Modification 2 :

The acid/base dissociations have been considered for AA, PA, BA, NH_4^+ and $CO2/HCO_3^-$ in addition to the existing dissociations for VA and CA. The dissociation HCO_3^-/CO_3^{2-} has been omitted because it introduces an error in the computation of solvated CO2 .

Modification 3 :

The molar masses of NH_4^+, OM_Carb and Amino_A have been set to their correct value.

Modification 4 :

The partition coefficient of CO2 has been set to 3082 at 55 °C (instead of 2837 at 0 °C) accordingly to the formula established in TN23.1 by LGCB..

Modification 5 :

The liquid flow rate at reactor output has been set at 450 l/h (instead of 3 l/h) as it is the case on the EPAS prototype reactor.

The inputs and the initial state are the same on both simulators and are remembered hereafter (Table 8 and Table 9).

The input and filtrate flow rates are equal to 0.07875 l/h. The drain flow rate is null.

Table 8. Input concentrations.

Compound	Input concentration (g/l)
Faeces	3.968
Wheat	7.936
Salad	7.936
Potato	7.936
AA	0.091
PA	0.018
BA	0.021
VA	0.006
CA	0.007
NH3	0.025

The concentrations of the dissociated compounds are given for the total form.

Table 9. Initial state concentrations

Compound	Input concentration (g/l)
Faeces	0
Wheat	0
Salad	0
Potato	0
AA	2.03
PA	0
BA	2
VA	0.047
CA	0.1
NH3	0
CO2	0
SolubleInert	0
SolidInert	0
MonoSacch	0
AminoA	0
OMFibre	0
BioDead	0
OMCarb	0.05
OMProt	0.02
OMLip	0
BioSugar	10^{-3}
BioAA	10^{-3}
BioLCFA	10^{-3}
BioSugar2	10^{-3}

.

The concentrations of the dissociated compounds are given for the total form.

The liquid compounds are :
AA, PA, BA, VA, CA, NH3, CO2,iMonoSacch, AminoA, SolubleInert.
The solid compounds are :
Faeces, Wheat, Potato, Salad, OMProt, OMLip, OMCarb, OMFibre, BioSugar, BioSugar2, BioAA, BioLCFA, BioDead, SolidInert.

What is simulated is the addition of 125 g of AA- at time t=720 h and the addition of 55 g of NH_4^+ at time t=2256 h as it is done in the 'awc_ms' on 30 July 2004.

Both simulators give the same results globally as one can check on the plotting of annex 4 (figures A4.1 to A4.25). For each compound, the results of the simplified simulator and of the 'awc_ms' simulator are plotted in the upper and lower graphs, respectively. However, a few slight differences can be observed :

- In figure A4.11 the dynamic of CO2 is a little bit quicker in 'awc_ms'. There is no confirmed explanation.
- In figure A4.25 the production rate of CO2 gas falls to zero in 'awc_ms' because simulation is interrupted for the impulses of acetate and ammonium.

Comparison of running times :
The running time has been measured on a PC equipped with a Pentium 4 CPU 2.4 GHz. The test consists in the computing of the above simulation.

1.3.1.1 Simulator	**Running time**
awc_ms with 152 ODE's	30.5 mn
simplified simulator with 25 ODE's	6 s

The 'simplified simulator' is about 300 times as quick as 'awc_ms'.

1.4 Conclusions

Both simulators 'awc_ms' and 'simplified simulator', give the same results when they run in the same conditions.
The system of Ordinary Differential Equations has been reduced from 152 to 25.
The Acid/Base dissociation reactions are assumed very quick in 'awc_ms' (where the kinetics constants of these reactions are set to 10^6 h) and instantaneous in the 'simplified model', which allows the sampling period to be greater in the last case because the high frequency signals are cancelled out.
Consequently the running time of the 'simplified simulator' is highly decreased : it is 300 times as quick as 'awc_ms'.

This simplified simulator was used to study the general technical specifications of the Control Command System in one hand and, in the other hand, the analysis of the physical system.

2. Technical specifications of the Control Command System

The control is in charge of the process after manual starting around a steady state point of functioning. The control does not take into account a deteriorated functioning of the reactor (for example when the temperature or the pH is out of range or when a sensor or an actuator is out of work).

2.1 Introduction

This section gathers :

- the CCS technical specifications already elaborated on June 2004 in the document 'EWC_ControlFunctionAnalysisV3.doc'. This last document is obsolete from now on.
- the tests plan for the validation of the specifications : plan for the tests of the performances and compliance with the constraints.

2.2 Description of the process and of the functioning scenario

The process is composed mainly of a bioreactor and a filtration unit. The waste (solid particles) is mixed apart in a specific vessel. The resulting mixture and water are introduced in the influent tank before being transferred into the reactor. The products are extracted via the gas and liquid output flows. A drain is performed regularly to prevent accumulation of solid (particles and biomass).

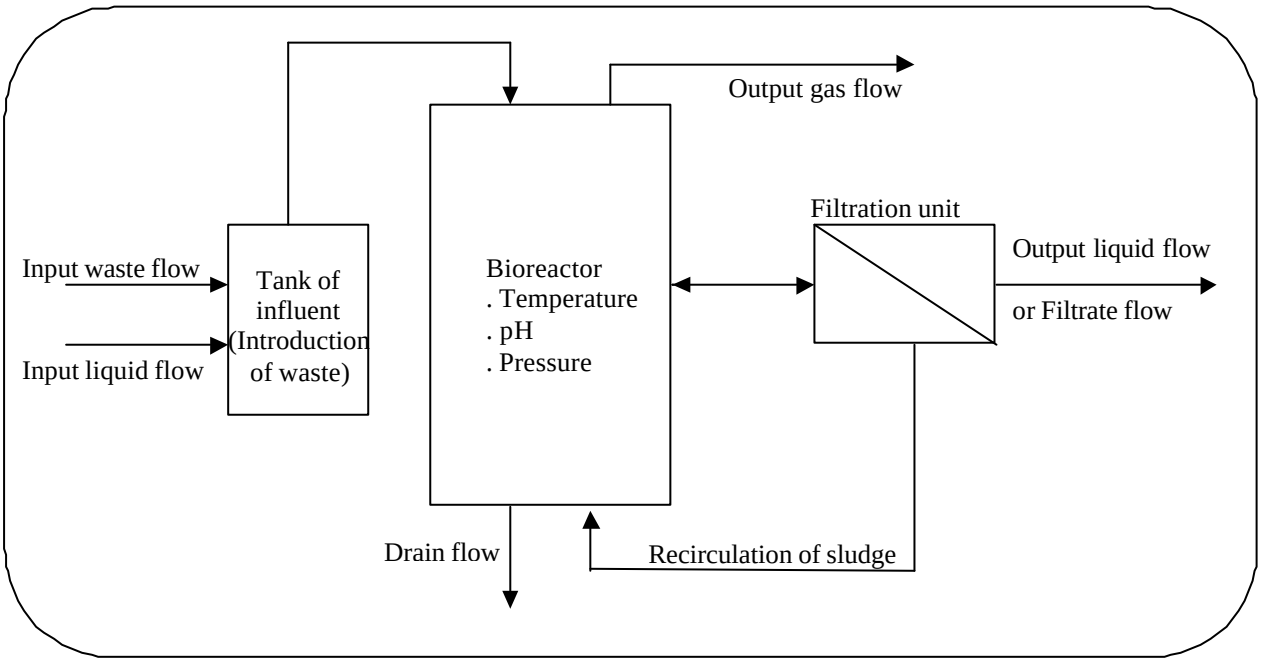


Figure 2. Representation of the first compartment

2.3 External functional analysis

2.3.1 Main functions

The aim of the control is to maintain the operating conditions so that the Liquefying compartment:

- degrades the maximum of OM (solid and soluble compounds: non edible parts of plant material (lettuce, beet, wheat straw), human faecal matter and toilet paper);
- produces the maximum of ammonia and VFA without inhibiting the transformation reactions.

2.3.2 Constraints functions

The control has to fulfil the main functions regarding the following constraints:

- the reactor must produce the minimum of methane because methane cannot be consumed in the other compartments of the MELISSA loop;
- the reactor must produce the minimum of hydrogen for safety reason and to avoid the hydrolysis inhibition and the conversion inhibition of propionic and butyric acids into acetic acid.

The requirement of maximum solid degradation has to be compliant with a maximum solid concentration due to the operating condition of the filtration unit.

The production of NH_4^+ has to be optimised between 0 and a maximum constraint to avoid hydrolysis inhibition.
The low production of methane is ensured by means of the pH.
The production of H2 is actually not controlled. It is expected that H2 will be removed by gas/gas exchange.

At this step of the study, the conditions of temperature, pressure and pH are pre-selected and the level 1 control is not in charge of optimising them. This optimizing function will be required when the process knowledge has increased and when the modelling is able to quantify the effects of these variables on the process.

2.4 Control system architecture

In the present study, the temperature, pH and pressure of the reactor are fixed parameters and the optimiser is not in charge of optimising them. This will be done in a further study and it is recalled for the record.

2.4.1 Present study

Maximising the VFA production is equivalent to maximising the OM degradation and the NH_4^+ and CO2 productions. So given the nominal input waste flow rate, the VFA production is the only one criterion to optimize.

The optimiser takes into account the constraints (maximum NH_4^+ concentration, maximum OM matter concentration) and the process data in order to compute the VFA setpoint, at any moment.
The 2 main VFA are acetic and butyric acids whose sum of concentrations is about 90 % of the total VFA.

2.4.1.1 Optimiser and Level 1 control

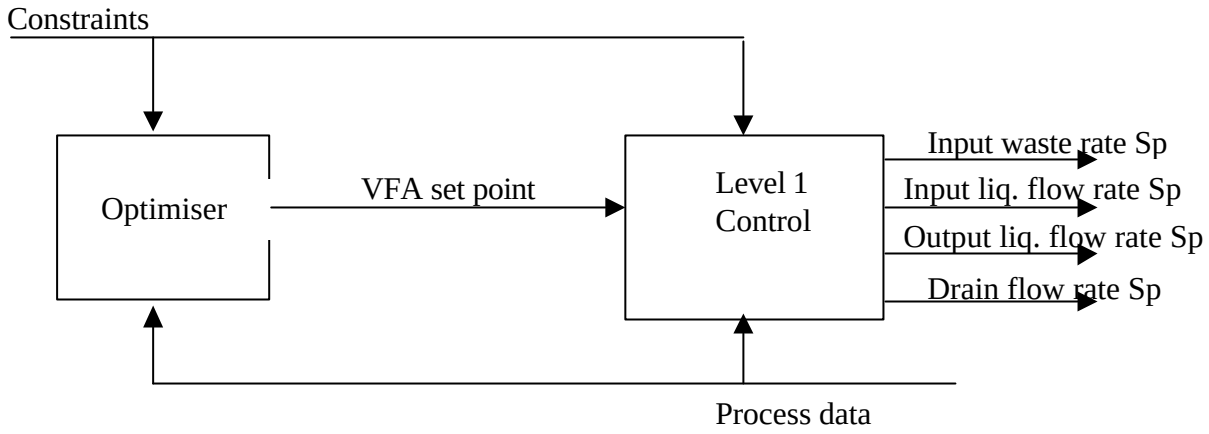


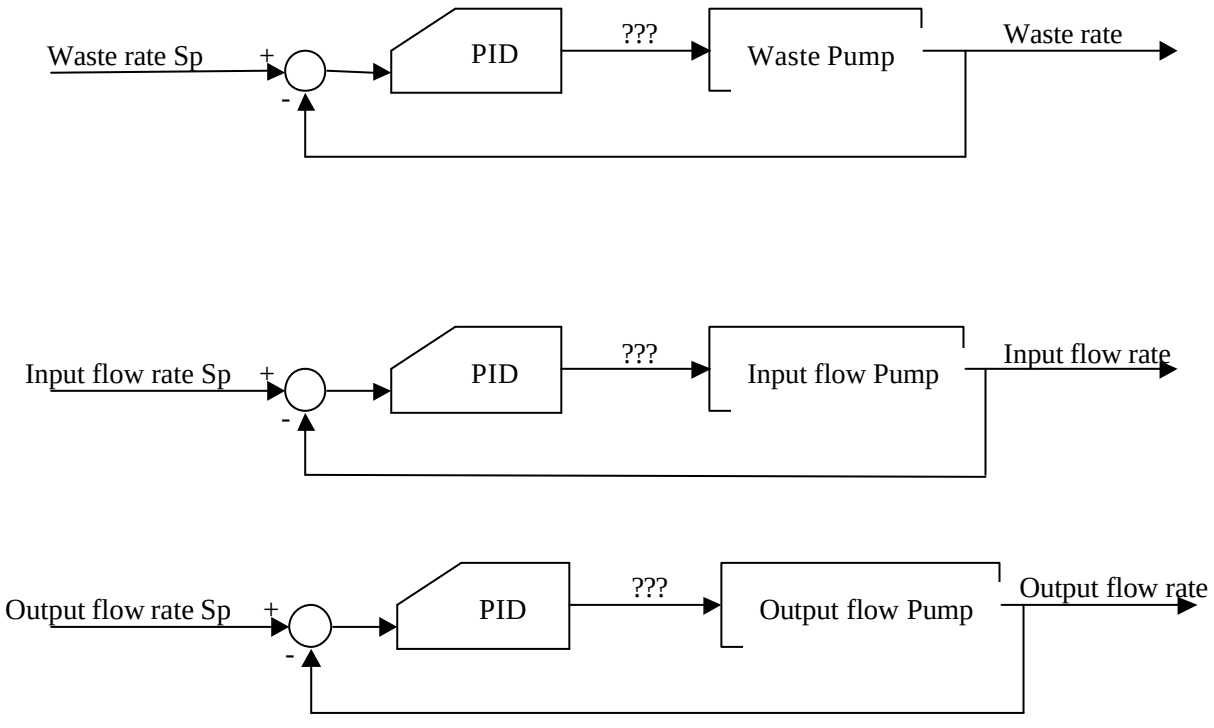
Figure 3. Control architecture: Optimiser and level 1 control

2.4.1.2 Level 0 controls

List of the Level 0 Controlled Variables:

- Waste rate
- Input liquid flow rate
- Filtrate flow rate
- Drain flow rate
- Reactor temperature
- pH
- Pressure.

The following closed loop systems are designed for the record.



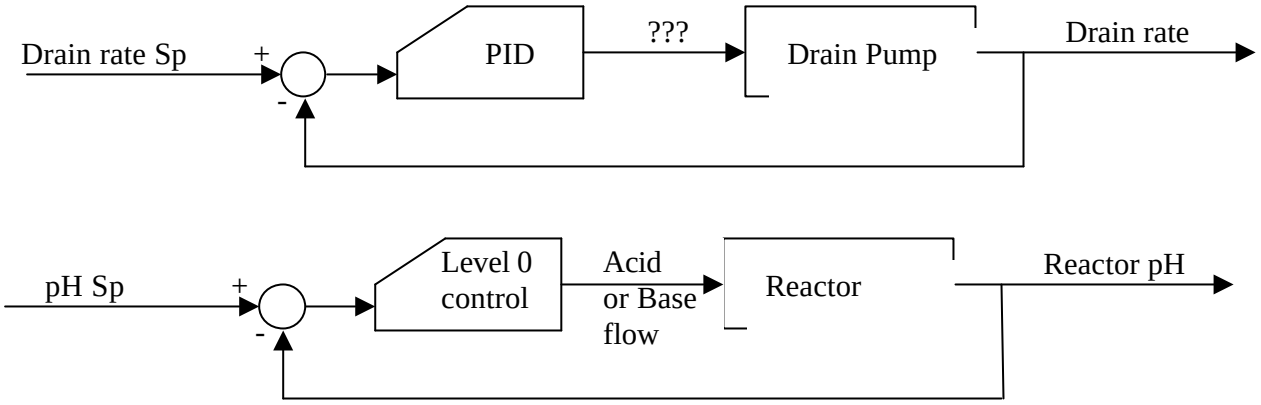


Figure 4. Level 0 controller

The '???' means that the manipulated variable computed by the PID is not specified (it could be the rotation speed of a volumetric pump for example)

2.4.2 Further study

In a further study, the temperature and pH setpoints will be variable and no more constant. The optimiser will have 2 more degrees of freedom to fulfil the high level requirements.

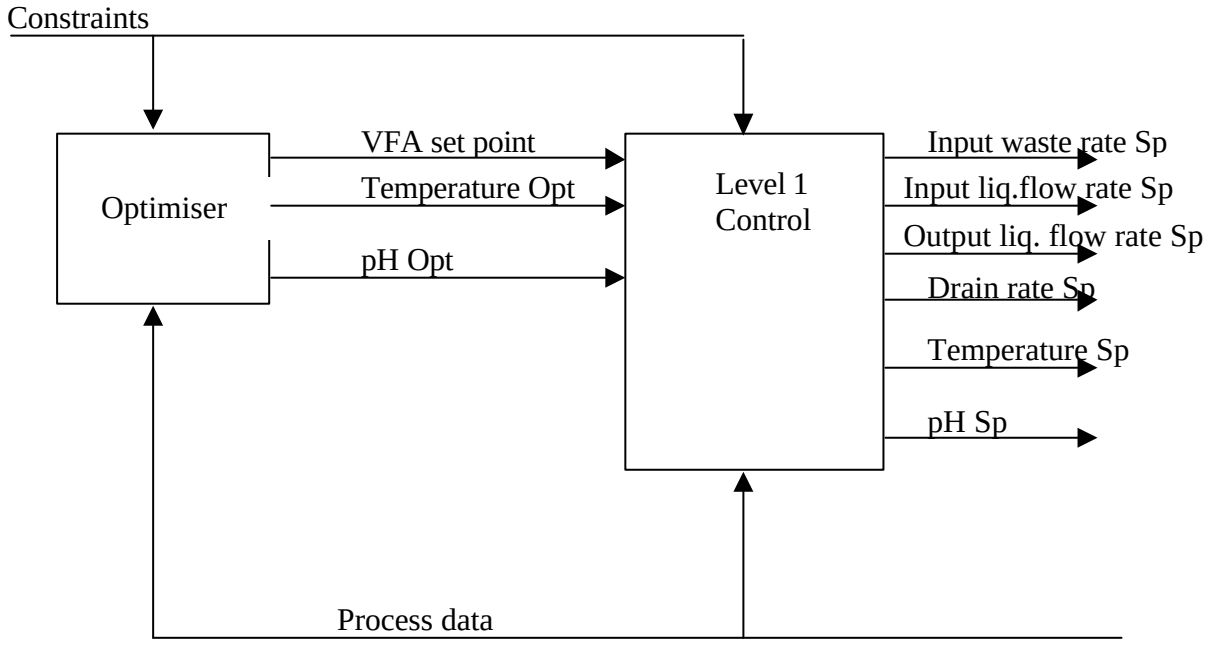


Figure 5. Future control architecture: Optimiser and level 1 control with 2 more freedom degrees (temperature and pH)

2.5 Criteria and qualitative parameters bound to the requirements of the external functional analysis

The requirement 'Max VFA production' is equivalent to the 'Max OM degradation', 'Max NH_4^+ production' and 'Max CO2 production' requirements.
So only the requirement 'Max VFA production' must be fulfilled by the control. The 3 other ones will follow. This will be checked.

2.5.1 Requirement 'Max VFA production'

Each VFA production rate r_{VFA} is measured in mg cumulated on a given time period Δt:

$$r_{VFA} = \frac{VFA_{eff} - VFA_{inf}}{\Delta t}$$

where VFA_{eff} is the cumulative amount of VFA during Δt in effluent;
VFA_{inf} is the cumulative amount of VFA during Δt in influent.

The criterion to be optimised is the sum of the production rate of the main VFA. According to the present tests results, these VFA are acetic and butyric acids that represent 90% of the total VFA. This choice may change in case of shift in the VFA proportion.
According to [4], the cumulative time period Δt is defined as (at the moment):

$$1 \le \Delta t \le 7 \text{ days}$$

This definition is expected to evolve by means of the simulator.
For optimisation, the prediction horizon is foreseen to be 30 days. The control sampling period is foreseen to be 1 day. These values will be checked on the simulator.

The optimiser and the level 1 control are in charge of the requirement under the following constraints:

- the solid concentration limited by the operating condition of the filtration unit.
- the NH_4^+ maximum concentration to avoid hydrolysis inhibition.

One of the manipulated variables is the input waste flow rate that will vary around its nominal value. But its mean value on a significant period should be equal to 210 gDM/day for the 100 l reactor (and the quarter of 210 gDM/day for the 25 l prototype). This period is such that the corresponding max volume of storage is about 2-3 days of nominal waste input flow rate.

It is already known that the temperature and the pH have an influence on the production of VFA and NH_4^+. On the present study they are constant.

2.5.2 Requirement 'Max OM degradation'

There are two possible ways for the definition of the solid degradation efficiency. It has to be noticed that these formulas are based on a simplified model of the effective efficiency, since some variables (such as intermediary degradation products or soluble, non-VFA species, ethanol, lactate...) are not included in the calculations. These formulas could be thus adapted in the future.

1. Biological biodegradation efficiency

$$h_{OM1} = \frac{OM_{biod}}{OM_{inf}} = \frac{(VFA_{eff} - VFA_{inf}) + CO_2 + CH_4}{OM_{inf}}$$

Where:

- h_{OM1} = OM biological degradation efficiency

- OM_{biod} = cumulative biodegraded OM mass (mg)

- VFA_{inf} = cumulative VFA mass at input of the reactor (mg)

- CO_2 = cumulative mass of CO2 produced (mg)

- CH_4 = cumulative mass of CH4 produced (mg)

Remark: In the formula above, instead of mg, a better measurement unit would be the number of C (Carbon) mole.
When there is no production of VFA, CO_2 or CH_4, the efficiency η_{OM1} is zero. And when all the organic matter is degraded, the efficiency should be 1.

- **2. Biological degradation and mechanical removal efficiency:**

$$h_{OM2} = \frac{OM_{\inf} - OM_{eff}}{OM_{\inf}}$$

Where:

- h_{OM2} = OM biological degradation and mechanical removal efficiency

- OM_{eff} = cumulative mass of organic matter in effluent (mg)

The optimiser and the level 1 control are not in charge of the requirement. It will be followed by computing the 2 above efficiencies.

2.5.3 Requirement 'Max NH_4^+ production'

There are three possible ways for the definition of nitrogen degradation efficiency:

- **1. Nitrogen biodegradation efficiency**

$$h_{N1} = \frac{Norg_{biod}}{Norg_{\inf}} = \frac{NH4_{eff} - NH4_{\inf}}{Norg_{\inf}}$$

Where:

- h_{N1} = nitrogen biodegradation efficiency

- $Norg_{biod}$ = cumulative biodegraded organic nitrogen mass (mg)

- $Norg_{inf}$ = cumulative organic nitrogen mass in influent (mg)

- $NH4_{inf}$ = cumulative ammonium mass in influent (mg)

- $NH4_{eff}$ = cumulative ammonium mass in effluent (mg)

- **2. Nitrogen biodegradation and mechanical removal efficiency:**

$$h_{N2} = \frac{Norg_{\inf} - Norg_{eff}}{Norg_{\inf}}$$

Where:

- h_{N2} = nitrogen biodegradation and mechanical removal efficiency

- $Norg_{eff}$ = cumulative organic nitrogen mass in effluent (mg)

- **3. Proteins removal efficiency**

$$h_{prot} = \frac{prot_{\inf} - prot_{efff}}{prot_{\inf}}$$

Where:

- h_{prot} = proteins removal efficiency

- $prot_{inf}$ = cumulative proteins mass in influent (mg)

-$prot_{eff}$ = cumulative proteins mass in effluent (mg)

The optimiser and the level 1 control are not in charge of the requirement. It will be followed by computing the 3 above efficiencies.

2.5.4 Requirement 'No methane production'

The production of methane should be avoided because no compartment of the MELISSA loop is designed to consume this compound. In fact this objective cannot be fulfilled and the acceptable CH4 concentration level is 1 % max.
So adequate operating conditions are defined to the process, particularly the pH must be maintained in a given range defined in the following section.
A level 0 control is in charge of the pH by adding an acid or a base into the reactor.

2.5.5 Requirement 'Minimum hydrogen production'

This requirement cannot be fulfilled by the optimiser and the level 1 control. The hydrogen production depends on pH also. A trade off is necessary; when pH increases, CH4 production increases and H2 production decreases.

2.6 Global description of the control system

2.6.1 Inputs and outputs of the optimiser

2.6.1.1 Inputs

The inputs of the optimiser are the following constraints (defined in Table 10) and the process data (Table 11).
Constraints:

Table 10. Quantification of the constraints

Constrained Variable	Constraint value	Admissible overshoot duration	Reason of constraint
NH_4^+_Max	3 g/l max	1 sampling period (1)	Inhibition of acidogenic bacteria
VFA_Max	To be optimised with the simulator (3)	1 sampling period (1)	Auto-inhibition of VFA hydrolysis
Suspended Solid_Max (2)	45 gDM/l max	1 sampling period (1)	Filtration unit requirement

(1) : sampling period is 2 hours on the pilot reactor (100 l) and 2 days on the prototype (25 l).
(2) : suspended solid is a specific measurement expressed in dry matter.

(3) : complementary information : the inhibition due to VFA is starting at 2000-3000 mg/l.

The nominal zone for NH_4^+ is 0.1-0.5 g/l where no inhibition is to be afraid of.
The nominal zone of the solid concentration is 25-35 gDM/l. The idea that the study will confirm probably is to stabilise the solid to the highest possible value and to minimise the drain flow rate (in order not to remove non-degraded matter). The minimization of time to reach stabilisation is not an objective for the control.

Process data: measured concentrations and flow rates.

Table 11. Process data for the CCS

List of the measured process data
Waste flow rate
Input flow rate
Filtrate flow rate
Drain flow rate
Gas flow rate
Influent composition
Solid concentration in the reactor
NH_4^+ in the filtrate flow
VFA in the filtrate flow
CO2 in the gas output flow
CH4 in the gas output flow

A particular input of the reactor is the influent composition (Table 3). The mixture is prepared in sufficient amount to feed the reactor during one week. In fact the composition is not measured on line but is assumed constant and known (except the noise).

Table 12. Influent composition

	Nominal	**Variation range**	**Constraint**
Influent composition	Lettuce : 26 % DM Beet : 26 % DM Wheat straw : 26 % DM Toilet paper : 8 % DM Faecal material : 14 % DM	Will be measured and delivered by EPAS.	None

2.6.1.2 Outputs

The output is VFA_Sp.

2.6.2 Inputs and outputs of the level 1 control

2.6.2.1 Inputs

All the inputs of the optimiser are also inputs of the level 1 control. A supplementary input is the output of the optimiser:

Table 13. Inputs of the level 1 control

Input	**Nominal**
VFA_Sp	To be optimised below the constraint

2.6.2.2 Outputs

Table 14. Outputs of the level 1 control

Outputs	Nominal	Absolute Constraints
Input waste rate Sp	210 DM/day (1)	none
Input flow rate Sp (Q_{in})	10 l/day (1)	none
Output liquid flow rate Sp	Q_{in} -Q_{drain}	[0 20-80] l/day (1)
Drain flow rate Sp (Q_{drain})	[0.4 - 1] l/day (1)	none

(1): values for the pilot reactor corresponding to clogged (20 l/day) or clean (80 l/day) filter. They are 4 times as small for the prototype.

Remark: the different liquid flow rates (that are computed by the level 1 control) are bound by a constraint on the volume of liquid inside the reactor. The nominal volume is 100 l and the bounds are: [80 120] litres for the pilot reactor (These values are 4 times as small for the prototype).

The drain strategy (frequency and volume) is an important issue for the process. In the present study the drain flow rate is considered continuous. In a future study, the consequences of a discontinuous drain flow rate should be investigated (particularly the consequence on the 'maximum solid concentration' constraint).
The introduction of waste is semi-continuous (the suitable amount every hour).
The withdrawing of liquid is done every hour, and of drain every day.

2.6.3 Inputs and outputs of the level 0 controls

Each level 0 control is one input / one output control.

Table 15. Inputs of the level 0 controls.

Inputs	Outputs	Constraint on outputs
Input waste rate Sp	?	?
Input liq. flow rate Sp	?	?
Output liq. flow rate Sp	?	?
Drain flow rate Sp	?	?
Temperature Sp	Warm water recirculation	?
pH Sp	Acid or base flow rate	?
Pressure Sp	Compressor and valve	?

Recall of the nominal and constraint values of temperature, pH and pressure :

Table 16. Variation range of temperature, pH and pressure.

Variables	Nominal	Constraint	Reason of constraint
Reactor temperature	55	[53 57]	Optimisation of acidogenesis, inhibition of pathogens.
pH	5.6	[5.5 5.8]	To avoid methanogenesis
Pressure	100 mbar	[50 100]	To avoid O2 introduction into the reactor

2.7 Tests plan for validation of the CCS specifications

The tests must check that the constraints on solid and NH_4^+ concentrations are respected in the previously defined conditions (Table 10). As the present model does not describe the production of CH4 and H2, the checking of these constraints does not make sense. The tests must also check that the requirement 'Max VFA production' is fulfilled. The other secondary requirements 'Max OM degradation' , 'Max NH_4^+ production' and 'Max CO2 production' will be checked too.

It is foreseen to proceed in 2 successive steps :

- checking the constraints without taking care of the optimisation;
- checking optimisation with respect of the constraints.

Checking the constraints without taking care of the optimisation

The aim of these tests is to check the specific part of the CCS that is in charge of the constraints.
Making a variable stay under a max constraint is equivalent to assign the variable to a setpoint that is lower than the max constraint. The distance between the setpoint and the constraint depends on the fluctuations magnitude of the variable around its setpoint and on the authorized overflow of the constraint (if a constraint can be transgressed from time to time, the setpoint can be nearer the maximum than if the constraint must never be overflowed).
This is illustrated in Figure 6 and Figure 7.

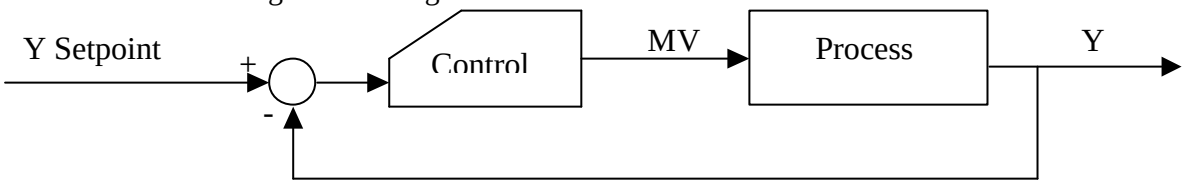


Figure 6. Control of a constraint Y

The setpoint of Y is set at a adequate distance of the constraint value.

The tests of a constrained variable control (solid or NH_4^+ concentration) will consist in steps of constraint value. The Manipulated Variable (MV) will be one of the following variables : drain flow rate, input flow rate or filtrate flow rate. The controller will be tuned so that the constrained variable respects its maximum value in the previously defined conditions (Table 1).
At this step of the study, the tests will be done with the simplified model elaborated by Sherpa running on simulator.

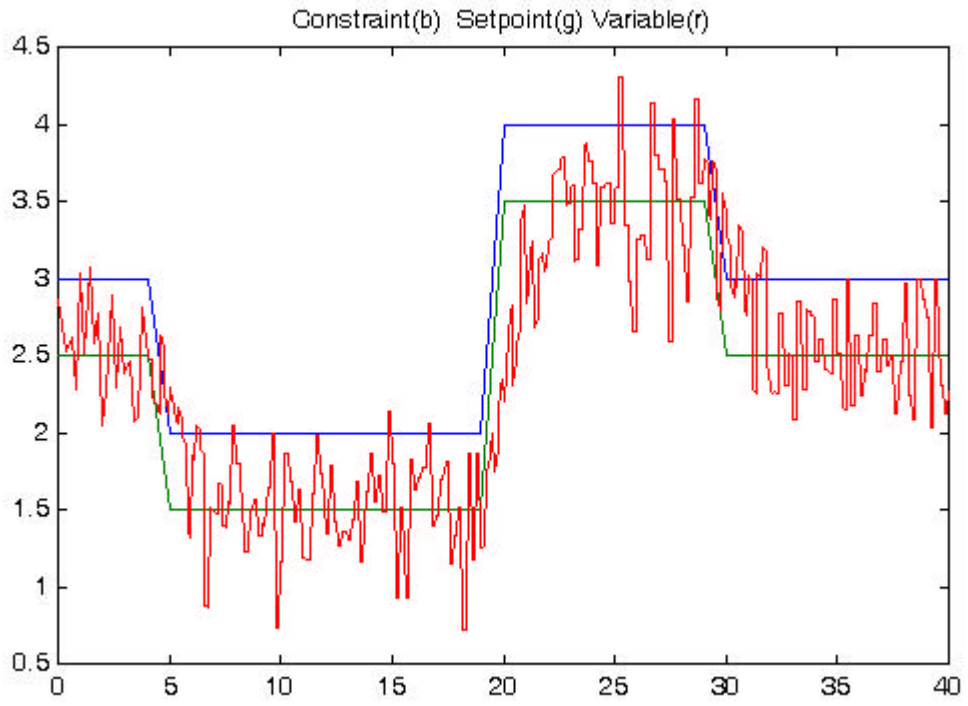


Figure 7. Foreseen test of constraint control (X and Y values are arbitrary).

Checking the optimisation with respect of the constraints

An optimisation study will be done with the simplified model running on simulator. This study will establish the operating conditions that are necessary to have the optimum functioning of the simulated process (reactor and filtration unit).

The aim is to check that the CCS, tested on simulator in equivalent operating conditions environment, is able to make the simulated process work at the theoretical optimum.

The simulated operating conditions will be steps of waste concentrations and of input flow rate (Figure 8). The amplitude of the steps will be 50 % of the nominal functioning and the length will be one and a half response time.

Note : One reminds the definition of the response time (more rigorously, the 95 % response time) of a transfer between an input and an output. When a step is applied to the input, it is the time past until the output reach, in a stable way, 95 % of its incremental variation at infinite.

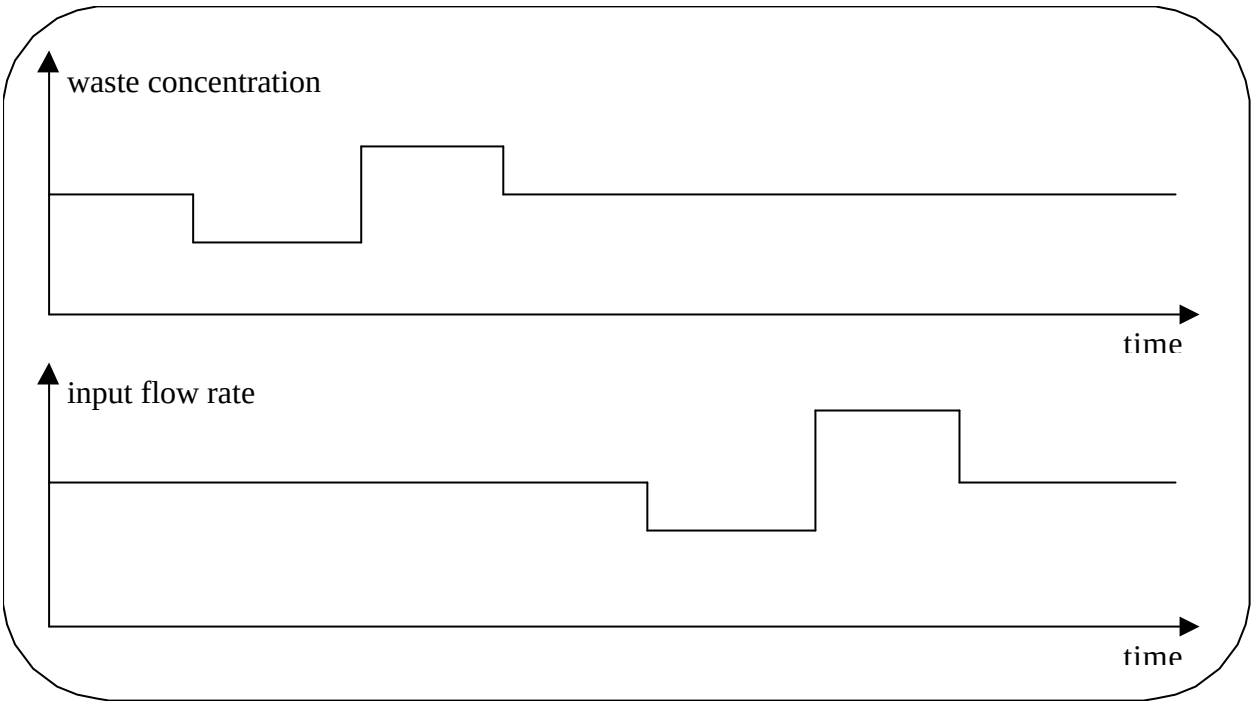


Figure 8. Foreseen test of CCS.

2.8 Conclusion

The expected specifications of the Control Command System are defined now. The CCS that will be built and tested in a future study will have to respect them. The way it will be tested is defined.

3. Analysis of the physical system

3.1 Introduction

A simulator of the process has been built from the LGCB First Principles model of the Liquefying Compartment (reactor and filtration unit).
The aim of this section is to analyse the simulated process before the optimisation study of its working conditions.

Among all the reactions of the model ([E 1] to [E 16] recalled in section 5), the reactions [E 4] and [E 5] (gathered in Table 17) have same kinetics type (Monod/Pirt type) and have same substrates: MonoSacch and NH3. No other reaction has the same substrates together. Reaction [E 7] consumes also NH3; but it is assumed in a first step that it is negligible and it will be taken into account for the study of the whole process [E 1] to [E 16] (justification is detailed in annex).

Table 17. Sub-process limited to biomasses BioSugar and BioSugar2

[E 4] acidogenesis	$1.091\ \mathrm{MonoSacch} + 0.1091\mathrm{NH_3} \longrightarrow 0.1091[\mathrm{CHONSP}]_{\mathrm{BioSugar}} + 0.6667\mathrm{Acetate} + 1.3333\mathrm{Propionate} + 0.6667\mathrm{CO_2} + 0.9939\mathrm{H_2O}$
[E 5] acidogenesis	$1.0833\ \mathrm{MonoSacch} + 0.1\mathrm{NH_3} \longrightarrow 0.1[\mathrm{CHONSP}]_{\mathrm{BioSugar2}} + \mathrm{C3H7COOH} + 2\,\mathrm{CO_2} + 0.3\,\mathrm{H_2O}$
[E 11] Decay biomass	$[\mathrm{CHONSP}]_{\mathrm{BioSugar}} \longrightarrow [\mathrm{CHONSP}]_{\mathrm{BioDead}}$
[E 15] Decay Biomass	$[\mathrm{CHONSP}]_{\mathrm{BioSugar2}} \longrightarrow [\mathrm{CHONSP}]_{\mathrm{BioDead}}$

When one adds to the previous reactions [E 4] and [E 5], the biomass degradation reactions [E11] and [E15], these 4 reactions together can be treated as a group isolated from the other reactions.
So it appears interesting to study this group composed of these 4 reactions as a sub-process apart from the whole process (Figure 9) in order to see if one biomass will prevail over the other and in what conditions. As it will be seen, one biomass among the two disappears from the medium and the related reactions can be eliminated from the list.

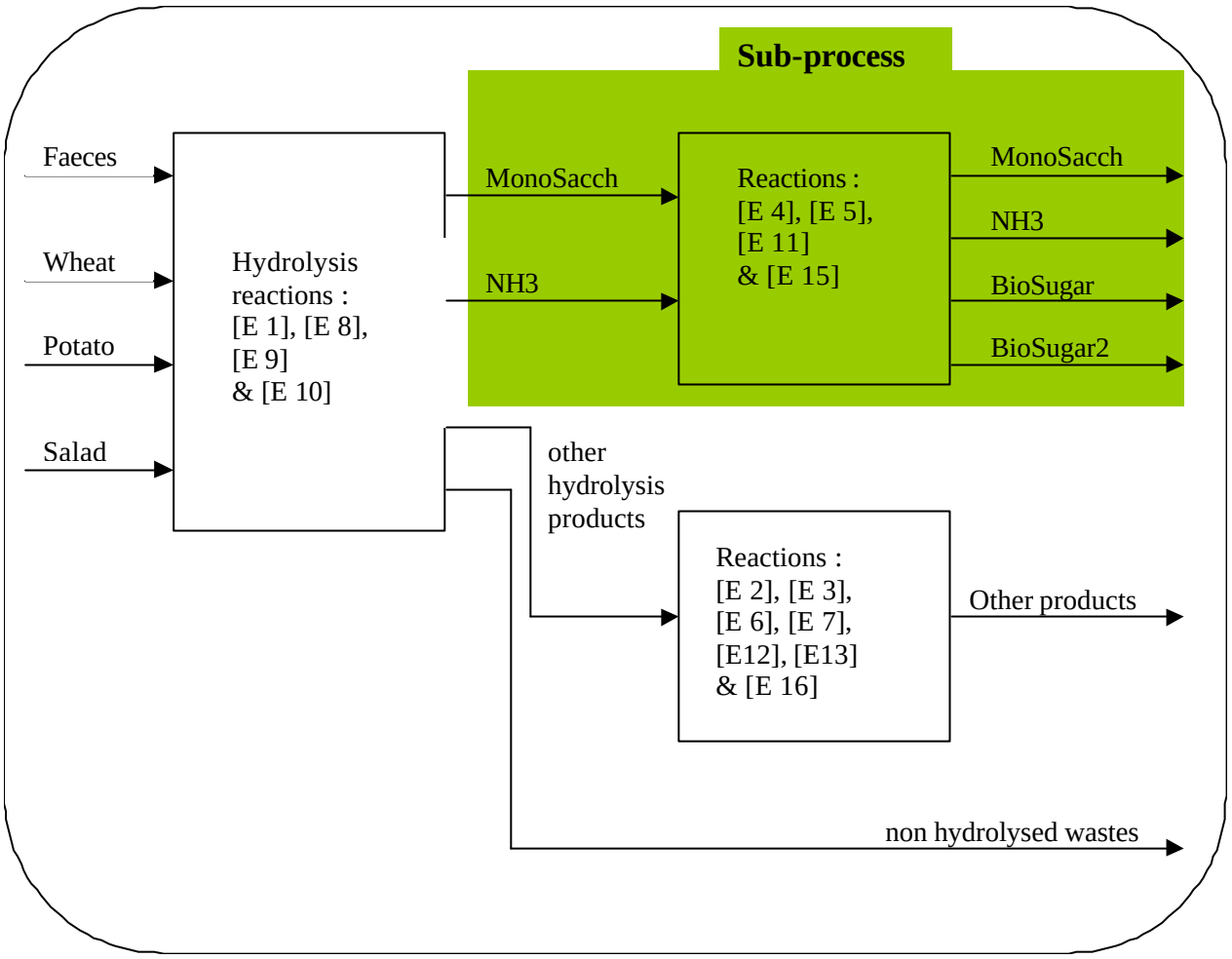


Figure 9. Limits of the studied sub-process (green area) inside the whole process

Then the study will take an interest in :
- description of the steady state of the whole process (reactions [E 1] to [E 16]);
- description of the response times of the transfers input/output.

Note : One reminds the definition of the response time (more rigorously, the 95 % response time) of a transfer between an input and an output. When a step is applied to the input, it is the time past until the output reach, in a stable way, 95 % of its incremental variation at infinite.

3.2 Study of the sub-process defined by the reactions E4, E5, E11 & E15

3.2.1 Introduction

So as said in the general introduction, the sub-process composed of the 4 reactions [E 4], [E 5], [E 11] and [E 15] have been studied as a group apart from the whole process in order to see if one biomass will prevail over the other and in what conditions.
This sub-process is defined as follows :
on the one hand, the inputs are the concentrations of MonoSacch and NH3 and,
on the other hand, the state is composed of the concentrations of the four compounds : MonoSacch, NH3, BioSugar and BioSugar2 (Figure 10).

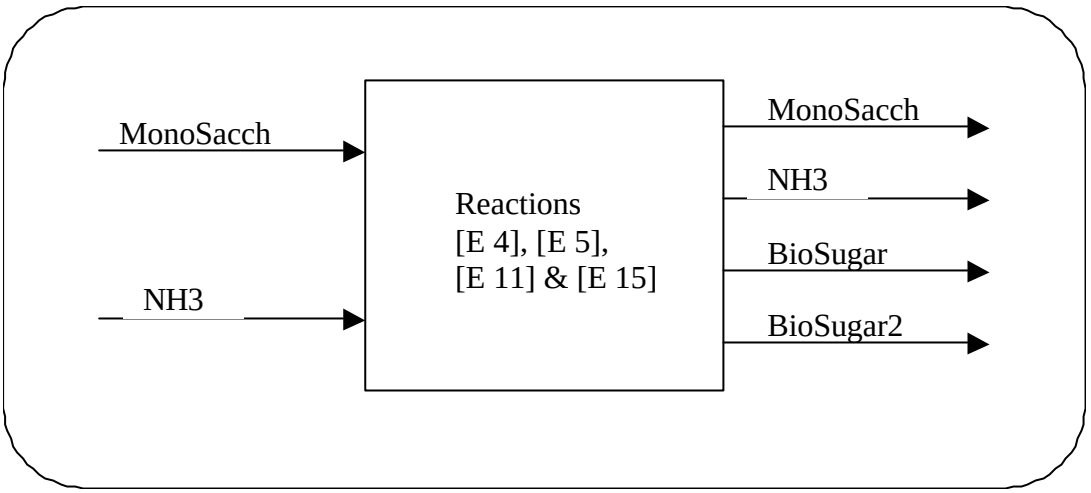


Figure 10. Sub-system limited to BioSugar and BioSugar2

The aim is to point out the time evolution of the biomasses.
It is recalled that for these reactions, the general expression of the chemical kinetics 'r' (expressed in g/l/h) is (TN 74.1 by LGCB) :

$$r = \mu_M \cdot \frac{[S_1]}{k_{S1} + [S_1]} \cdot \frac{[S_2]}{k_{S2} + [S_2]} \cdot \frac{1}{1 + \frac{[S_I]}{k_I}} \cdot [\text{Biomass}]$$

with the following parameters :

Table 18. Parameters of equations E4 and E5

Reaction	Biomass (g/l)	μ_M (h^{-1})	S_1		S_2		S_I	
				k_S (g/l)		k_S (g/l)		k_I (g/l)
E4	Bio_Sugar	$\frac{0.4}{0.1091}$	NH3	10^{-4}	Mono_Sacch	10^{-2}	none	
E5	Bio_Sugar2	$\frac{0.1}{0.1}$	NH3	10^{-4}	Mono_Sacch	10^{-4}	none	

Particularly the products (Acetate, Propionate, CO2 …) have no effect on the kinetics of the 4 reactions. Consequently they are not taken into consideration.

3.2.2 Expression of the state system

The following notation will be used to describe the sub-process mathematically.
Notation :
The concentration of a compound (substrate or product of a reaction) is designed 'a'.
In a reaction [E i] , a given compound is referred to by the indices 'i' and 'j', where 'j' is the rank of the compound from left hand side to right hand side as it appears in the reactions [E 1] to [E 16] in annex.
For example :

- a_{41} and a_{43} are the concentrations of MonoSacch and BioSugar, respectively;
- the concentration of NH3 is designed 'a_{42}' or 'a_{52}' as NH3 appears at the second rank of the reactions [E 4] and [E 5].

In the analytical expression of chemical kinetics, the stoechiometric coefficients are designed 'α' and are signed. The left hand side compounds have negative sign as they are consumed and right hand side compounds have positive one.
For example :

- the coefficient of NH3 in [E 5] is $\alpha_{52} = -0.1$;
- the coefficient of BioSugar2 in [E 5] is $\alpha_{53} = +0.1$.

3.2.2.1 Differential equations system

The time evolution of the complete sub-process is fully described when one considers the 4 compounds : MonoSacch, NH3, BioSugar and BioSugar2.

MonoSacch:
MonoSacch is a soluble compound whose concentration follows the relation (2.5) established in section 1. :

$$\dot{a}_{41} = -\beta \cdot a_{41} + \beta \cdot a_{i41} + r_{A41}$$

with $\beta = \frac{q_i}{V}$

q_i : liquid input flow rate;
V : liquid volume in the reactor;
a_{i41} : input concentration of MonoSacch;
r_{A41} : variation rate of MonoSacch.

The reaction [E 4] is a Monod/Pirt type reaction whose characteristics are detailed in Table 3:

$$r_{A41} = \alpha_{41} \cdot \mu_4 \cdot C_4 \cdot a_{43} + \alpha_{51} \cdot \mu_5 \cdot C_5 \cdot a_{53}$$

with $C_4 = \frac{a_{41}}{k_{S41} + a_{41}} \cdot \frac{a_{42}}{k_{S42} + a_{42}}$

$$C_5 = \frac{a_{41}}{k_{S51} + a_{41}} \cdot \frac{a_{42}}{k_{S52} + a_{42}}$$

So the concentration of MonoSacch is expressed by :

$$\dot{a}_{41} = -\beta \cdot a_{41} + \beta \cdot a_{i41} + \alpha_{41} \cdot \mu_4 \cdot C_4 \cdot a_{43} + \alpha_{51} \cdot \mu_5 \cdot C_5 \cdot a_{53}$$

where μ_4 and μ_5 are the specific growth rates of BioSugar and BioSugar2 respectively and defined as μ_M in Table 3.

NH3:
NH3 is a soluble and dissociated compound whose concentration follows the relation (2.7) established in section 1 and whose kinetics is the same as MonoSacch. So :

$$\dot{a}_{42} = -\beta \cdot a_{42} + \beta \cdot a_{i42} + \frac{1}{K} \cdot r_{A42}$$

with

$$r_{A42} = \alpha_{42} \cdot \mu_4 \cdot C_4 \cdot a_{43} + \alpha_{52} \cdot \mu_5 \cdot C_5 \cdot a_{53}$$

BioSugar :
BioSugar is a solid compound whose concentration follows the relation (2.6) established in section 1. So, taking into account the decay rate (section 1.2.2.3) and the fact that there is no input of biomass :

$$\dot{a}_{43} = -\beta_S \cdot a_{43} + r_{A43}$$

with

$$\beta_S = \frac{q_o}{q_o + q_d - q_i} \cdot \frac{q_d}{V}$$

q_i, q_o and q_d : input, output and drain flow rates

and $r_{A43} = \alpha_{43} \cdot \mu_4 \cdot C_4 \cdot a_{43} + \alpha_{11,1} \cdot k_{D11} \cdot a_{43}$

where k_D is the specific decay rate defined in Table 4.

BioSugar2 :
The behaviour of BioSugar2 is quite similar to the BioSugar one :

$$\dot{a}_{53} = -\beta_S \cdot a_{53} + r_{A53}$$

with $r_{A53} = \alpha_{53} \cdot \mu_5 \cdot C_5 \cdot a_{53} + \alpha_{15,1} \cdot k_{D15} \cdot a_{53}$

Summary table of the state system
The sub-process limited to the biomasses BioSugar and BioSugar2 of the reactions [E 4], [E 5], [E 11] and [E 15], can be described by the following state system :

$$\begin{aligned}
\dot{a}_{41} &= -\beta \cdot a_{41} + \beta \cdot a_{i41} + \alpha_{41} \cdot \mu_4 \cdot C_4 \cdot a_{43} + \alpha_{51} \cdot \mu_5 \cdot C_5 \cdot a_{53} \\
\dot{a}_{42} &= -\beta \cdot a_{42} + \beta \cdot a_{i42} + \frac{1}{K} \cdot \alpha_{42} \cdot \mu_4 \cdot C_4 \cdot a_{43} + \frac{1}{K} \cdot \alpha_{52} \cdot \mu_5 \cdot C_5 \cdot a_{53} \\
\dot{a}_{43} &= \left(-\beta_S + \alpha_{43} \cdot \mu_4 \cdot C_4 + \alpha_{11,1} \cdot k_{D11}\right) \cdot a_{43} \\
\dot{a}_{53} &= \left(-\beta_S + \alpha_{53} \cdot \mu_5 \cdot C_5 + \alpha_{15,1} \cdot k_{D15}\right) \cdot a_{53}
\end{aligned} \tag{2.14}$$

with

a_{41} : MonoSacch concentration in the sub-process;
a_{i41} : MonoSacch concentration at sub-process input
a_{42} : NH3 molecular form concentration in the sub-process;
a_{i42} : NH3 molecular form concentration at sub-process input
a_{43} : BioSugar concentration in the sub-process;
a_{53} : BioSugar2 concentration in the sub-process;
α_{jk} : signed stoechiometric coefficient (convention of indices in the notation rules above);

$$\beta = \frac{q_i}{V}$$

$$\beta_S = \frac{q_o}{q_o + q_d - q_i} \cdot \frac{q_d}{V}$$

q_i : flow rate at reactor input;
q_o : flow rate at reactor output (defined as ‘q’ in section 1);
q_d : drain flow rate;
μ_4 and μ_5 : specific growth rates of BioSugar and BioSugar2 respectively defined as μ_M inTable 3;

$$C_4 = \frac{a_{41}}{k_{S41} + a_{41}} \cdot \frac{a_{42}}{k_{S42} + a_{42}}$$

$$C_5 = \frac{a_{41}}{k_{S51} + a_{41}} \cdot \frac{a_{42}}{k_{S52} + a_{42}}$$

k_S : half saturation constants defined in table 2.2 of TN1;
k_D : the specific decay rates defined in table 2.3 of TN1;
K : ratio of NH3 total on NH3 molecular.

3.2.2.2 Discussion

From relation (2.14), the differential equations relative to the biomasses concentrations can be written :

$$\dot{a}_{43} = f_4(t) \cdot a_{43}$$
$$\dot{a}_{53} = f_5(t) \cdot a_{53}$$
with (2.15)
$$f_4(t) = -\beta_S + \alpha_{43} \cdot \mu_4 \cdot C_4 + \alpha_{11,1} \cdot k_{D11}$$
$$f_5(t) = -\beta_S + \alpha_{53} \cdot \mu_5 \cdot C_5 + \alpha_{15,1} \cdot k_{D15}$$

The sums of the form '$-\beta_S + \alpha_{j,1} \cdot k_D$' are negative constants because $\alpha_{j,1}$ is negative. As α_{j3} is positive, the terms $\alpha_{j3} \cdot \mu_j \cdot C_j$ are positive time variables depending on C_j, i.e. on a_{41} and a_{42} (MonoSacch and NH3 concentrations). So the function f_4 and f_5 can be :

- positive → the biomass concentration is increasing exponentially;
- negative → the biomass concentration is decreasing exponentially to zero;
- null → the biomass concentration is stable at a given value;

3.2.2.3 Examples of simulation

The discussion is illustrated in the 2 following examples. The first simulation is based on the wastes inputs of the LGCB model dated 30 July 2004 : Faeces (3.968 g/l); Wheat, Salad and Potato (7.936 g/l). The concentrations of MonoSacch and NH3 at input of the sub-process are deduced from the complete transformation of the wastes inputs : it gives the concentrations of MonoSacch and NH3 (total form) equal to 11.95 and 0.592 g/l, respectively. The second simulation is the same as the first one except that the input NH3 concentration is chosen low (divided by a factor 6) so that to illustrate the 2 different behaviours of the sub-process.

In both simulation :

- The inputs MonoSacch and NH3 are constant along the simulation;
- The initial states of MonoSacch and NH3 are equal to the inputs;
- The initial biomass concentrations are the same and equal to 1 10^{-3} g/l .

In the first simulation (Figure 11), the input NH3 concentration (0.562 g/l of total form) is 'high' compared to the input MonoSacch concentration (11.95 g/l). During the 19 first hours, the functions f_4 and f_5 are positive, quasi constant (to 0.35 and 0.08, respectively) and consequently the biomasses grow exponentially. Beyond t=19h, f_4 falls very quickly to a negative value; then the evolution of BioSugar is exponentially decreasing to 0. Concerning f_5, it decreases to 0 until t=500h; during this period, BioSugar2 grows until it reaches the steady state value of 0.218 g/l.

In the second simulation (Figure 12), the input NH3 concentration (9.37 10^{-2} g/l of total form) is 'low' compared to the input MonoSacch concentration (11.95 g/l.). In the first step (about 30 first hours), the biomasses grow exponentially as in the first simulation. In the next time period, f4 tend to 0 and BioSugar decreases to a non null value : 0.193 g/l, while f5 falls to a negative value and BioSugar2 tends to 0.

The 2 following examples illustrate also the 2 main behaviours of the sub-system. Depending on the relative input concentration of NH3 compared to the one of MonoSacch, only one biomass remains in the medium, the other one going to 0. This will be studied with the steady state and will justify the simplification of the group of reactions [E 4], [E 5], [E 11] and [E 15].

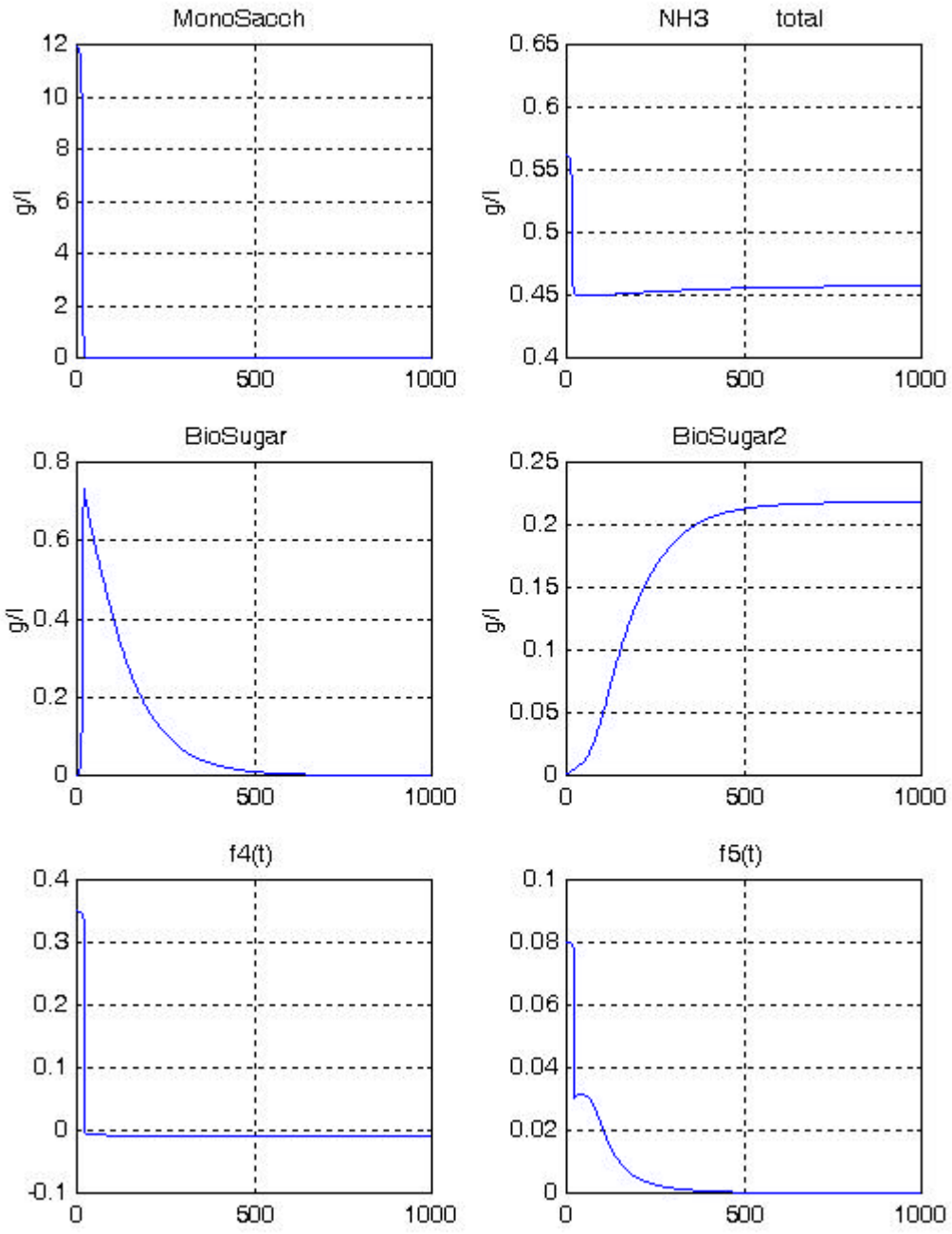


Figure 11. Simulation 1; Evolution function of time expressed in hour.

NH3 is 'high' compared to MonoSacch
Inputs: 0.562 g/l of NH3 total form and 11.95 g/l of MonoSacch

⇒

- The functions $f_4(t)$ and $f_5(t)$ are positive, quasi constant during the 19 first hours; so the biomasses are growing exponentially ;
- Beyond t=19h, the function $f_4(t)$ is negative and BioSugar tends to 0;
- The function $f_5(t)$ tends to 0 and BioSugar2 tends to a non null value : 0.218 g/l.

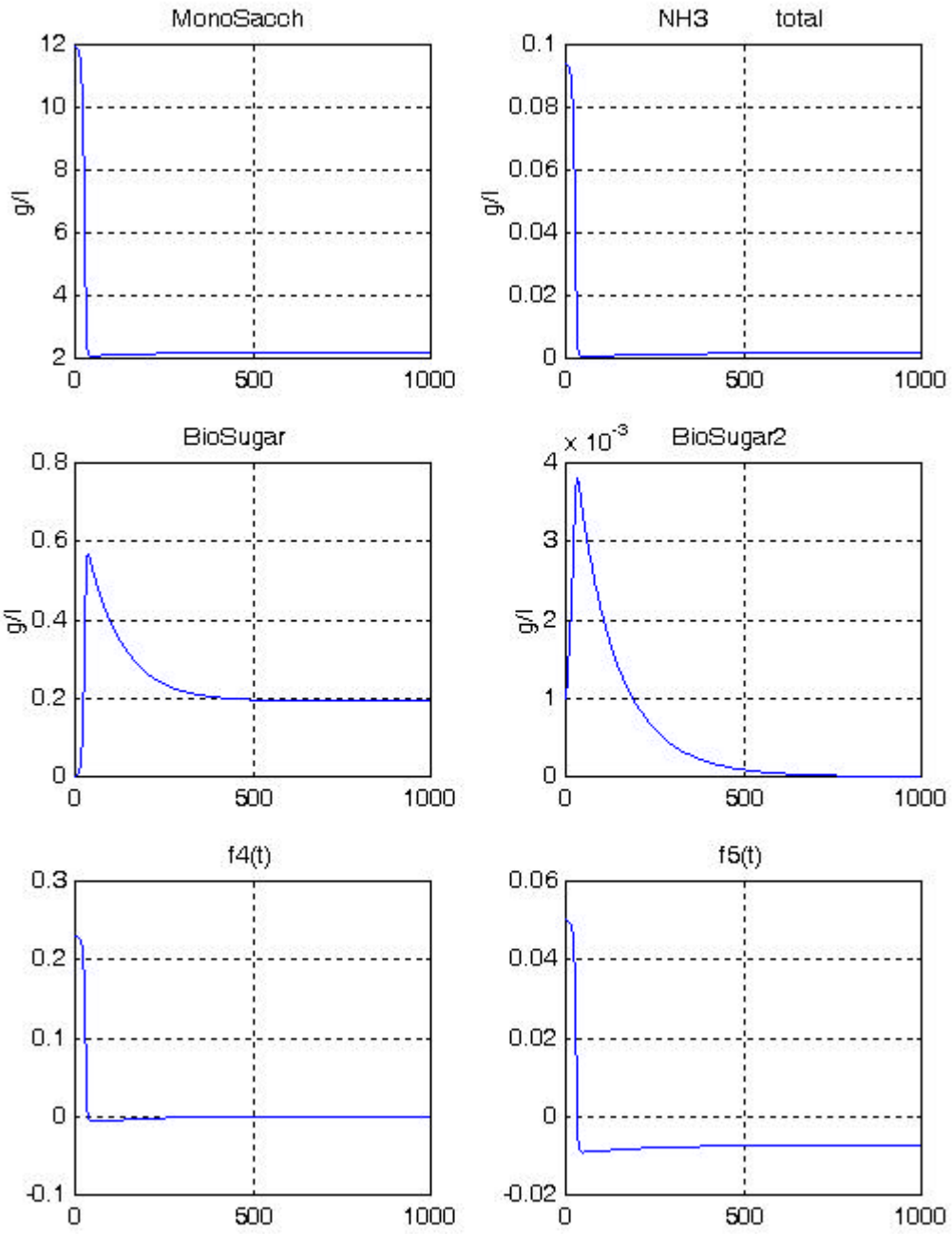


Figure 12. Simulation 2; Evolution function of time expressed in hour.

NH3 is 'low' compared to MonoSacch
Inputs: 9.37 10^{-2} g/l of NH3 total form and 11.95 g/l of MonoSacch

⇒

- The functions $f_4(t)$ and $f_5(t)$ are positive, quasi constant during the 19 first hours; so the biomasses are growing exponentially ;
- Beyond this time period, the function $f_4(t)$ tends to 0 and BioSugar tends to 0.193 g/l;
- The function $f_5(t)$ is negative and BioSugar2 tends to 0.

3.2.2.4 Analysis of the steady state

It has been established in relation (2.14) of section 3.2.2.1 that the sub-process limited to the biomasses BioSugar and BioSugar2 of the reactions [E 4], [E 5], [E 11] and [E 15], can be described by the following state system :

$$\dot{a}_{41} = -\beta \cdot a_{41} + \beta \cdot a_{i41} + \alpha_{41} \cdot \mu_4 \cdot C_4 \cdot a_{43} + \alpha_{51} \cdot \mu_5 \cdot C_5 \cdot a_{53}$$

$$\dot{a}_{42} = -\beta \cdot a_{42} + \beta \cdot a_{i42} + \frac{1}{K} \cdot \alpha_{42} \cdot \mu_4 \cdot C_4 \cdot a_{43} + \frac{1}{K} \cdot \alpha_{52} \cdot \mu_5 \cdot C_5 \cdot a_{53}$$

$$\dot{a}_{43} = \left(-\beta_S + \alpha_{43} \cdot \mu_4 \cdot C_4 + \alpha_{11,1} \cdot k_{D11}\right) \cdot a_{43} \quad \Leftrightarrow \quad \dot{a}_{43} = f_4 \cdot a_{43}$$

$$\dot{a}_{53} = \left(-\beta_S + \alpha_{53} \cdot \mu_5 \cdot C_5 + \alpha_{15,1} \cdot k_{D15}\right) \cdot a_{53} \quad \Leftrightarrow \quad \dot{a}_{53} = f_5 \cdot a_{53}$$

with

a_{41} : MonoSacch concentration in the sub-process;
a_{i41} : MonoSacch concentration at sub-process input
a_{42} : NH3 molecular form concentration in the sub-process;
a_{i42} : NH3 molecular form concentration at sub-process input
a_{43} : BioSugar concentration in the sub-process;
a_{53} : BioSugar2 concentration in the sub-process;

For constant inputs, the necessary and sufficient condition of steady state is the null state derivative. So from (2.1) recalled here above, the necessary and sufficient condition is :

$$\left|\begin{array}{l} \dot{a}_{41} = 0 \\ \dot{a}_{42} = 0 \\ \dot{a}_{43} = 0 \\ \dot{a}_{53} = 0 \end{array}\right. \tag{2.16}$$

From this necessary and sufficient condition (2.3), several sets of sufficient condition can be extracted. To obtain $\dot{a}_{43} = 0$, one of the 2 conditions is sufficient : $f_4 = 0$ or $a_{43} = 0$. In the same way, to fulfil $\dot{a}_{53} = 0$, one of the 2 conditions is sufficient : $f_5 = 0$ or $a_{53} = 0$. So 4 combinations are possible:

- $a_{43} = 0$ and $a_{53} = 0$ → set 1
- $f_4 = 0$ and $f_5 = 0$ → set 2
- $f_4 = 0$ and $a_{53} = 0$ → set 3
- $f_5 = 0$ and $a_{43} = 0$ → set 4

In set 3, to make a_{53} tends to 0 when initial a_{53} is not null, another condition must be fulfilled implicitly : $f_5 < 0$.
In the same way, in set 4, to make a_{43} tends to 0 when initial a_{43} is not null, another condition must be fulfilled implicitly : $f_4 < 0$.

<u>set 1</u>

$$\left|\begin{array}{l} -\beta \cdot a_{41} + \beta \cdot a_{i41} + \alpha_{41} \cdot \mu_4 \cdot C_4 \cdot a_{43} + \alpha_{51} \cdot \mu_5 \cdot C_5 \cdot a_{53} = 0 \\ -\beta \cdot a_{42} + \beta \cdot a_{i42} + \frac{1}{K} \cdot \alpha_{42} \cdot \mu_4 \cdot C_4 \cdot a_{43} + \frac{1}{K} \cdot \alpha_{52} \cdot \mu_5 \cdot C_5 \cdot a_{53} = 0 \\ a_{43} = 0 \\ a_{53} = 0 \end{array}\right. \tag{2.17}$$

<u>set 2</u>

$$
\begin{aligned}
&-\beta \cdot a_{41} + \beta \cdot a_{i41} + \alpha_{41} \cdot \mu_4 \cdot C_4 \cdot a_{43} + \alpha_{51} \cdot \mu_5 \cdot C_5 \cdot a_{53} = 0 \\
&-\beta \cdot a_{42} + \beta \cdot a_{i42} + \frac{1}{K} \cdot \alpha_{42} \cdot \mu_4 \cdot C_4 \cdot a_{43} + \frac{1}{K} \cdot \alpha_{52} \cdot \mu_5 \cdot C_5 \cdot a_{53} = 0 \\
&-\beta_S + \alpha_{43} \cdot \mu_4 \cdot C_4 + \alpha_{11,1} \cdot k_{D11} = 0 \\
&-\beta_S + \alpha_{53} \cdot \mu_5 \cdot C_5 + \alpha_{15,1} \cdot k_{D15} = 0
\end{aligned}
\qquad (2.18)
$$

<u>set 3</u>

$$
\begin{aligned}
&-\beta \cdot a_{41} + \beta \cdot a_{i41} + \alpha_{41} \cdot \mu_4 \cdot C_4 \cdot a_{43} + \alpha_{51} \cdot \mu_5 \cdot C_5 \cdot a_{53} = 0 \\
&-\beta \cdot a_{42} + \beta \cdot a_{i42} + \frac{1}{K} \cdot \alpha_{42} \cdot \mu_4 \cdot C_4 \cdot a_{43} + \frac{1}{K} \cdot \alpha_{52} \cdot \mu_5 \cdot C_5 \cdot a_{53} = 0 \\
&-\beta_S + \alpha_{43} \cdot \mu_4 \cdot C_4 + \alpha_{11,1} \cdot k_{D11} = 0 \\
&-\beta_S + \alpha_{53} \cdot \mu_5 \cdot C_5 + \alpha_{15,1} \cdot k_{D15} < 0 \quad \text{to have} \quad a_{53} = 0 \quad \text{at infinite}
\end{aligned}
\qquad (2.19)
$$

<u>set 4</u>

$$
\begin{aligned}
&-\beta \cdot a_{41} + \beta \cdot a_{i41} + \alpha_{41} \cdot \mu_4 \cdot C_4 \cdot a_{43} + \alpha_{51} \cdot \mu_5 \cdot C_5 \cdot a_{53} = 0 \\
&-\beta \cdot a_{42} + \beta \cdot a_{i42} + \frac{1}{K} \cdot \alpha_{42} \cdot \mu_4 \cdot C_4 \cdot a_{43} + \frac{1}{K} \cdot \alpha_{52} \cdot \mu_5 \cdot C_5 \cdot a_{53} = 0 \\
&-\beta_S + \alpha_{43} \cdot \mu_4 \cdot C_4 + \alpha_{11,1} \cdot k_{D11} < 0 \quad \text{to have} \quad a_{43} = 0 \quad \text{at infinite} \\
&-\beta_S + \alpha_{53} \cdot \mu_5 \cdot C_5 + \alpha_{15,1} \cdot k_{D15} = 0
\end{aligned}
\qquad (2.20)
$$

The study of these 4 sets of sufficient condition is detailed in annex 5 (section 5.3.1). The results are gathered hereafter.
The set 1 of equations leads to a trivial solution : the 2 biomasses concentrations are null, which has no interest.
The set 2 of equations leads to a mathematical solution whose value is negative and cannot be accepted as a concentration value.
The sets 3 and 4 lead to solutions where only one biomass (BioSugar or BioSugar2) remains in the medium at steady state. The existence of one of the 2 biomasses depends on the relative concentrations of MonoSacch and NH3 in the input flow. It is summed up in Figure 13 that gives the biomasses concentrations in function of MonoSacch and NH3 inputs.
When BioSugar is not null (i.e. for 'low' NH3 input), it is a linear function of NH3 whose slope is constant independent of the 2 inputs and equal to 2.09.
When BioSugar2 is not null (i.e. for 'high' NH3 input), it is independent of NH3 input and dependent of MonoSacch input only.

The case of the complete model dated 30 July 2004 can be situated on the middle graph (where MonoSacch input conc. is 11.945 g/l) at the x abscissa of 0.562 g/l of NH3 total form input. At this point, BioSugar is null and BioSugar2 equal to 0.218 g/l . These values are also obtained in section 5.3.1 as illustration of the analytical computation of the biomasses at steady state.
The behaviour of the complete model dated 30 July 2004 is confirmed : the evolution of the 2 biomasses will be of the type of the Figure 13. So BioSugar will disappear from the medium within 1000 hours after the starting of the reactor. Consequently the reactions [E 4] and [E 11] can be eliminated from the list of the reactions when the process is observed in a long term functioning. Of course, these reactions [E 4] and [E 11] cannot be removed for a study of the process at starting.

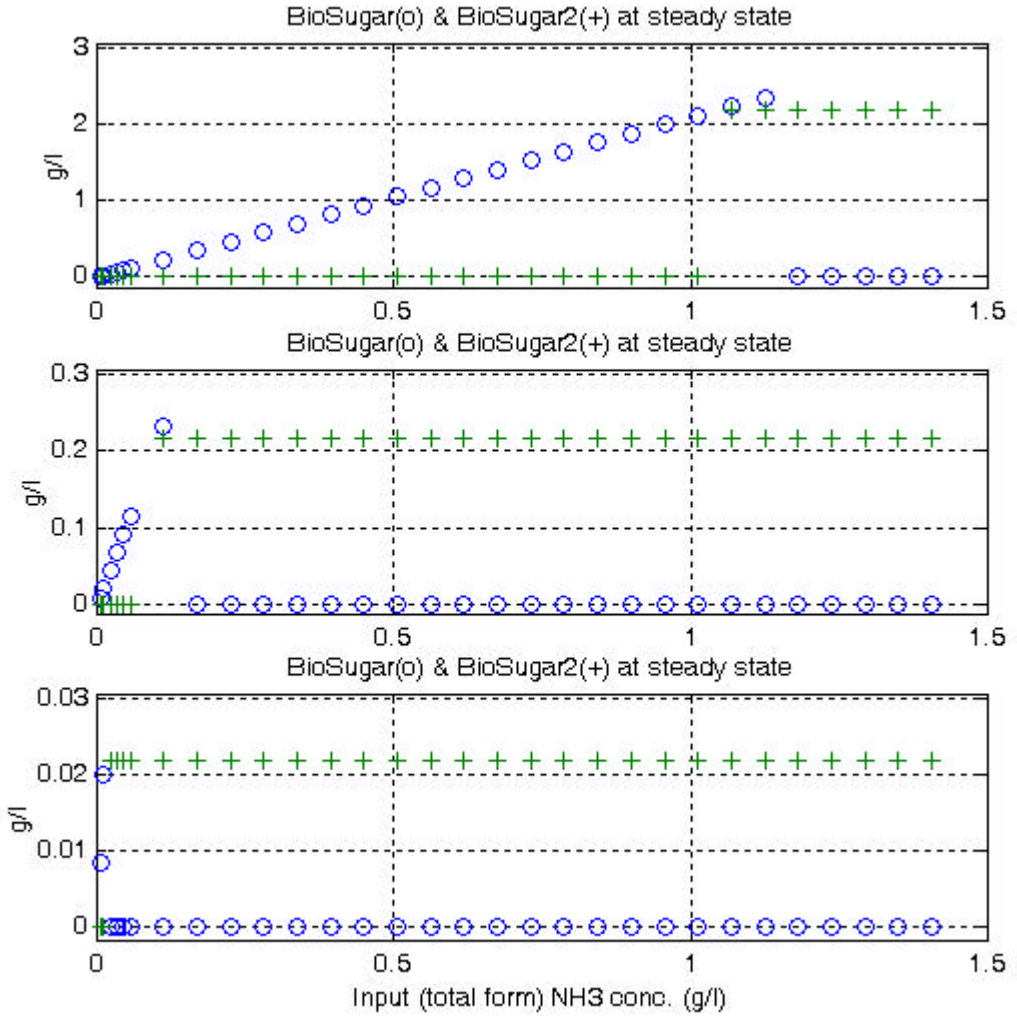


Figure 13. Biomasses at steady state in function of the MonoSacch and NH3 inputs.

The BioSugar conc. is plotted by blue circles and BioSugar2 one by green crosses.
The 3 graphs represent the biomasses evolution
for different values of MonoSacch : 119.45, 11.945 & 1.1945 g/l from top to bottom.
When BioSugar is not null (i.e. for low NH3 input), its evolution is a linear function of NH3 whose slope is constant independent of the 2 inputs and equal to 2.09 .
When BioSugar2 is not null, its evolution is independent of NH3 input and dependent of MonoSacch input only.

3.3 Description of the response times of the whole process (reactions [E 1] to [E 16])

The response times are estimated by simulations of input steps around the standard steady state point defined by the inputs of the LGCB model on 30 July 2004 (Annex 3). They are gathered in Table 19 for the different kinds of step : input flow step, drain flow step and concentrations step.

Table 19. Response times (expressed in hours and days) of the outputs for the different kinds of process excitation and for the nominal simulated process of 30 July 2004 by LGCB.

Process excitation / Component	Input flow rate		Drain flow rate		Input concentrations	
	(hours)	(days)	(hours)	(days)	(hours)	(days)
Wastes (faeces, wheat, potato, salad)	15	0.625	15		15	
VFA (AA, PA, BA, VA, CA)	1000	40	1000	40	1000	40
NH3	1000	40	1500	60	1500	60
Mono_Sacch **OM_Lip** **OM_Carb** **OM_Fibre**	500	20	500	20	500	20
OM_Prot	30	1.25	30	1.25	30	1.25
Amino_A	500	20	500	20	500	20
Biomasses (BioSugar2, Bio_AA, Bio_LCFA)	500	20	500	20	500	20
SolubleInert	1000	40	1000	40	1000	40
SolidInert, BioDead, CO2	∞	∞	10000	400	∞	∞

The hydrolysis reactions of faeces, wheat, potato and salad are quick (15 hours). This is confirmed by the analytical expression of the time constant :

$$\tau = \frac{1}{\beta_S + k} \qquad (3.1)$$

with $\beta_S = \frac{q_d}{V}$ (see (2.6))

V : liquid volume of the reactor

k : rate coefficient of the hydrolysis reactions [E 1], [E 8], [E 9] or [E 10], previously defined in Table 2.

The evolution of τ in function of the drain flow q_d can be plotted in Figure 14.

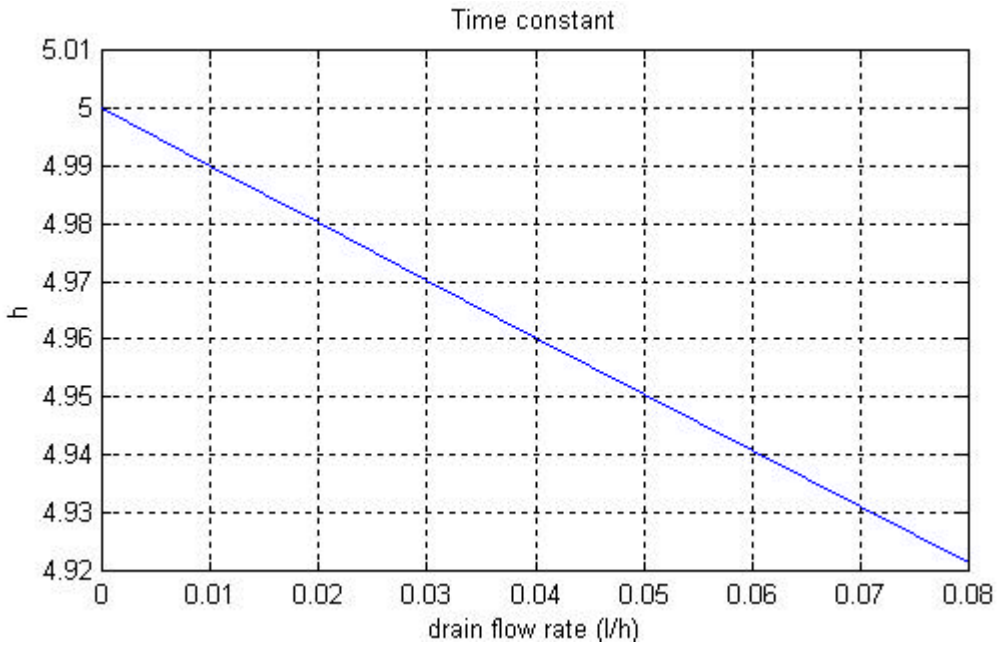


Figure 14. Evolution of time constant in function of drain flow rate

Then, remembering that the 95 % time response is equal to 3 times the time constant, it is confirmed that the time response is equal to 15 hours for q_d=0 and decreases to 14.8 hours when q_d increases to its maximum value (equal to the input flow rate = 0.08 l/h). One notes that the response time varies a little (less than 2 %) on the whole range of variation of the drain flow rate.

So the dynamics of the wastes hydrolysis can be cancelled : these reactions can be considered instantaneous compared to the other reactions and the hydrolysis can be expressed as a simple static gain.
The gain of the hydrolysis reaction is, for each waste (faeces, wheat, potato and salad) :

$$\frac{\text{ReactorWasteConcentration}}{\text{InputWasteConcentration}} = \frac{\beta}{\beta_S + k} \qquad (3.2)$$

with $\beta = \frac{q_i}{V}$.

which can be expressed in another way:

$$\frac{\text{ReactorWasteConcentration}}{\text{InputWasteConcentration}} = \frac{q_i}{q_d + V \cdot k} \qquad (3.3)$$

3.4 Conclusion

It has been shown, in section 3.2, that 1000 hours after the starting of the simulated process (defined by the reactions [E 1] to [E 16]) with constant standard inputs (i.e. inputs defined in the LGCB model on 30 July 2004), the biomass BioSugar becomes null and will stay null beyond. So the reactions [E 4] and [E 11] can be removed. Of course if the kinetics parameters of the reactions [E 4], [E 5], [E 11] and [E 15] were modified, the behaviour of this sub-process should be reviewed.
The time constants of the wastes hydrolysis are very short (5 hours when the drain flow rate is null). So these hydrolysis reactions can be replaced by instantaneous reactions whose yields are expressed by relation (3.3) type.
A tool, attached in annex 4, is now available to study numerically the optimisation of the operating conditions.

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POUGHON L. "Anareobic Waste Compartment modelling and simulation toolbox 'AWC_MS'". ESTEC contract, Memorandum of Understanding TOS-MCT/2002/3161/In/CL Dated January 2002, February 2003, TN 74.1.

POUGHON L. "Anareobic Waste Compartment modelling and simulation toolbox 'AWC_MS' – AWC toolbox improvement". ESTEC contract, Memorandum of Understanding TOS-MCT/2002/3161/In/CL Dated January 2002, August 2003, TN 74.2.

PATOUX Philippe, "Rapport de stage de 2ième année – Modélisation d'un réacteur anaérobie", Septembre 2004.

5. ANNEXES

5.1 Stoechiometry of the reactions

This annex is a copy of the LGCB document 'equations_model.doc' on 16 July 2004.
Concerning particularly the stoechiometry of the compound 'OM_Carb' in the reactions [E8], [E9] and [E11], one has noted a difference between the pre-quoted document and the simulator 'awc_ms'.

Stoechio. of OM_Carb	**in 'equations_model.doc'**	**in 'awc_ms'**
Reaction [E8]	1.95915864	1.1141
Reaction [E9]	3.53060129	2.0076
Reaction [E10]	0.99985678	0.56856

Table 20. Difference of stoechiometry in 'equations_model.doc' and 'awc_ms'.

The values of awc_ms have been retained for the present study.

Content of the document 'equations_model.doc' on 16 July 2004 :

[E 1] Hydrolysis

$$FAECES \longrightarrow 0.00869\ [CHONSP]_{Mono\_sacche} + 0.7654\ [CHONSP]_{OM\_Prot} + 0.1956\ [CHONSP]_{OM\_lipe} + 0.7828\ Inert soluble$$

[E 2] OM Carbohydrate hydrolysis

$$6\ [CHONS]_{carbohydrates} + 1.5\ H_2O \longrightarrow [CHONP]_{oses}$$

[E 3] OM proteins hydrolysis

$$[CHONS]_{proteins} + 0.2057\ H_2O \longrightarrow [CHONP]_{poolAA}$$

[E 4] acidogenesis

$$1.091\ [CHONSP]ose + 0.1091 NH_3 \longrightarrow 0.1091 [CHONSP]_{Bio\_sugar} + 0.6667 Acetate + 1.3333 Propionate + 0.6667 CO_2 + 0.9939 H_2O$$

[E 5] acidogensis

$$1.0833\ [CHO]_{oses} + 0.1\ NH_3 \longrightarrow 0.1 [CHONSP]_{Bio\_sugar2} + + C3H7COOH + 2\ CO_2 + 0.3\ H_2O$$

[E 6] acidogenesis (amino-acids)

$$[CHONS]_{poolAA} + 0.3482\ H_2O \Downarrow$$
$$0.0241\ [CHONSP]_{Bio\_AA} + 0.16373\ CH_3COOH + 0.0612\ C_2H_5COOH + 0.019\ C_3H_7COOH + 0.0177\ C_4H_9COOH + 0.01734\ C_5H_{11}COOH + 0.11816\ CO_2 + 0.2489 NH_3$$

[E 7] acidogenesis (lipids)

$$0.95\ [CHON]_{lipids} + 0.05\ NH_3 + 0.68125\ H_2O \longrightarrow 0.05 [CHONSP]_{Bio\_LCFA} + 0.35\ CH_3COOH$$

[E 8] Wheat hydrolysis	$WHEAT \longrightarrow 0.24574166[CHONSP]_{OM\_Prot} + 0.05824135[CHONSP]_{OM\_Lip} + 1.95915864[CHONSP]_{OM\_Carb} + 0.04799087[CHONSP]_{Fibre} + 0.60395883\ Inert\ solide$
[E 9] Potatoe hydrolysis	$POTATOE \longrightarrow 0.3049197[CHONSP]_{OM\_Prot} + 0.02285434[CHONSP]_{OM\_Lip} + 3.53060129[CHONSP]_{OM\_Carb} + 0.08343911[CHONSP]_{Fibre} + 0.33315195\ Inert\ solide$
[E 10] Salad hydrolysis	$SALAD \longrightarrow 0.74076846[CHONSP]_{OM\_Prot} + 0.18122404[CHONSP]_{OM\_Lip} + 0.99985678[CHONSP]_{OM\_Carb} + 0.20033494[CHONSP]_{Fibre} + 0.46094085\ Inert\ solide$
[E 11] Decay biomass	$[CHONSP]_{Bio\_sugar} \longrightarrow [CHONSP]_{Bio\_dead}$
[E 12] Decay biomass	$[CHONSP]_{Bio\_AA} \longrightarrow [CHONSP]_{Bio\_dead}$
[E 13] Decay biomass	$[CHONSP]_{Bio\_LCFA} \longrightarrow [CHONSP]_{Bio\_dead}$
[E 14] Decay biomass	$[CHONSP]_{Bio\_HVFA} \longrightarrow [CHONSP]_{Bio\_dead}$
[E 15] Decay Biomass	$[CHONSP]_{Bio\_sugar2} \longrightarrow [CHONSP]_{Bio\_dead}$
[E 16] Fiber hydrolysis	$[CHONSP]_{OM\_Fibre} \longrightarrow 3.9216[CHONSP]_{OM\_Carb}$

FAECES : CHONSP undefined – Molar Mass 100g/mol
Inert Soluble : CHONSP undefined : Molar Mass 100g/mol
Inert Solid : CHONSP undefined : Molar Mass 100g/mol
$[CHONSP]_{OM\_carbo}=CH_{1.6667}O_{0.8333}$ $[CHONSP]_{bses}=C_6H_{12}O_6$
$[CHONSP]_{OM\_roteins}=CH_{1.56828}O_{0.3063}N_{0.2693}S_{0.00635}$ $[CHONSP]_{poolAA}=CH_{1.9800}O_{0.5122}N_{0.2693}S_{0.00635}$
$[CHONSP]_{Lipids}=CH_2O_{0.125}$
$[CHONSP]_{Bio}=C_5H_7O_2N$

[E 1] Hydrolysis	N order kinetic
[E 2] OM Carbohydrate hydrolysis	N order kinetic
[E 3] OM proteins hydrolysis	N order kinetic
[E 4] acidogenesis	Pirt + non-competitive inhibition + pH inhibition
[E 5] acidogensis	Pirt + non-competitive inhibition + pH inhibition
[E 6]	Pirt + non-competitive inhibition + pH inhibition

acidogenesis (amino-acids)	
[E 7] acidogenesis (lipids)	Pirt + non-competitive inhibition + pH inhibition
[E 8] Wheat hydrolysis	N order kinetic
[E 9] Potatoe hydrolysis	N order kinetic
[E 10] Salad hydrolysis	N order kinetic
[E 11] Decay biomass	Lethal model
[E 12] Decay biomass	Lethal model
[E 13] Decay biomass	Lethal model
[E 14] Decay biomass	Lethal model
[E 15] Decay Biomass	Lethal model
[E 16] Fiber hydrolysis	N order kinetic

5.2 Molar mass

```
Faeces       : 100.000000
Wheat        : 100.000000
Potato       : 100.000000
Salad        : 100.000000
AA           : 60.000000
PA           : 74.000000
BA           : 88.000000
VA           : 102.000000
CA           : 116.000000
NH3          : 17.000000
CO2          : 44.000000
MonoSacch    : 180.000000
OMProt       : 22.442480
OMLip        : 16.000000
OMCarb       : 26.999500
OMFibre      : 100.000000
AminoA       : 26.148600
BioSugar     : 113.000000
BioSugar2    : 113.000000
BioAA        : 113.000000
BioLCFA      : 113.000000
BioDead      : 113.000000
SolubleInert : 100.000000
SolidInert   : 100.000000
```

5.3 Plotting of the 2 simulators results

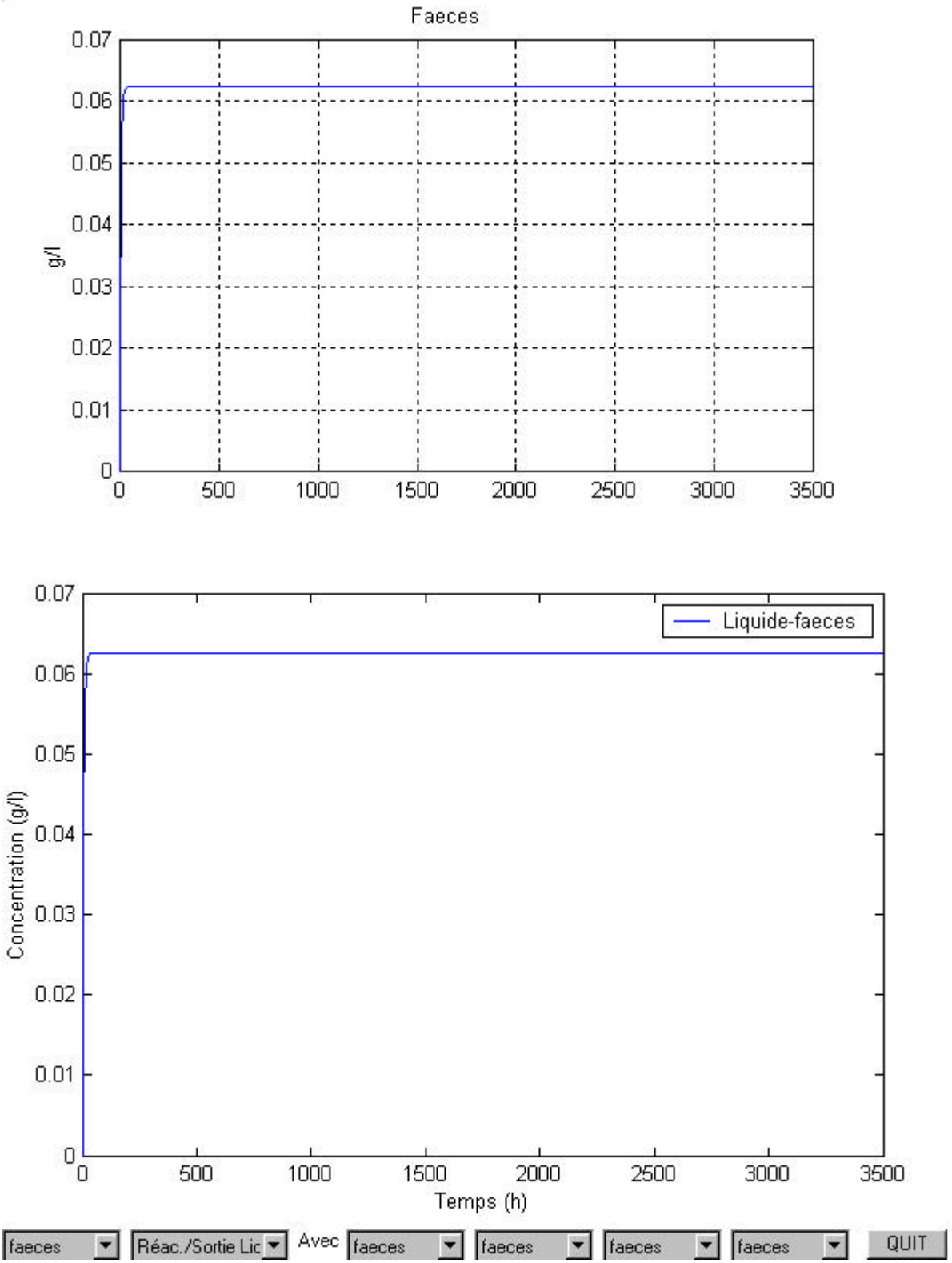

Figure 15. Faeces

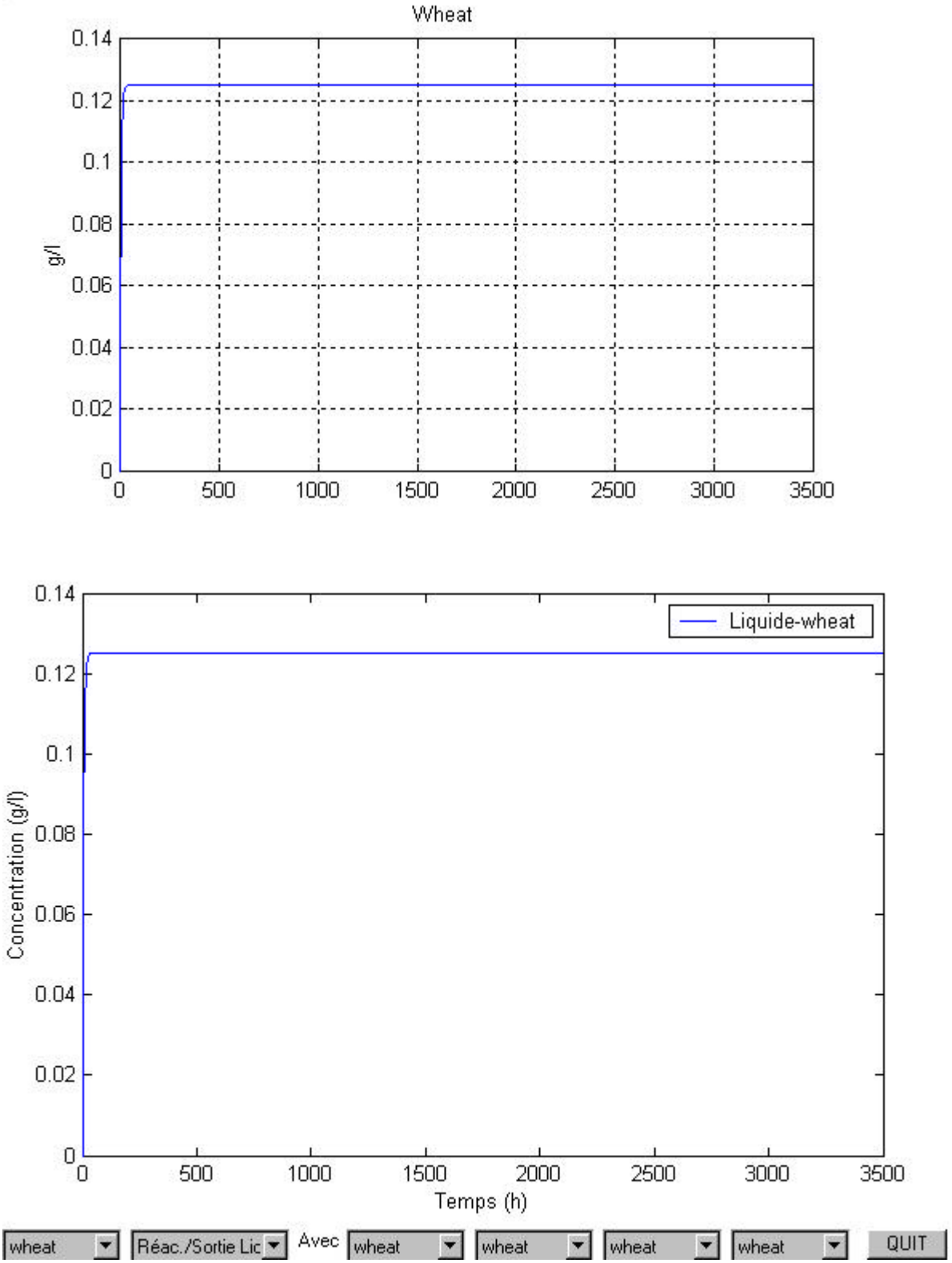

Figure 16. Wheat

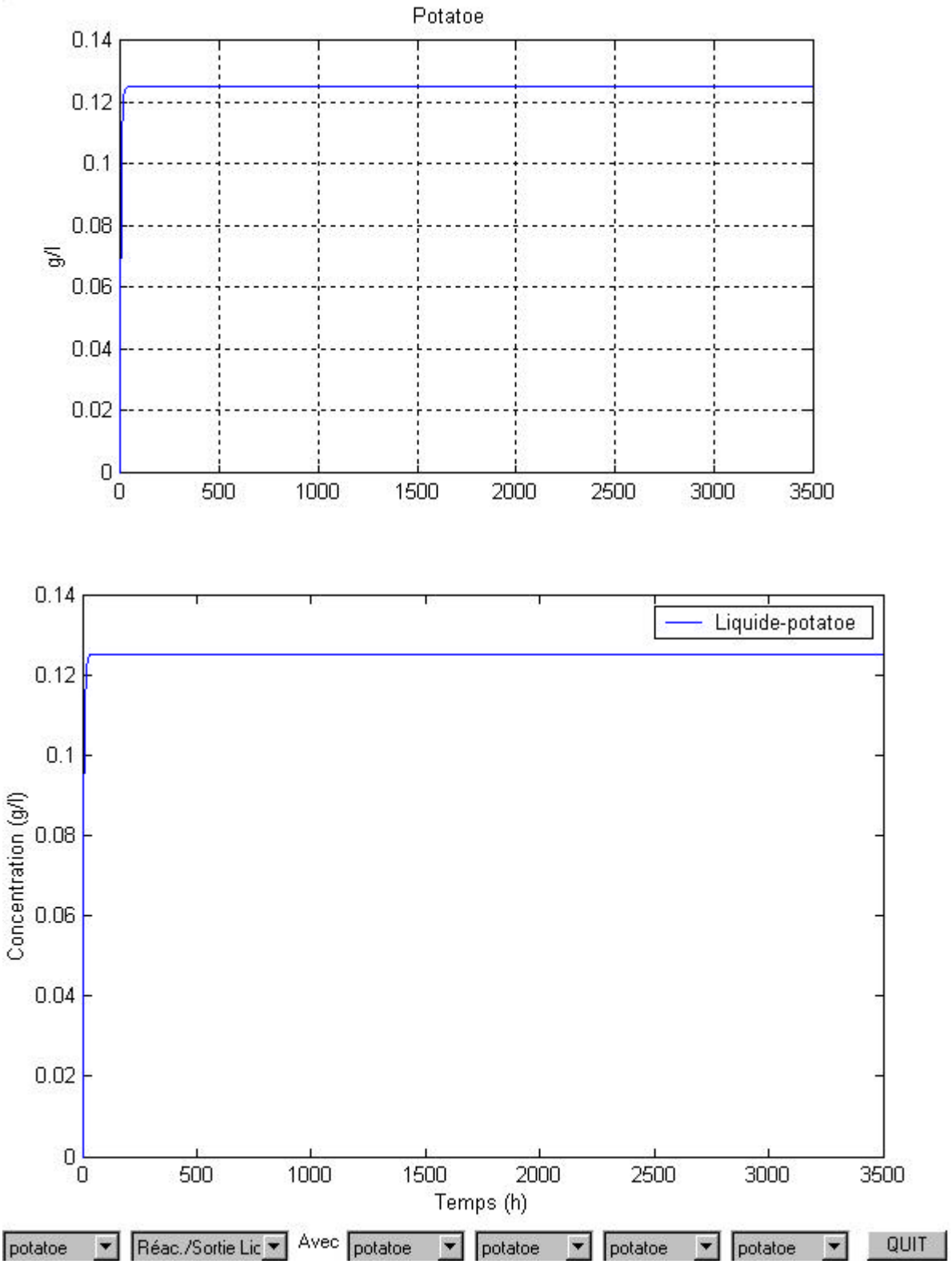

Figure 17. Potatoe

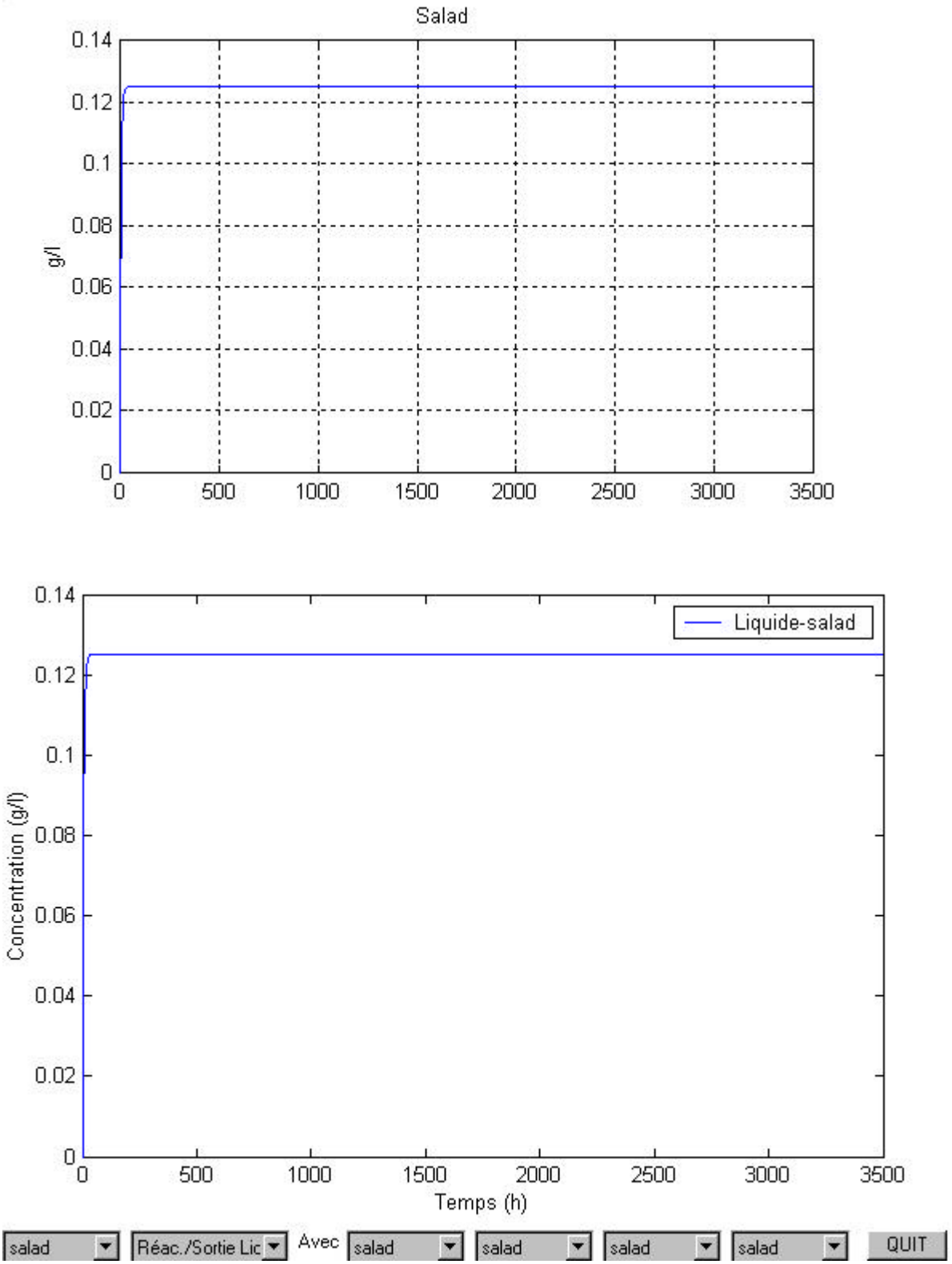

Figure 18. Salad

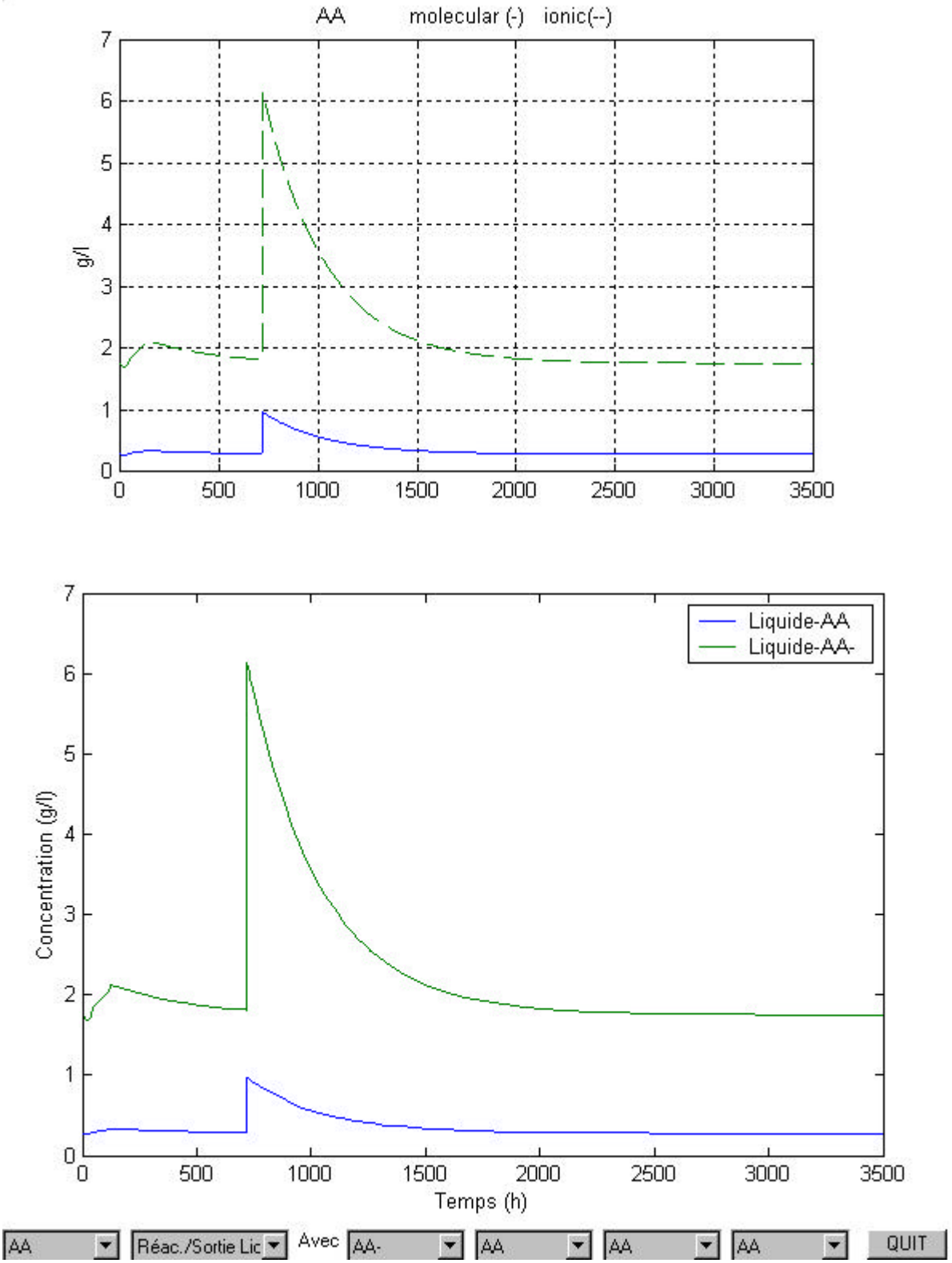

Figure 19. AA: Molecular (blue curve) and Ionic (green curve) forms

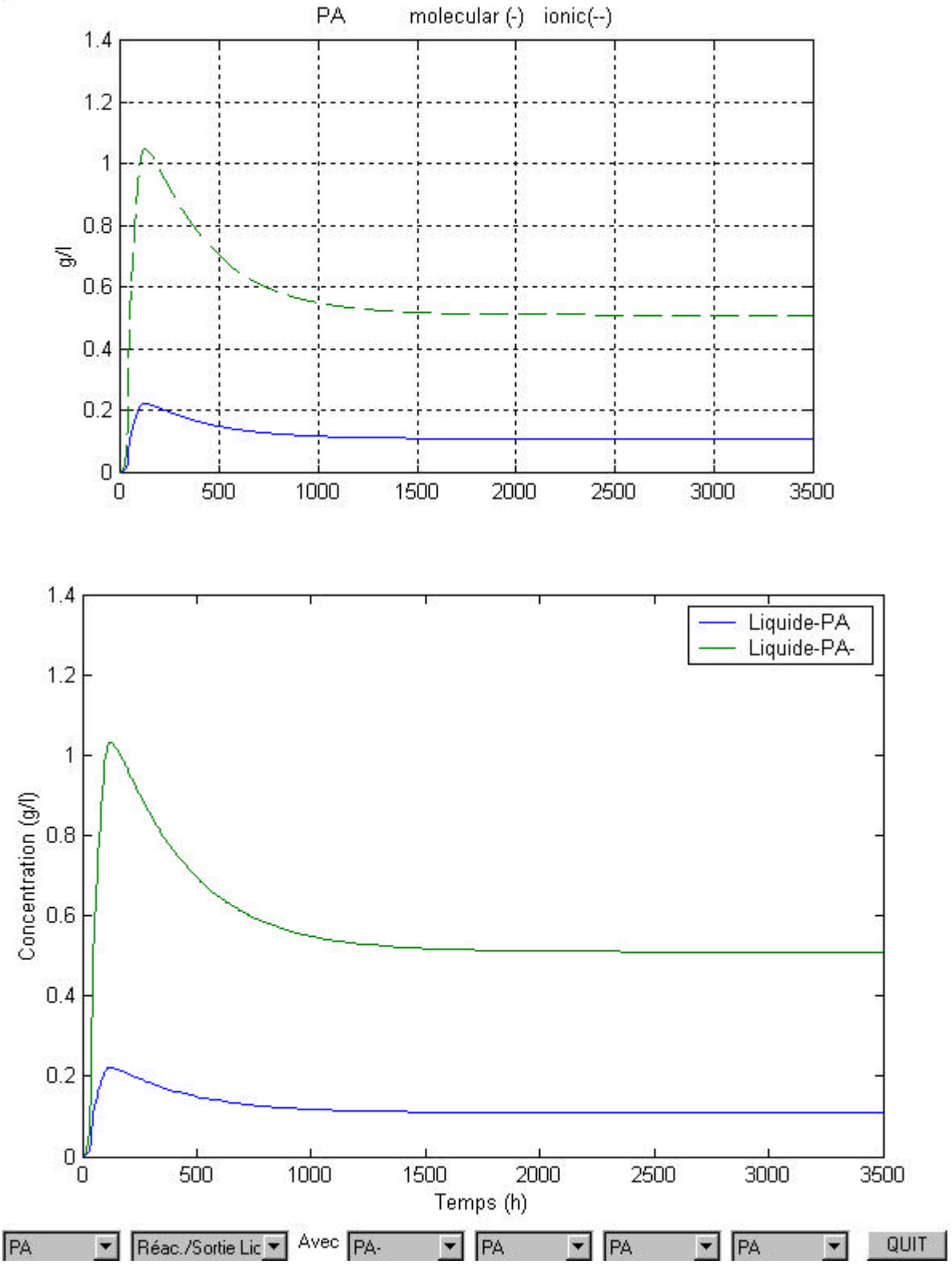

Figure 20. PA : Molecular (blue curve) and Ionic (green curve) forms

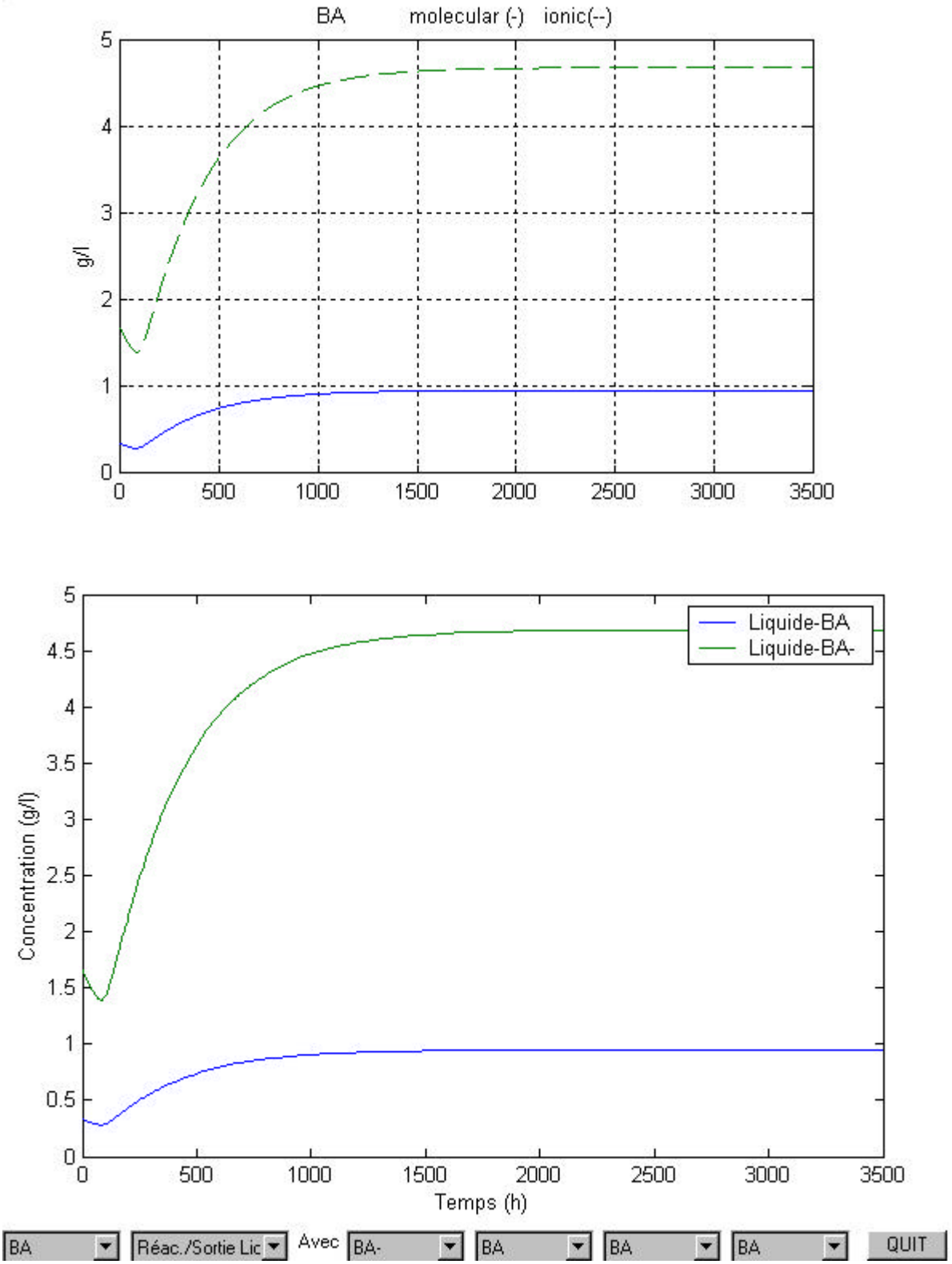

Figure 21. BA : Molecular (blue curve) and Ionic (green curve) forms

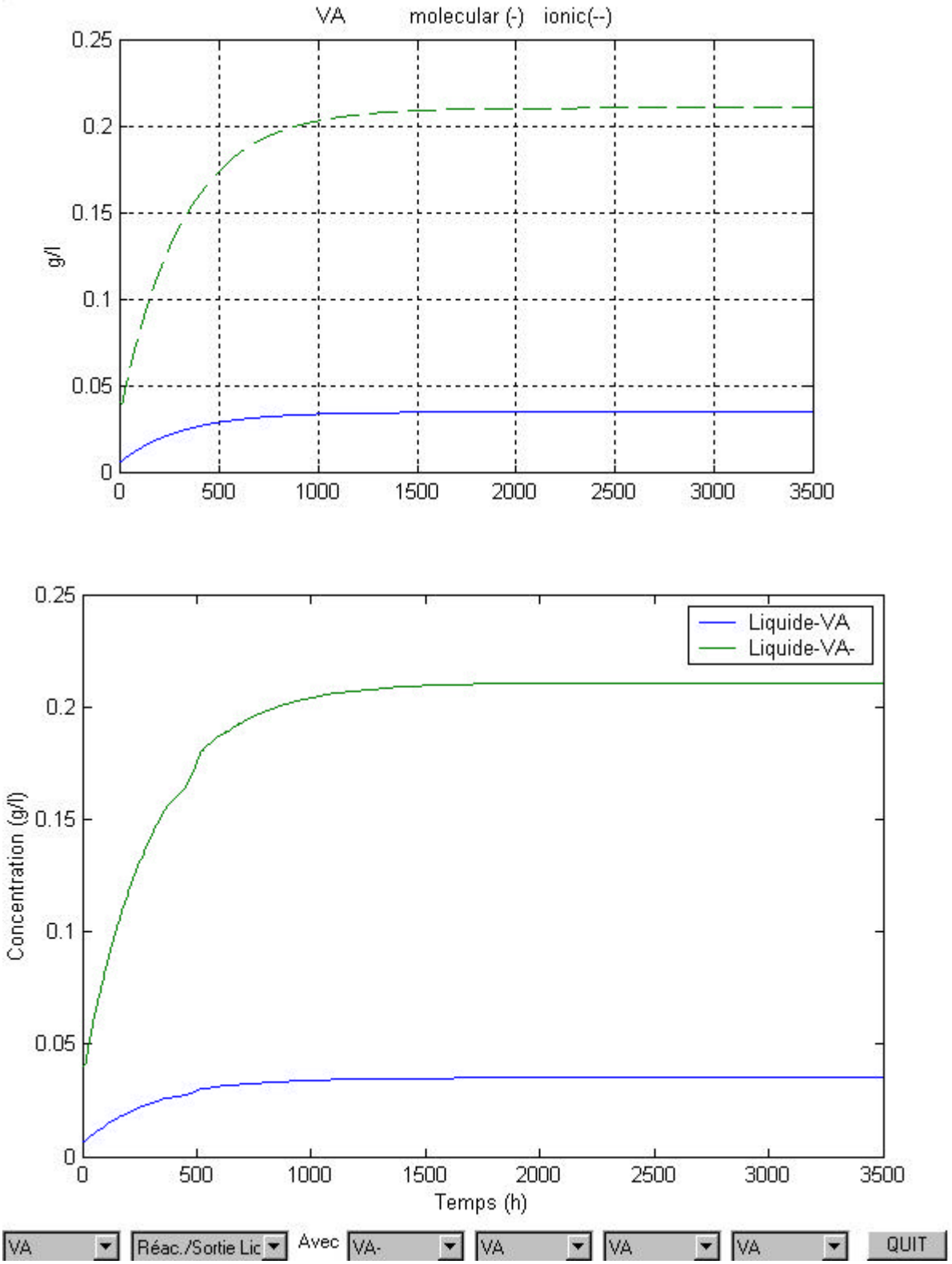

Figure 22. VA : Molecular (blue curve) and Ionic (green curve) forms

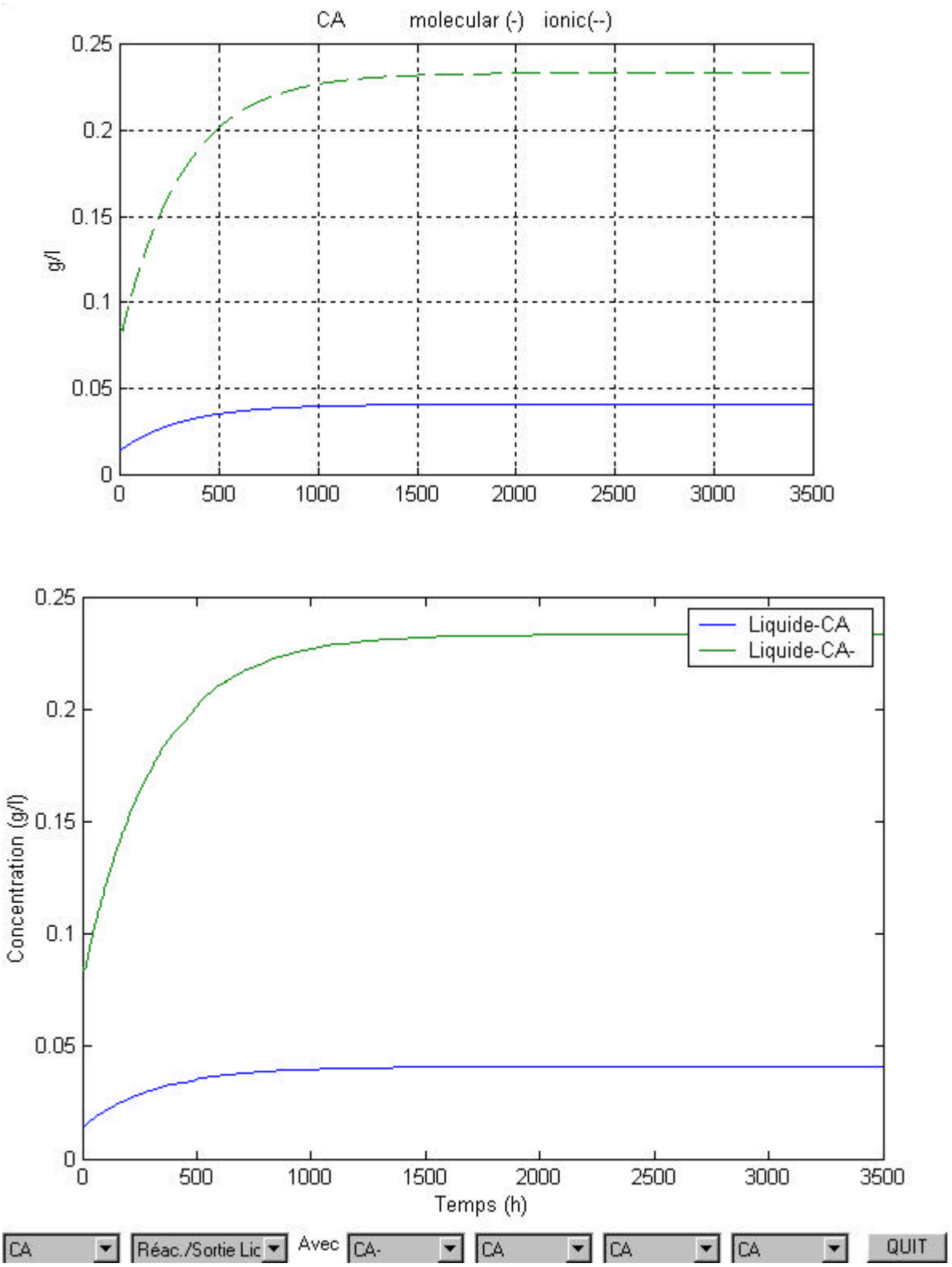

Figure 23. CA : Molecular (blue curve) and Ionic (green curve) forms

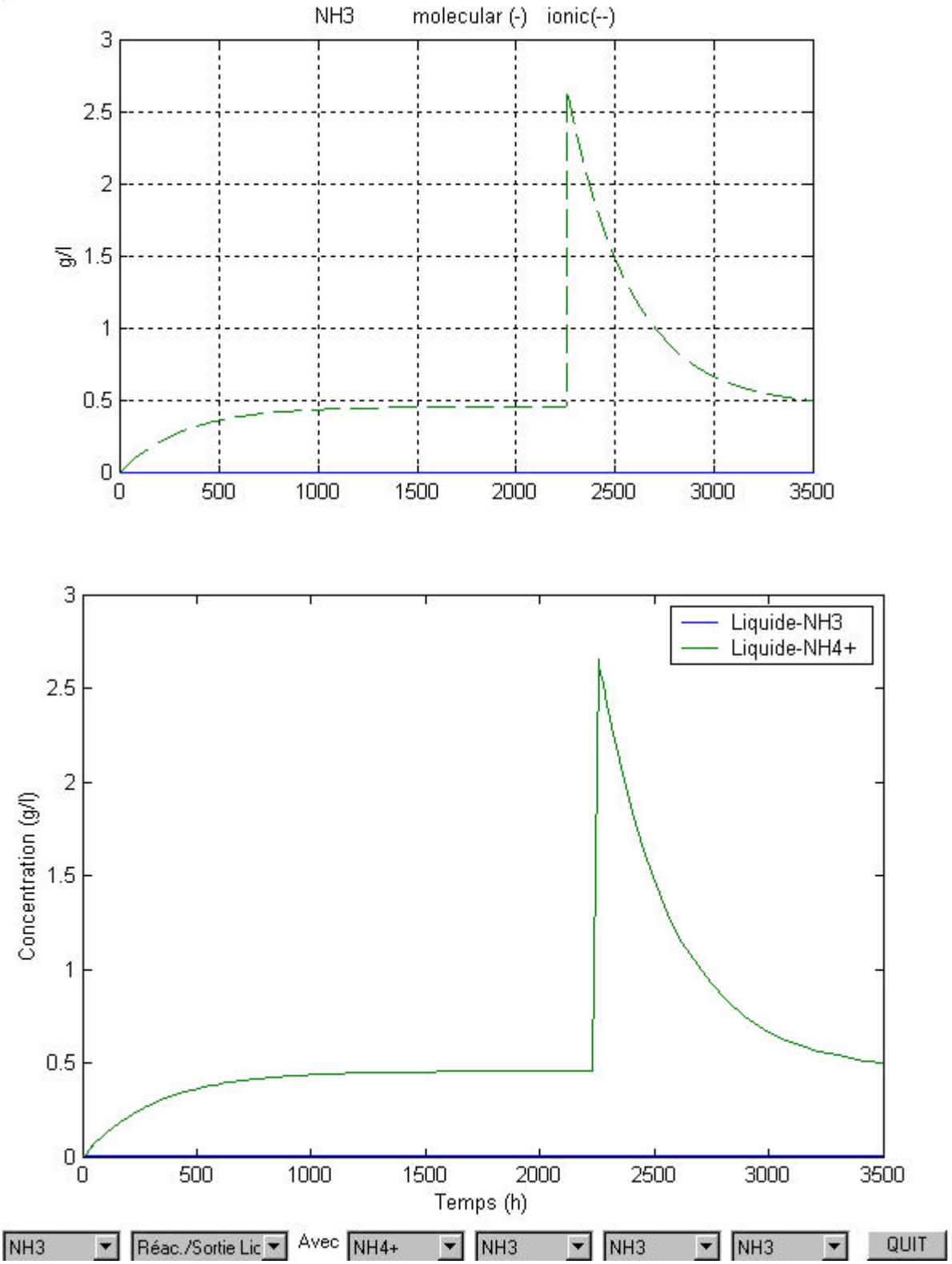

Figure 24. NH3 : Molecular (blue curve) and Ionic (green curve) forms

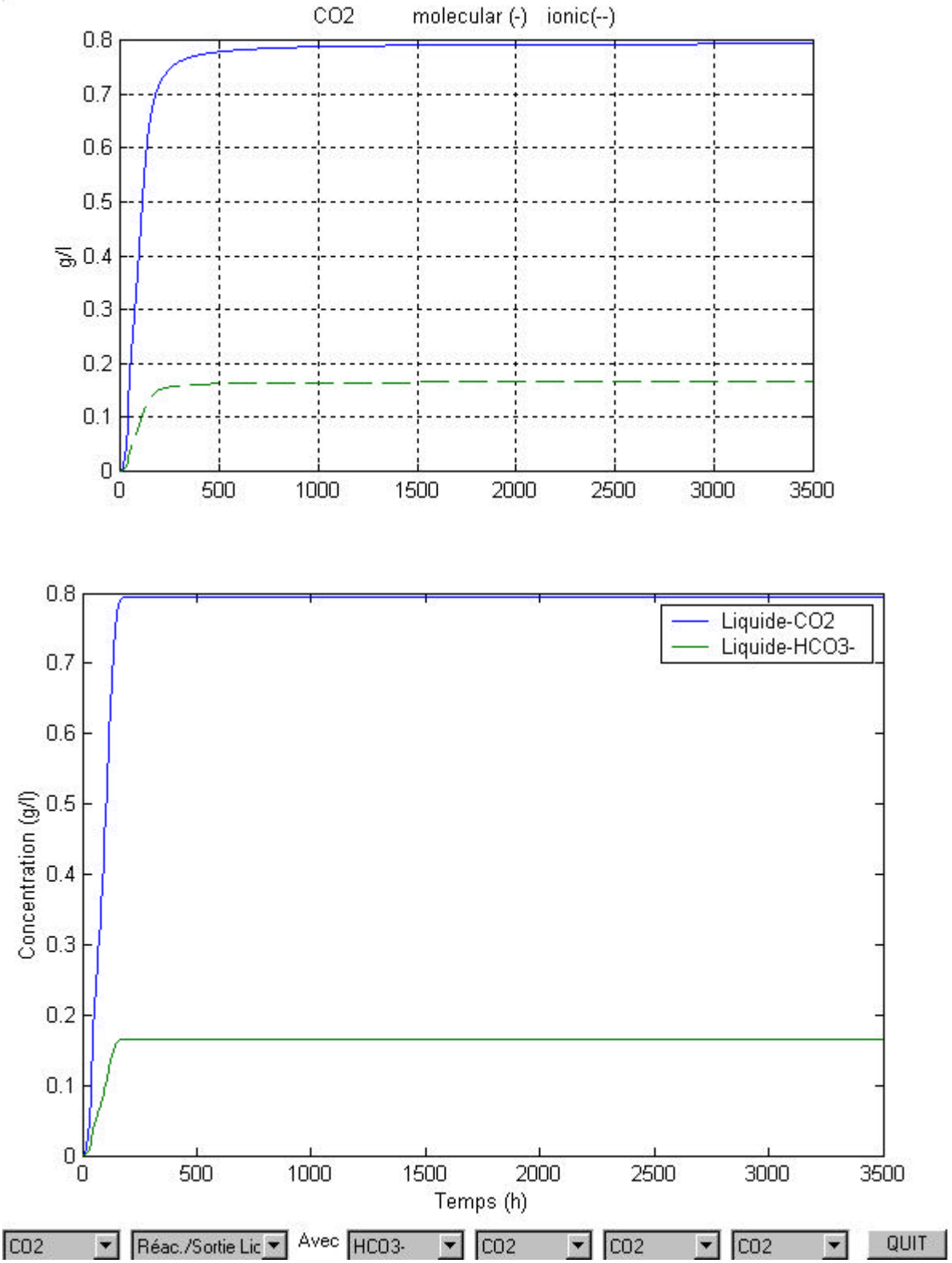

Figure 25. CO2 : Molecular (blue curve) and Ionic (green curve) forms

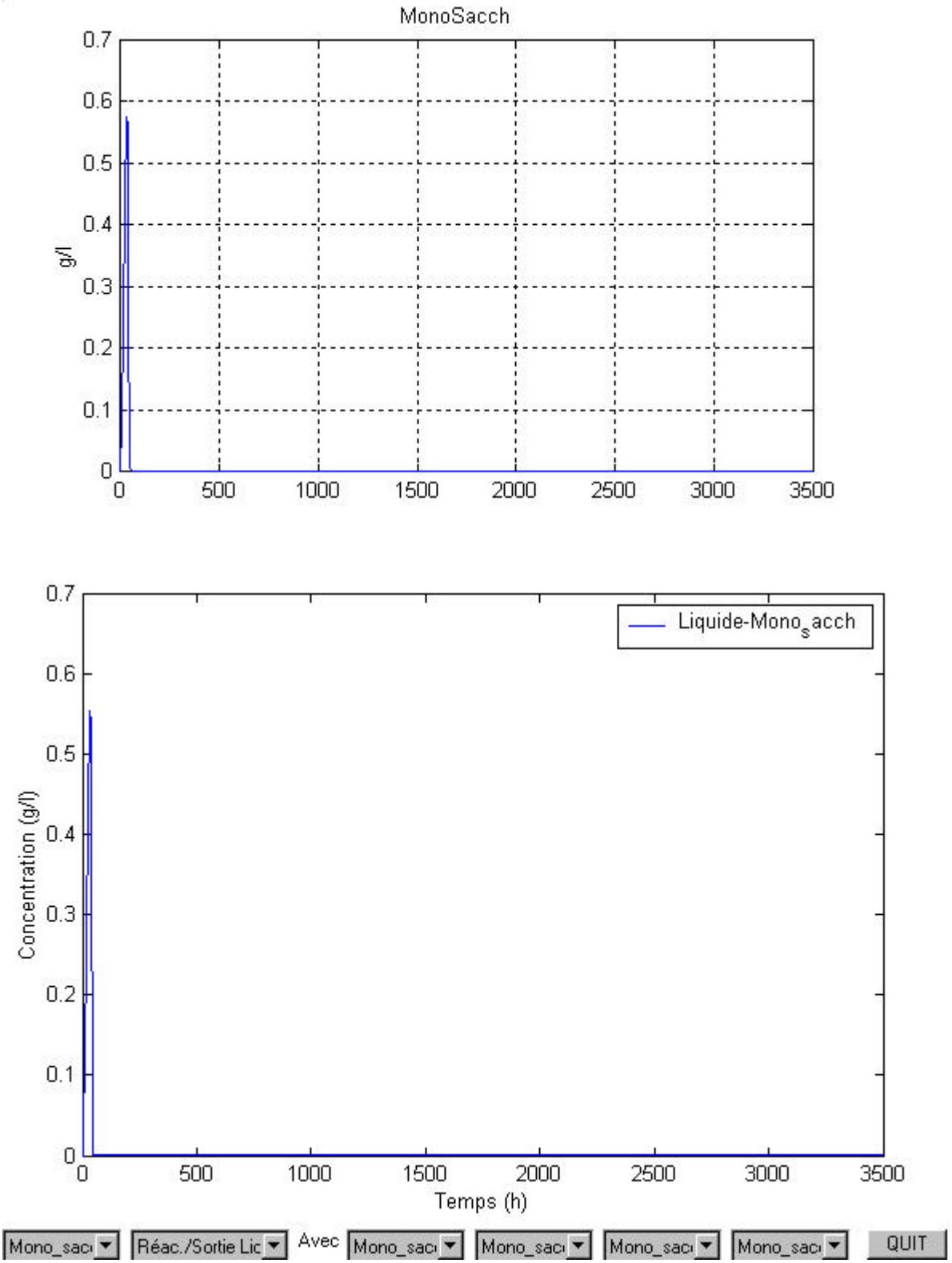

Figure 26. Mono_Sacch

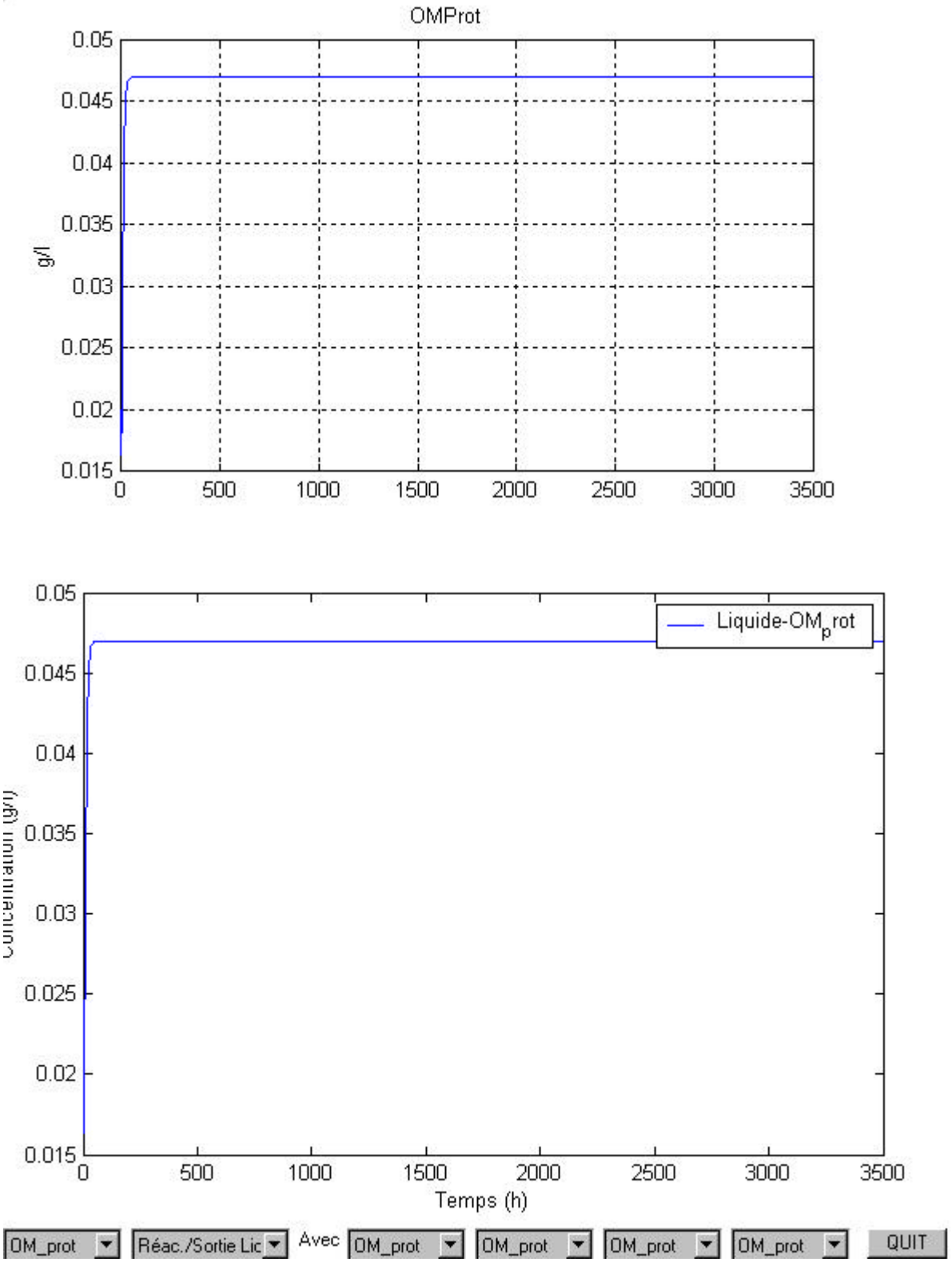

Figure 27. OM_Prot

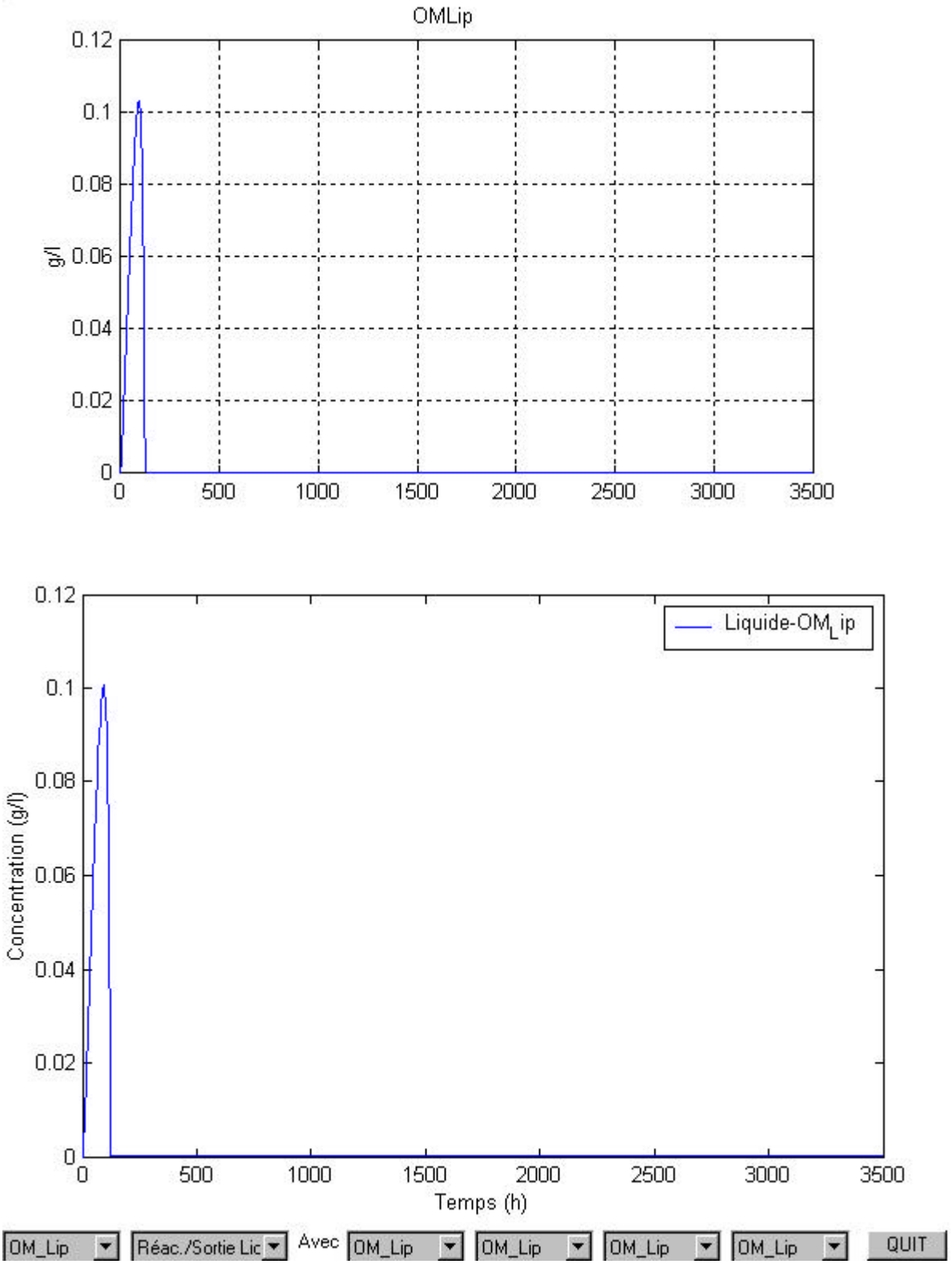

Figure 28. OM_Lip

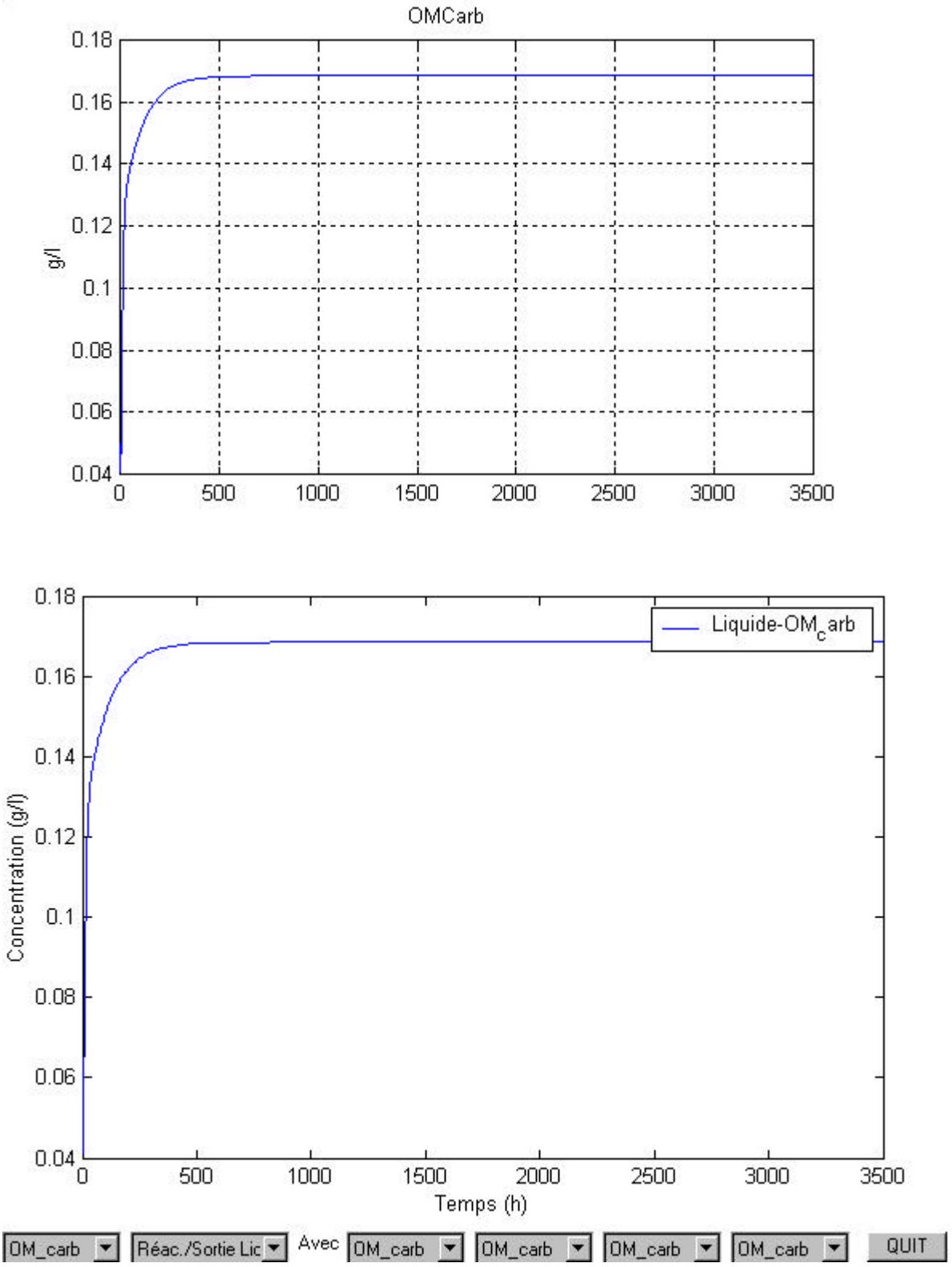

Figure 29. OM_Carb

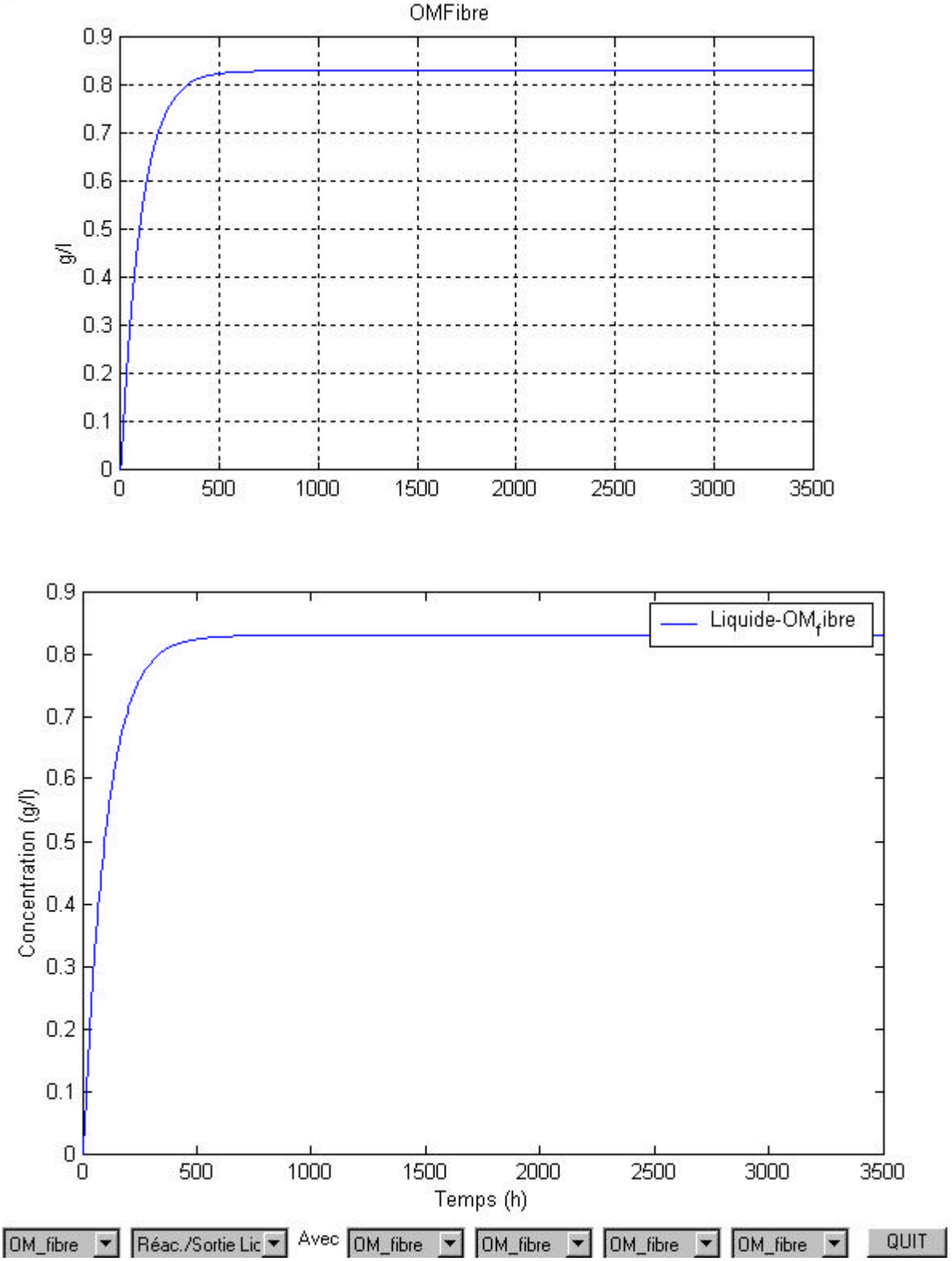

Figure 30. OM_Fibre

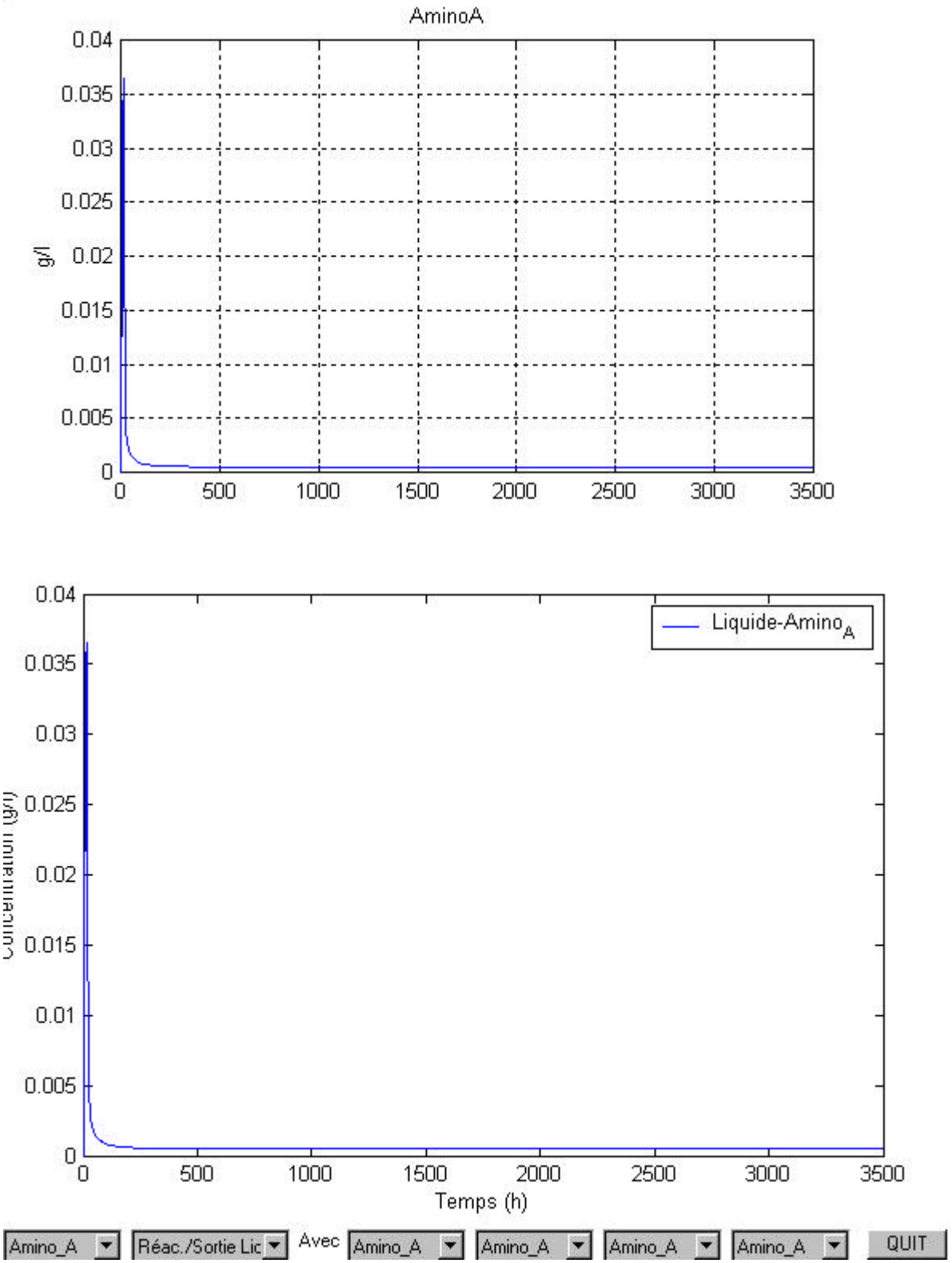

Figure 31. Amino_A

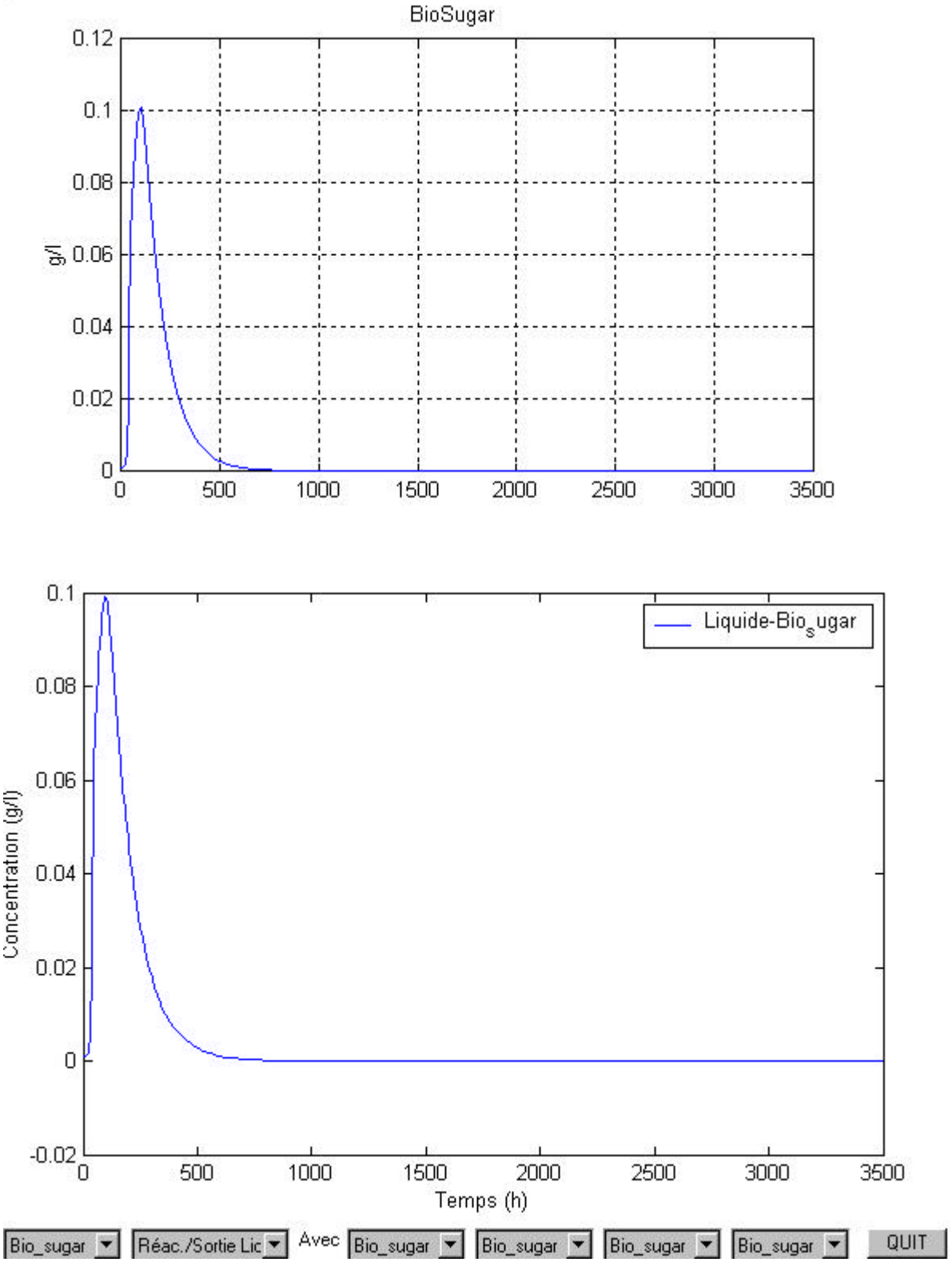

Figure 32. Bio_Sugar

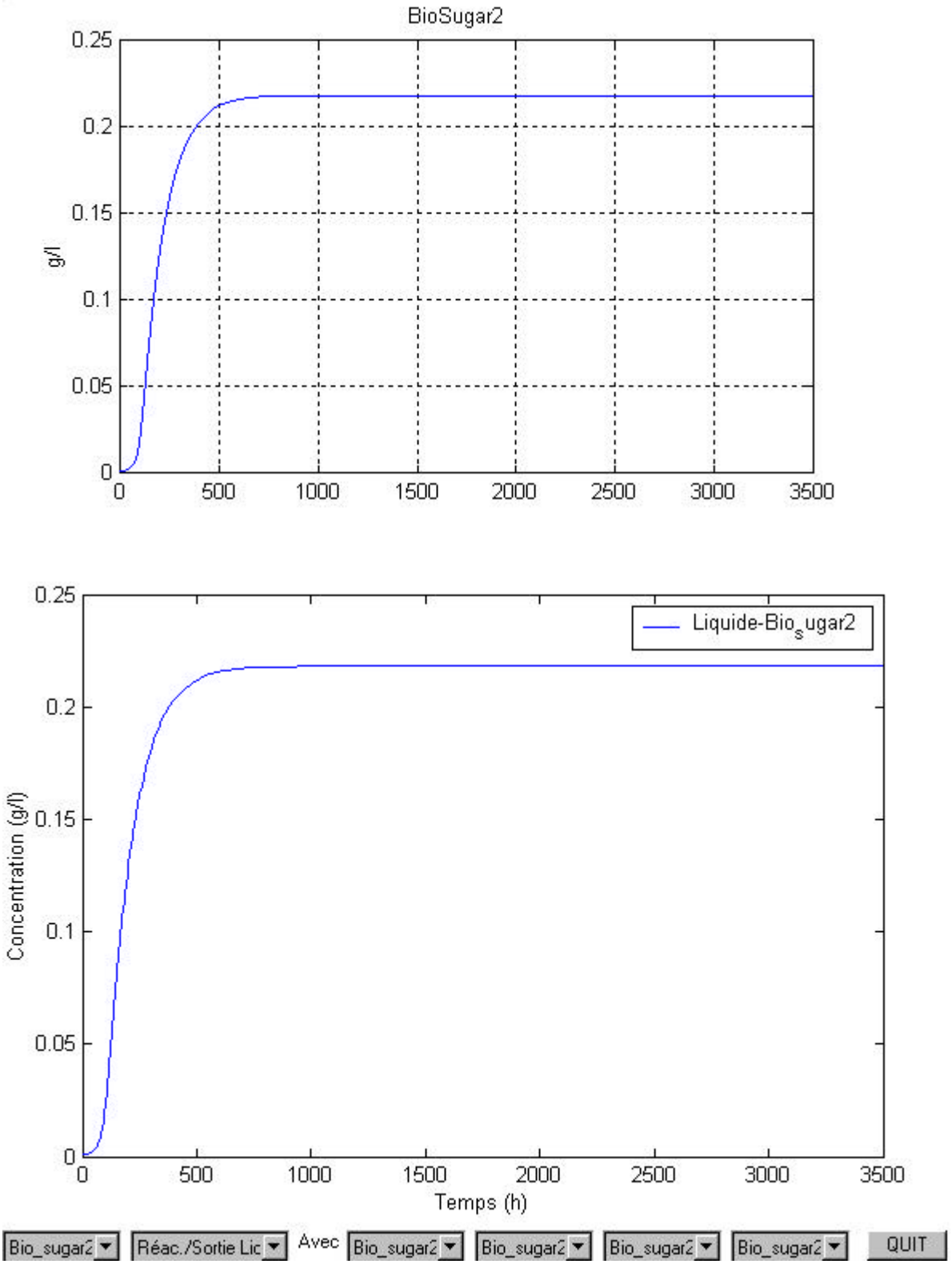

Figure 33. Bio_Sugar2

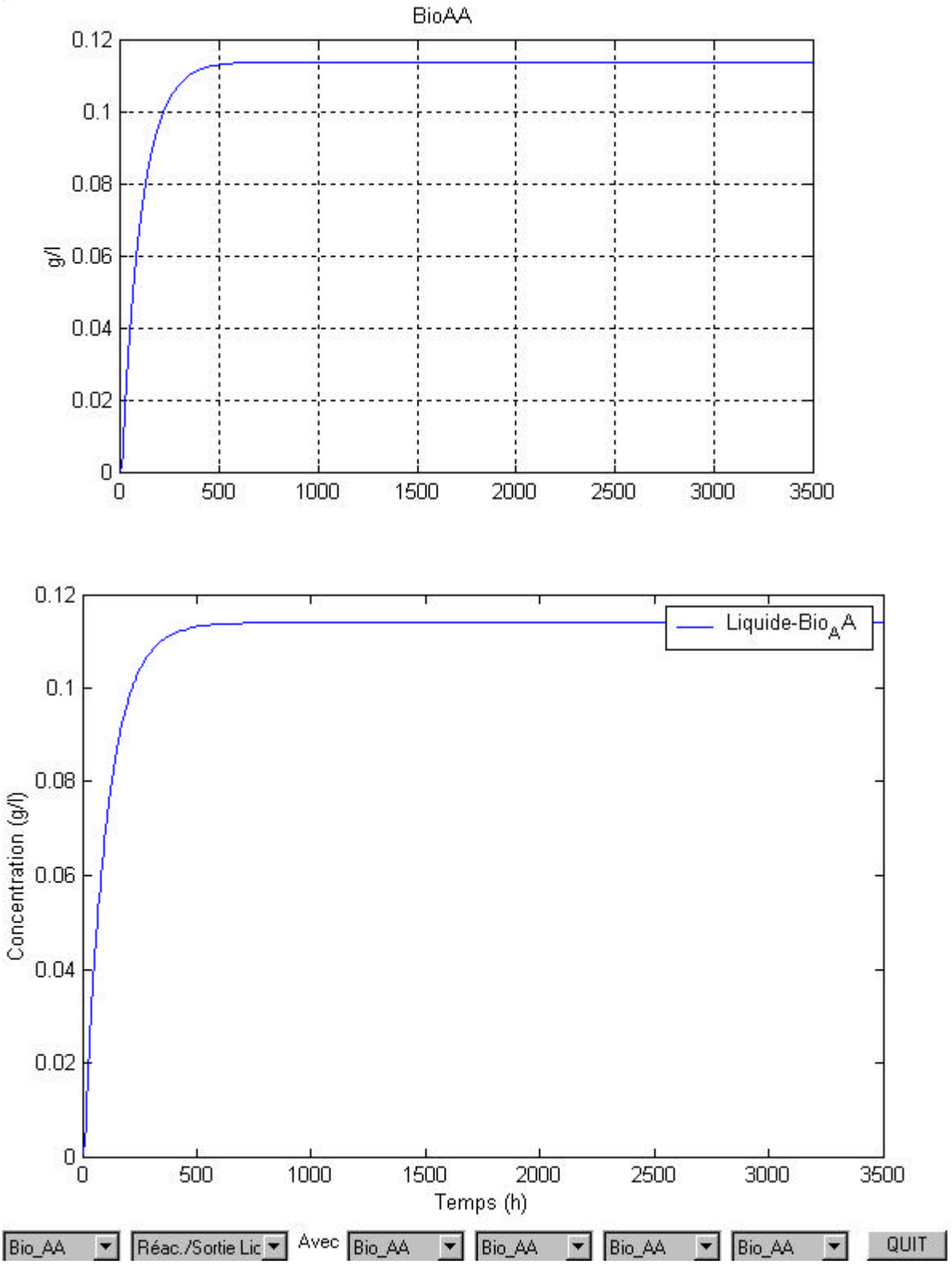

Figure 34. Bio_AA

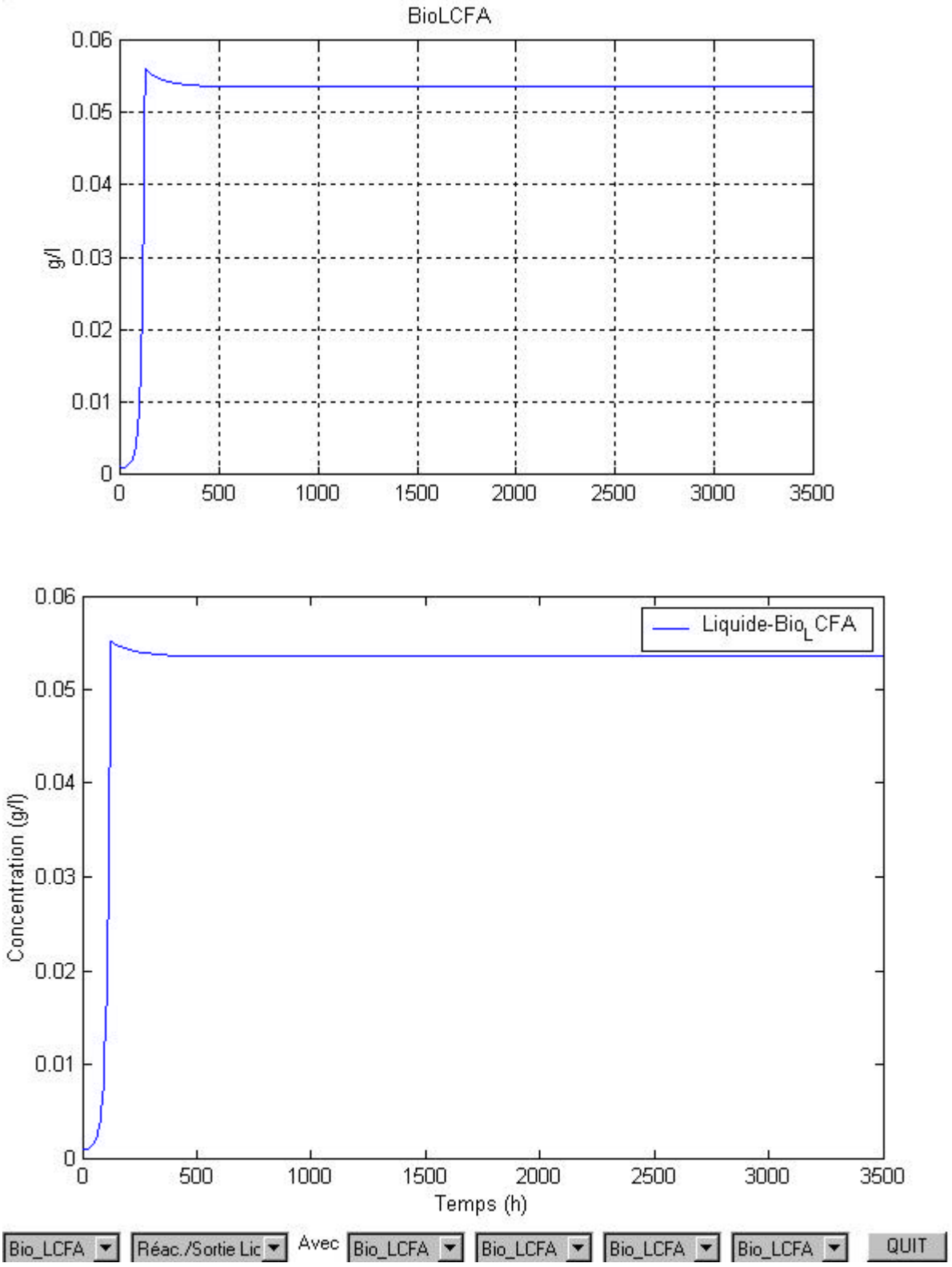

Figure 35. Bio_LCFA

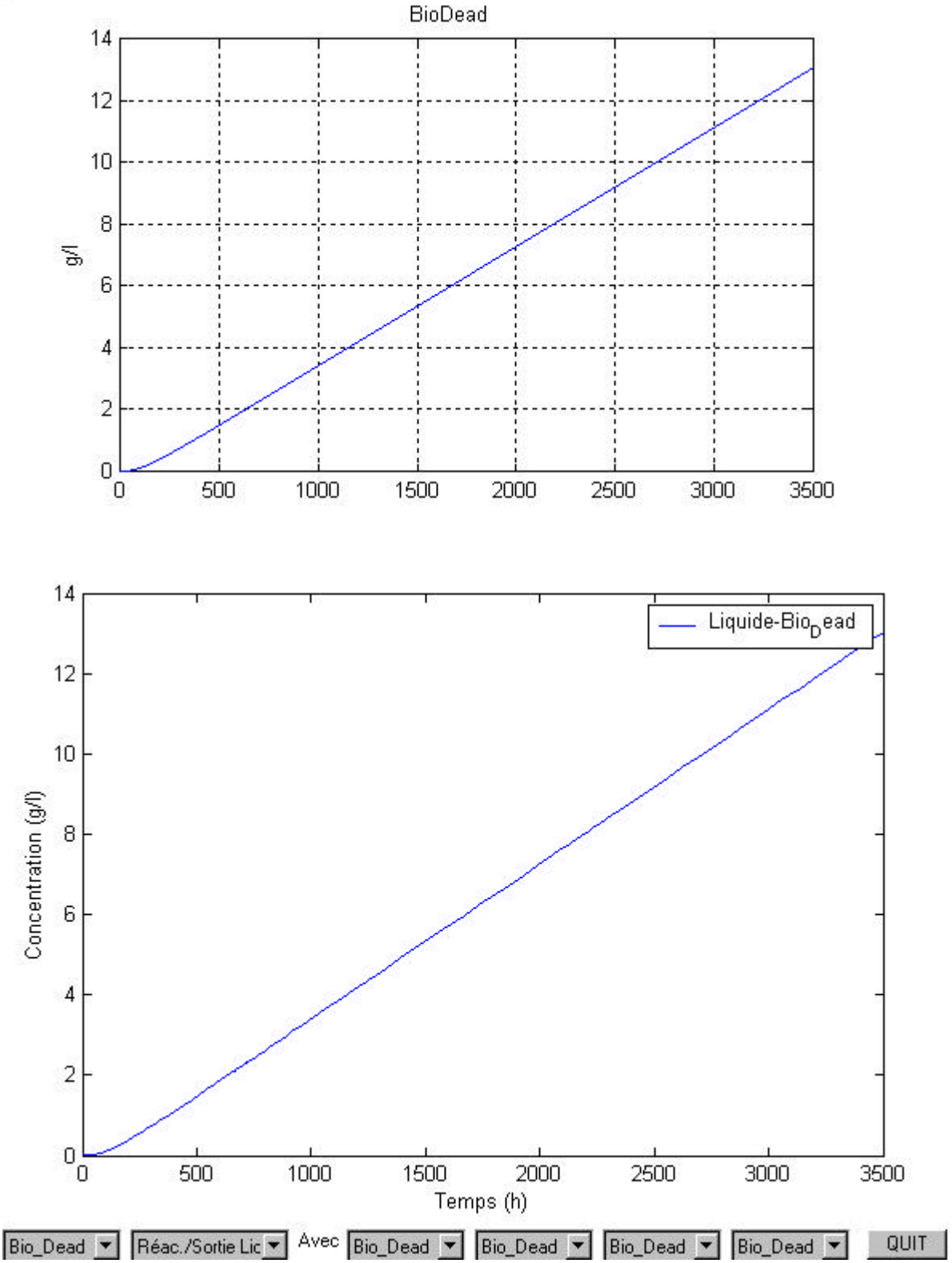

Figure 36. Bio_Dead

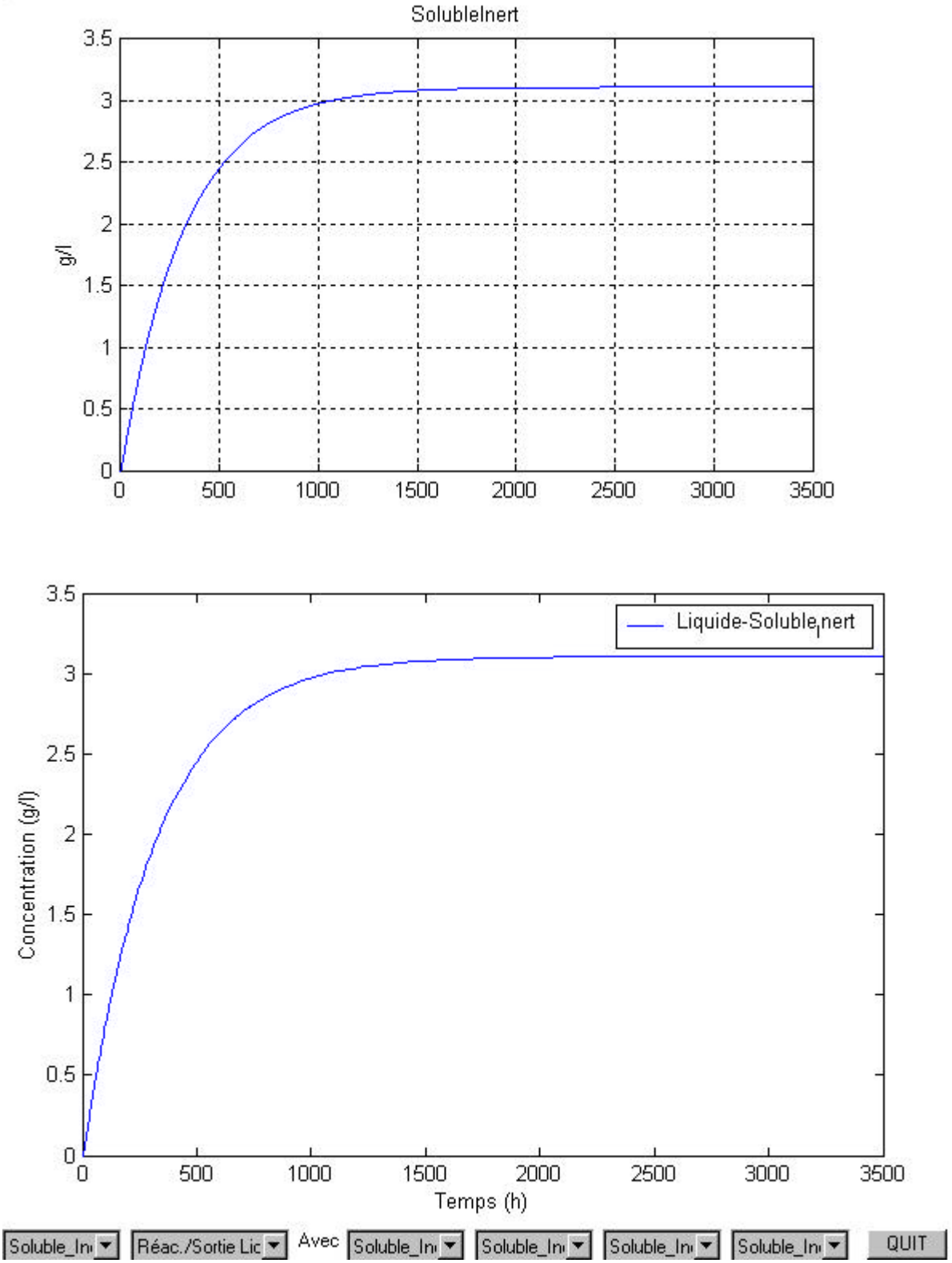

Figure 37. Soluble_Inert

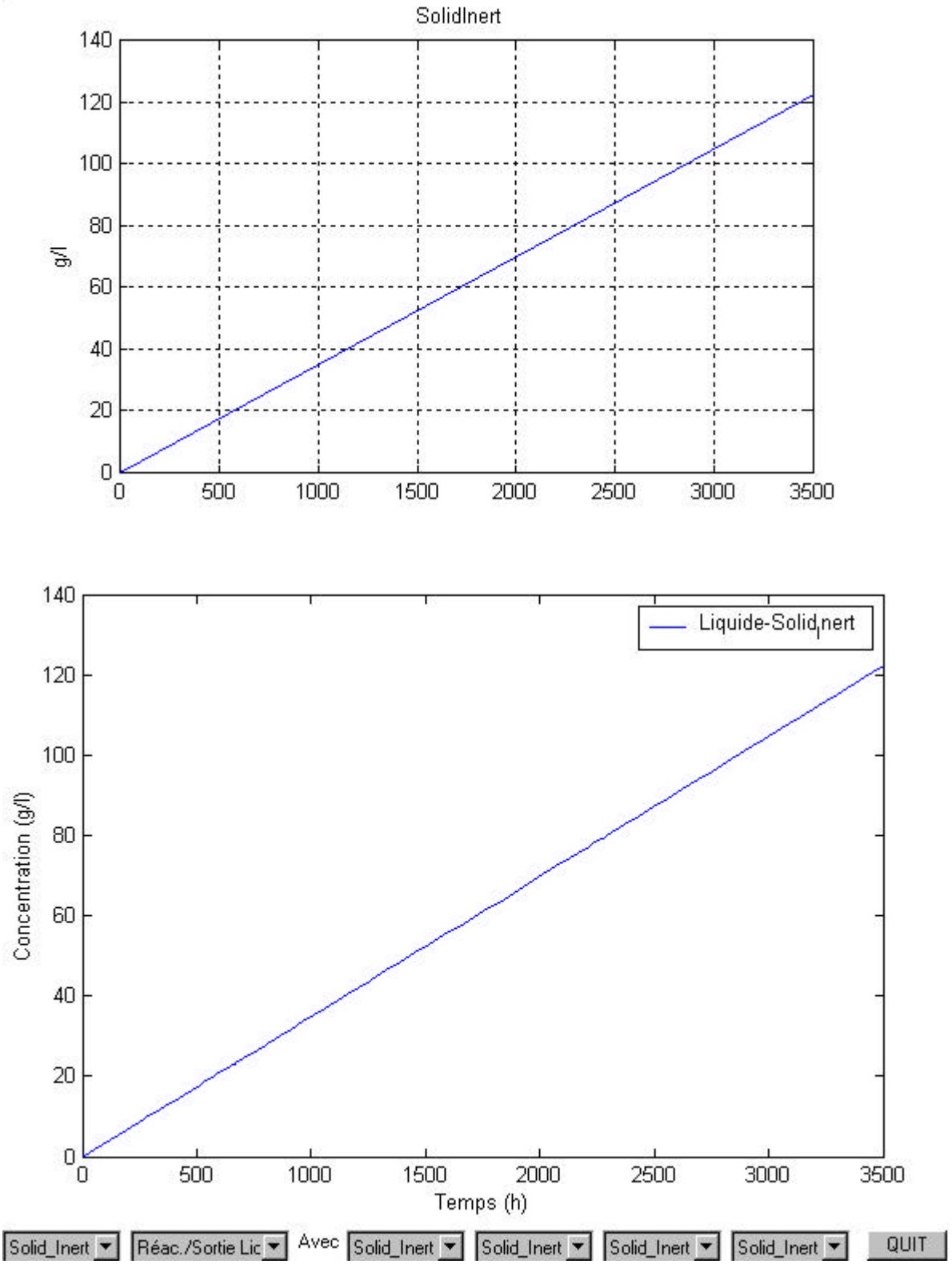

Figure 38. Solid_I

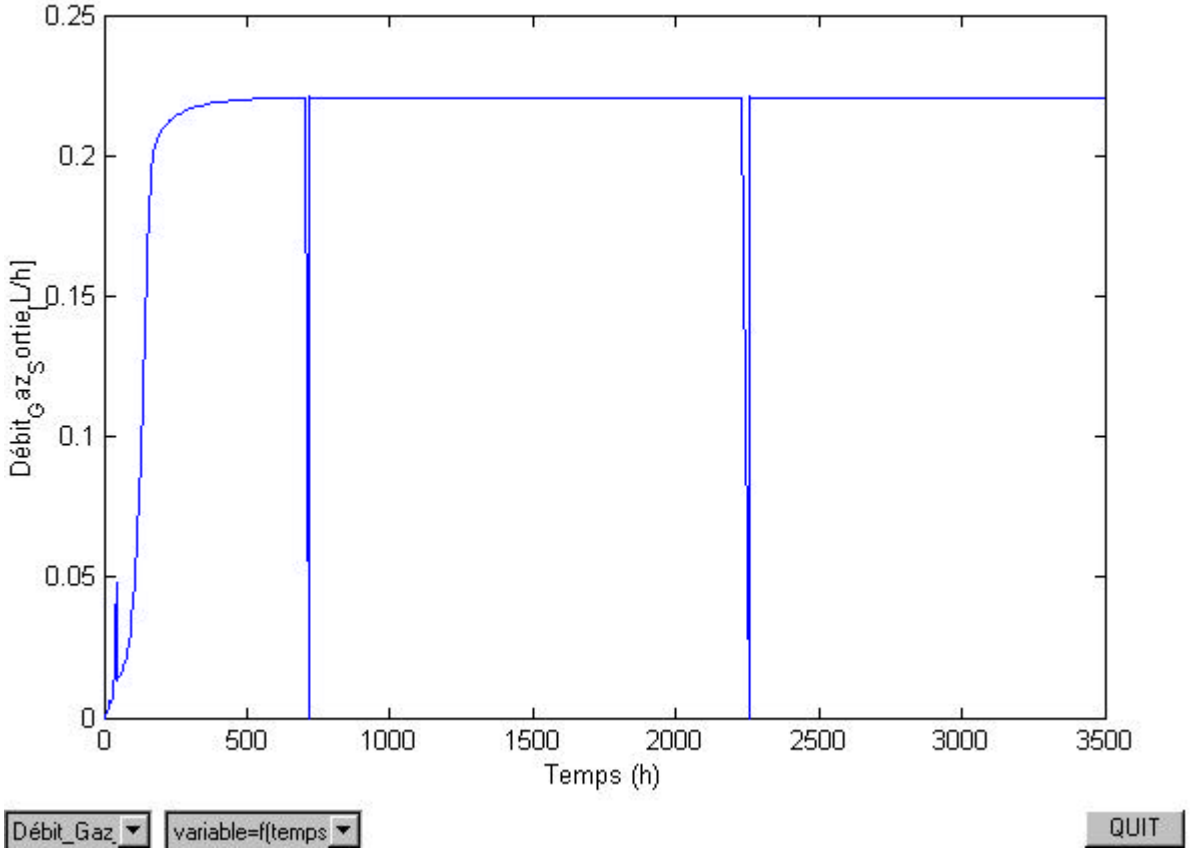

Figure 39. CO2 gas production rate (in l/h at 20 °C and 1 atm)

5.3.1 Steady state of the sub-process defined by the reactions E4, E5, E11 and E15

It has been established that the sub-process limited to the biomasses BioSugar and BioSugar2 of the reactions [E 4], [E 5], [E 11] and [E 15], can be described by the following state system :

$$\dot{a}_{41} = -\beta \cdot a_{41} + \beta \cdot a_{i41} + \alpha_{41} \cdot \mu_4 \cdot C_4 \cdot a_{43} + \alpha_{51} \cdot \mu_5 \cdot C_5 \cdot a_{53}$$

$$\dot{a}_{42} = -\beta \cdot a_{42} + \beta \cdot a_{i42} + \frac{1}{K} \cdot \alpha_{42} \cdot \mu_4 \cdot C_4 \cdot a_{43} + \frac{1}{K} \cdot \alpha_{52} \cdot \mu_5 \cdot C_5 \cdot a_{53}$$

$$\dot{a}_{43} = \left(-\beta_S + \alpha_{43} \cdot \mu_4 \cdot C_4 + \alpha_{11,1} \cdot k_{D11}\right) \cdot a_{43} \quad \Leftrightarrow \quad \dot{a}_{43} = f_4 \cdot a_{43}$$

$$\dot{a}_{53} = \left(-\beta_S + \alpha_{53} \cdot \mu_5 \cdot C_5 + \alpha_{15,1} \cdot k_{D15}\right) \cdot a_{53} \quad \Leftrightarrow \quad \dot{a}_{53} = f_5 \cdot a_{53}$$

with

a_{41} : MonoSacch concentration in the sub-process;
a_{i41} : MonoSacch concentration at sub-process input
a_{42} : NH3 molecular form concentration in the sub-process;
a_{i42} : NH3 molecular form concentration at sub-process input
a_{43} : BioSugar concentration in the sub-process;
a_{53} : BioSugar2 concentration in the sub-process;

For constant inputs, the necessary and sufficient condition of steady state is the null state derivative. So from (2.1) recalled here above, the necessary and sufficient condition is :

$$\begin{cases} \dot{a}_{41} = 0 \\ \dot{a}_{42} = 0 \\ \dot{a}_{43} = 0 \\ \dot{a}_{53} = 0 \end{cases}$$

From this necessary and sufficient condition here above, several sets of sufficient condition can be extracted. To obtain $\dot{a}_{43} = 0$, one of the 2 conditions is sufficient : $f_4 = 0$ or $a_{43} = 0$. In the same way, to fulfil $\dot{a}_{53} = 0$, one of the 2 conditions is sufficient : $f_5 = 0$ or $a_{53} = 0$. So 4 combinations are possible:

- $a_{43} = 0$ and $a_{53} = 0$ → set 1
- $f_4 = 0$ and $f_5 = 0$ → set 2
- $f_4 = 0$ and $a_{53} = 0$ → set 3
- $f_5 = 0$ and $a_{43} = 0$ → set 4

In set 3, to make a_{53} tends to 0 when initial a_{53} is not null, another condition must be fulfilled implicitly : $f_5 < 0$.
In the same way, in set 4, to make a_{43} tends to 0 when initial a_{43} is not null, another condition must be fulfilled implicitly : $f_4 < 0$.

<u>set 1</u>

$$\begin{cases} -\beta \cdot a_{41} + \beta \cdot a_{i41} + \alpha_{41} \cdot \mu_4 \cdot C_4 \cdot a_{43} + \alpha_{51} \cdot \mu_5 \cdot C_5 \cdot a_{53} = 0 \\ -\beta \cdot a_{42} + \beta \cdot a_{i42} + \frac{1}{K} \cdot \alpha_{42} \cdot \mu_4 \cdot C_4 \cdot a_{43} + \frac{1}{K} \cdot \alpha_{52} \cdot \mu_5 \cdot C_5 \cdot a_{53} = 0 \\ a_{43} = 0 \\ a_{53} = 0 \end{cases} \qquad \text{(A2.1)}$$

<u>set 2</u>

$$
\begin{aligned}
&-\beta \cdot a_{41} + \beta \cdot a_{i41} + \alpha_{41} \cdot \mu_4 \cdot C_4 \cdot a_{43} + \alpha_{51} \cdot \mu_5 \cdot C_5 \cdot a_{53} = 0 \\
&-\beta \cdot a_{42} + \beta \cdot a_{i42} + \frac{1}{K} \cdot \alpha_{42} \cdot \mu_4 \cdot C_4 \cdot a_{43} + \frac{1}{K} \cdot \alpha_{52} \cdot \mu_5 \cdot C_5 \cdot a_{53} = 0 \\
&-\beta_S + \alpha_{43} \cdot \mu_4 \cdot C_4 + \alpha_{11,1} \cdot k_{D11} = 0 \\
&-\beta_S + \alpha_{53} \cdot \mu_5 \cdot C_5 + \alpha_{15,1} \cdot k_{D15} = 0
\end{aligned}
\qquad \text{(A2.2)}
$$

<u>set 3</u>

$$
\begin{aligned}
&-\beta \cdot a_{41} + \beta \cdot a_{i41} + \alpha_{41} \cdot \mu_4 \cdot C_4 \cdot a_{43} + \alpha_{51} \cdot \mu_5 \cdot C_5 \cdot a_{53} = 0 \\
&-\beta \cdot a_{42} + \beta \cdot a_{i42} + \frac{1}{K} \cdot \alpha_{42} \cdot \mu_4 \cdot C_4 \cdot a_{43} + \frac{1}{K} \cdot \alpha_{52} \cdot \mu_5 \cdot C_5 \cdot a_{53} = 0 \\
&-\beta_S + \alpha_{43} \cdot \mu_4 \cdot C_4 + \alpha_{11,1} \cdot k_{D11} = 0 \\
&-\beta_S + \alpha_{53} \cdot \mu_5 \cdot C_5 + \alpha_{15,1} \cdot k_{D15} < 0 \quad \text{to have} \quad a_{53} = 0 \quad \text{at infinite}
\end{aligned}
\qquad \text{(A2.3)}
$$

<u>set 4</u>

$$
\begin{aligned}
&-\beta \cdot a_{41} + \beta \cdot a_{i41} + \alpha_{41} \cdot \mu_4 \cdot C_4 \cdot a_{43} + \alpha_{51} \cdot \mu_5 \cdot C_5 \cdot a_{53} = 0 \\
&-\beta \cdot a_{42} + \beta \cdot a_{i42} + \frac{1}{K} \cdot \alpha_{42} \cdot \mu_4 \cdot C_4 \cdot a_{43} + \frac{1}{K} \cdot \alpha_{52} \cdot \mu_5 \cdot C_5 \cdot a_{53} = 0 \\
&-\beta_S + \alpha_{43} \cdot \mu_4 \cdot C_4 + \alpha_{11,1} \cdot k_{D11} < 0 \quad \text{to have} \quad a_{43} = 0 \quad \text{at infinite} \\
&-\beta_S + \alpha_{53} \cdot \mu_5 \cdot C_5 + \alpha_{15,1} \cdot k_{D15} = 0
\end{aligned}
\qquad \text{(A2.4)}
$$

5.3.2 . Analysis of the set 1 of equations

<u>Recall of set 1</u>

$$
\begin{aligned}
&-\beta \cdot a_{41} + \beta \cdot a_{i41} + \alpha_{41} \cdot \mu_4 \cdot C_4 \cdot a_{43} + \alpha_{51} \cdot \mu_5 \cdot C_5 \cdot a_{53} = 0 \\
&-\beta \cdot a_{42} + \beta \cdot a_{i42} + \frac{1}{K} \cdot \alpha_{42} \cdot \mu_4 \cdot C_4 \cdot a_{43} + \frac{1}{K} \cdot \alpha_{52} \cdot \mu_5 \cdot C_5 \cdot a_{53} = 0 \\
&a_{43} = 0 \\
&a_{53} = 0
\end{aligned}
\qquad \text{(A2.1)}
$$

This set of equations is equivalent to

$$
\begin{aligned}
&-\beta \cdot a_{41} + \beta \cdot a_{i41} = 0 \\
&-\beta \cdot a_{42} + \beta \cdot a_{i42} = 0
\end{aligned}
$$

which give the trivial solution (where index ‘0’ means ‘at steady state’) :

$$
\begin{aligned}
&a_{410} = a_{i41} \\
&a_{420} = a_{i42} \\
&a_{430} = 0 \\
&a_{530} = 0
\end{aligned}
\qquad \text{(A2.5)}
$$

Such a state

$$
X_0 = \begin{bmatrix} a_{410} \\ a_{420} \\ a_{430} \\ a_{530} \end{bmatrix}
$$

is a sufficient condition of steady state obviously but has no interest as it represents a process without biomass (a_{430}=0 and a_{530}=0) where nothing happens except a dilution phenomenon whose steady state

is precisely [a_{410}, a_{420}] : the concentrations of the compounds inside the reactor tend to the values of these compounds in the input flow.

5.3.3 Analysis of the set 2 of equations

Recall of set 2

$$\begin{aligned}
&-\beta \cdot a_{41} + \beta \cdot a_{i41} + \alpha_{41} \cdot \mu_4 \cdot C_4 \cdot a_{43} + \alpha_{51} \cdot \mu_5 \cdot C_5 \cdot a_{53} = 0 \\
&-\beta \cdot a_{42} + \beta \cdot a_{i42} + \frac{1}{K} \cdot \alpha_{42} \cdot \mu_4 \cdot C_4 \cdot a_{43} + \frac{1}{K} \cdot \alpha_{52} \cdot \mu_5 \cdot C_5 \cdot a_{53} = 0 \\
&-\beta_S + \alpha_{43} \cdot \mu_4 \cdot C_4 + \alpha_{11,1} \cdot k_{D11} = 0 \\
&-\beta_S + \alpha_{53} \cdot \mu_5 \cdot C_5 + \alpha_{15,1} \cdot k_{D15} = 0
\end{aligned} \qquad \text{(A2.2)}$$

The set of equations to be solved is composed of 4 equations and 4 unknowns. So at least one mathematical solution exists.

Remembering the expression of C4 and C5 in (2.1) :

$$C_4 = \frac{a_{41}}{k_{S41} + a_{41}} \cdot \frac{a_{42}}{k_{S42} + a_{42}}$$

$$C_5 = \frac{a_{41}}{k_{S51} + a_{41}} \cdot \frac{a_{42}}{k_{S52} + a_{42}}$$

and given the expression of an intermediate variable $C = \frac{C_4}{C_5} \cdot \frac{k_{S41} + a_{41}}{k_{S51} + a_{41}}$

the expression of a_{420} (a_{42} at steady state) can be obtained from the 2 last equations of (A2.2):

$$a_{420} = -\frac{k_{S52} - C \cdot k_{S42}}{1 - C}$$

In the present case, the half saturation constants of BioSugar and BioSugar2 growth related to NH3, k_{S42} and k_{S52}, are identical : $k_{S42} = k_{S52} = 10^{-4}$ g/l .
Then

$a_{420} = - k_{S42} = - 10^{-4}$ g/l.

which is a mathematical solution but not a physical one as a concentration cannot be negative.
So there is no physical solution to the sufficient condition (A2.2).

Of course, the present result depends on the equality of k_{S42} and k_{S52}. If the values of the half saturation constants were to be changed in the future, the problem should be considered again.

5.3.4 Analysis of the set 3 of equations

Recall of set 3

$$\begin{aligned}
&-\beta \cdot a_{41} + \beta \cdot a_{i41} + \alpha_{41} \cdot \mu_4 \cdot C_4 \cdot a_{43} + \alpha_{51} \cdot \mu_5 \cdot C_5 \cdot a_{53} = 0 \\
&-\beta \cdot a_{42} + \beta \cdot a_{i42} + \frac{1}{K} \cdot \alpha_{42} \cdot \mu_4 \cdot C_4 \cdot a_{43} + \frac{1}{K} \cdot \alpha_{52} \cdot \mu_5 \cdot C_5 \cdot a_{53} = 0 \\
&-\beta_S + \alpha_{43} \cdot \mu_4 \cdot C_4 + \alpha_{11,1} \cdot k_{D11} = 0 \\
&-\beta_S + \alpha_{53} \cdot \mu_5 \cdot C_5 + \alpha_{15,1} \cdot k_{D15} < 0 \quad \text{to have} \quad a_{53} = 0 \quad \text{at infinite}
\end{aligned} \qquad \text{(A2.3)}$$

It is recalled that the aim is to compute a peculiar value X_0 of the state :

$$X_0 = \begin{bmatrix} a_{410} \\ a_{420} \\ a_{430} \\ a_{530} \end{bmatrix}$$

such that the derivative of the state is null.
As $a_{53} = 0$, (A2.3) can be simplified into :

$$\begin{cases} -\beta \cdot a_{41} + \beta \cdot a_{i41} + \alpha_{41} \cdot \mu_4 \cdot C_4 \cdot a_{43} = 0 \\ -\beta \cdot a_{42} + \beta \cdot a_{i42} + \dfrac{1}{K} \cdot \alpha_{42} \cdot \mu_4 \cdot C_4 \cdot a_{43} = 0 \\ -\beta_S + \alpha_{43} \cdot \mu_4 \cdot C_4 + \alpha_{11,1} \cdot k_{D11} = 0 \end{cases}$$

From the 2 first equations, one of the variables a_{41} and a_{42} can be expressed in function of the other :

$$a_{42} = \frac{\alpha_{42}}{\alpha_{41}} \cdot \frac{1}{K} \cdot (a_{41} - a_{i41}) + a_{i42}$$

$$\Leftrightarrow$$

$$a_{41} = K \frac{\alpha_{41}}{\alpha_{42}} \cdot (a_{42} - a_{i42}) + a_{i41}$$

When these variables are replaced into the expression of C_4 of the third equation, one obtains a second order equation where a_{41} or a_{42} is the unknown (see relations (A2.5) and (A2.9) hereafter). So the system (A2.3) has 2 mathematical roots. Then the problem is to determine if these 2 roots are physical solutions. Fortunately it is possible to check that (A2.3) has only one positive solution.

1. Expression of a_{410} :
a_{410} is a solution of the second order equation where a_{41} is the unknown :

$$\begin{cases} A_1 \cdot a_{41}^2 + A_2 \cdot a_{41} + A_3 = 0 \\ \text{with} \quad A_1 = \left(1 - \dfrac{1}{C_{40}}\right) \cdot K_\alpha \\ A_2 = \left(1 - \dfrac{1}{C_{40}}\right) \cdot (a_{i42} - K_\alpha \cdot a_{i41}) + k_{S41} \cdot K_\alpha + k_{S42} \\ A_3 = k_{S41} \cdot (a_{i42} - K_\alpha \cdot a_{i41} + k_{S42}) \\ \dfrac{1}{C_{40}} = \dfrac{\alpha_{43} \cdot \mu_4}{\beta_S - \alpha_{11,1} \cdot k_{D11}} \quad (1) \\ K_\alpha = \dfrac{\alpha_{42}}{\alpha_{41}} \cdot \dfrac{1}{K} \end{cases} \qquad \text{(A2.5)}$$

Given $\Delta = A_2^2 - 4 \cdot A_1 \cdot A_3$

if $\Delta \geq 0$, the roots are: $a'_{410} = \dfrac{-A_2 + \sqrt{\Delta}}{2 \cdot A_1}$ and $a_{410} = \dfrac{-A_2 - \sqrt{\Delta}}{2 \cdot A_1}$ (A2.6)

with $a'_{410} < a_{410}$ because $A_1 < 0$ ([2]).

There is only one positive root a_{410} as long as $\dfrac{A_3}{A_1} < 0 \quad \Leftrightarrow \quad A_3 > 0$

$$\Leftrightarrow a_{i42} \geq a_{i42m}$$

$$\text{with} \quad a_{i42m} = \frac{\alpha_{42}}{\alpha_{41}} \cdot \frac{1}{K} \cdot a_{i41} - k_{S42} \tag{A2.7}$$

When $a_{i42} < a_{i42m}$, it is not easy to know if the roots are positive or negative because the sign of $\frac{A_2}{A_1}$ cannot be determined.

Moreover it is impossible to determine the sign of a_{420} when it is computed from:

$$a_{420} = \frac{\alpha_{42}}{\alpha_{41}} \cdot \frac{1}{K} \cdot (a_{410} - a_{i41}) + a_{i42} \tag{A2.8}$$

It is why it is preferable to extract a_{42} from the following second order equation (A2.9).

([1]) Remark 1: $\beta_S - \alpha_{11,1} \cdot k_{D11}$ is strictly positive as $\beta_S \geq 0$ and $\alpha_{11,1} < 0$

([2]) Remark 2: $A_1 < 0$ as long as $q_d < (\alpha_{43} \cdot \mu_4 + \alpha_{11,1} \cdot k_{D11}) \cdot V_L = 0.39 * 25 = 9.75 \ l/h$, which is true for the prototype reactor of 25 litres.

2. Expression of a_{420} :

a_{420} is a solution of the second order equation where a_{42} is the unknown :

$$\begin{aligned}
&A_1 \cdot a_{42}^2 + A_2 \cdot a_{42} + A_3 = 0 \\
&\text{with} \quad A_1 = \left(1 - \frac{1}{C_{40}}\right) \cdot K_\alpha \\
&A_2 = \left(1 - \frac{1}{C_{40}}\right) \cdot (a_{i41} - K_\alpha \cdot a_{i42}) + k_{S42} \cdot K_\alpha + k_{S41} \\
&A_3 = k_{S42} \cdot (a_{i41} - K_\alpha \cdot a_{i42} + k_{S41}) \\
&\frac{1}{C_{40}} = \frac{\alpha_{43} \cdot \mu_4}{\beta_S - \alpha_{11,1} \cdot k_{D11}} \\
&K_\alpha = \frac{\alpha_{41}}{\alpha_{42}} \cdot K
\end{aligned} \tag{A2.9}$$

Given $\Delta = A_2^2 - 4 \cdot A_1 \cdot A_3$

if $\Delta \geq 0$, the roots are: $a'_{420} = \frac{-A_2 + \sqrt{\Delta}}{2 \cdot A_1}$ and $a_{420} = \frac{-A_2 - \sqrt{\Delta}}{2 \cdot A_1}$ (A2.10)

with $a'_{420} < a_{420}$ because $A_1 < 0$.

There is only one positive root a_{420} as long as $\frac{A_3}{A_1} < 0 \quad \Leftrightarrow \quad A_3 > 0$

$$\Leftrightarrow a_{i42} \leq a_{i42M}$$

$$\text{with} \quad a_{i42M} = \frac{\alpha_{42}}{\alpha_{41}} \cdot \frac{1}{K} \cdot (a_{i41} + k_{S41}) \tag{A2.11}$$

When $a_{i42} > a_{i42M}$ there are 2 positive roots as the sign of A_2 is positive $\Leftrightarrow -\frac{A_2}{A_1} > 0$.

The lack of determination is cancelled in next section.

3. How to compute a_{410} and a_{420}

The previous results are gathered in Figure 40.

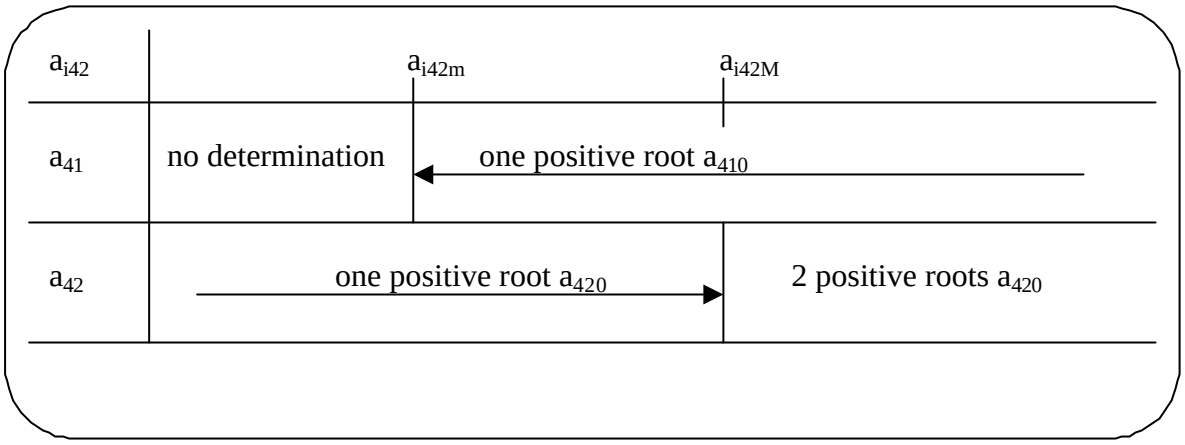

Figure 40. Domain of existence of only one positive root for a_{41} and a_{42}

So to be sure to get the only one positive solution, it is sufficient to compute :

- a_{410} of (A2.6) when a_{i42} is such that : $a_{i42} \geq a_{i42m}$ or $a_{i42} \geq a_{i42M}$
- a_{420} of (A2.10) when a_{i42} is such that : $a_{i42} < a_{i42M}$

When a_{410} is computed by (A2.6), a_{420} is computed by :

$$a_{420} = \frac{\alpha_{42}}{\alpha_{41}} \cdot \frac{1}{K} \cdot (a_{410} - a_{i41}) + a_{i42} \qquad \text{(A2.12)}$$

When a_{420} is computed by (A2.10), a_{410} is computed by :

$$a_{410} = K \frac{\alpha_{41}}{\alpha_{42}} \cdot (a_{420} - a_{i42}) + a_{i41} \qquad \text{(A2.13)}$$

The expression of BioSugar concentration is :

$$a_{430} = \frac{\beta}{\alpha_{41} \cdot \mu_4 \cdot C_{40}} \cdot (a_{410} - a_{i41}) \qquad \text{(A2.14)}$$

4. Taking into account the negative derivative of BioSugar2 concentration

Up to now only the 3 first equations of (A2.3) have been considered. The objective is to look for the implications of the inequality.

This inequality can be rewritten :

$$\frac{a_{41}}{k_{S51} + a_{41}} \cdot \frac{a_{42}}{k_{S52} + a_{42}} < C_{50}$$

$$\text{with} \quad C_{50} = \frac{\beta_S - \alpha_{15,1} \cdot k_{D15}}{\alpha_{53} \cdot \mu_5} \qquad \text{(A2.15)}$$

$$\text{Re call :} \quad \alpha_{53} > 0 \quad \text{and} \quad \alpha_{15,1} < 0$$

It implies :

$y > 0$

with $y = A_1 \cdot a_{42}^2 + A_2 \cdot a_{42} + A_3$

$$A_1 = \left(1 - \frac{1}{C_{50}}\right) \cdot K_\alpha$$

$$A_2 = \left(1 - \frac{1}{C_{50}}\right) \cdot \left(a_{i41} - K_\alpha \cdot a_{i42}\right) + k_{S52} \cdot K_\alpha + k_{S51} \qquad \text{(A2.16)}$$

$$A_3 = k_{S52} \cdot \left(a_{i41} - K_\alpha \cdot a_{i42} + k_{S51}\right)$$

$$\frac{1}{C_{50}} = \frac{\alpha_{53} \cdot \mu_5}{\beta_S - \alpha_{15,1} \cdot k_{D15}}$$

$$K_\alpha = \frac{\alpha_{41}}{\alpha_{42}} \cdot K$$

Given $\Delta = A_2^2 - 4 \cdot A_1 \cdot A_3$

if $\Delta \geq 0$, the roots of 'y = 0' are: $a_{421} = \dfrac{-A_2 + \sqrt{\Delta}}{2 \cdot A_1}$ and $a_{422} = \dfrac{-A_2 - \sqrt{\Delta}}{2 \cdot A_1}$ (A2.17)

with $a_{421} < a_{422}$ because $A_1 < 0$ ([3]).

The derivative of y is : $\dot{y} = 2 \cdot A_1 \cdot a_{42} + A_2$

Figure 41 shows that 'y' is positive for a_{42} belonging to the interval [a_{421} a_{422}].

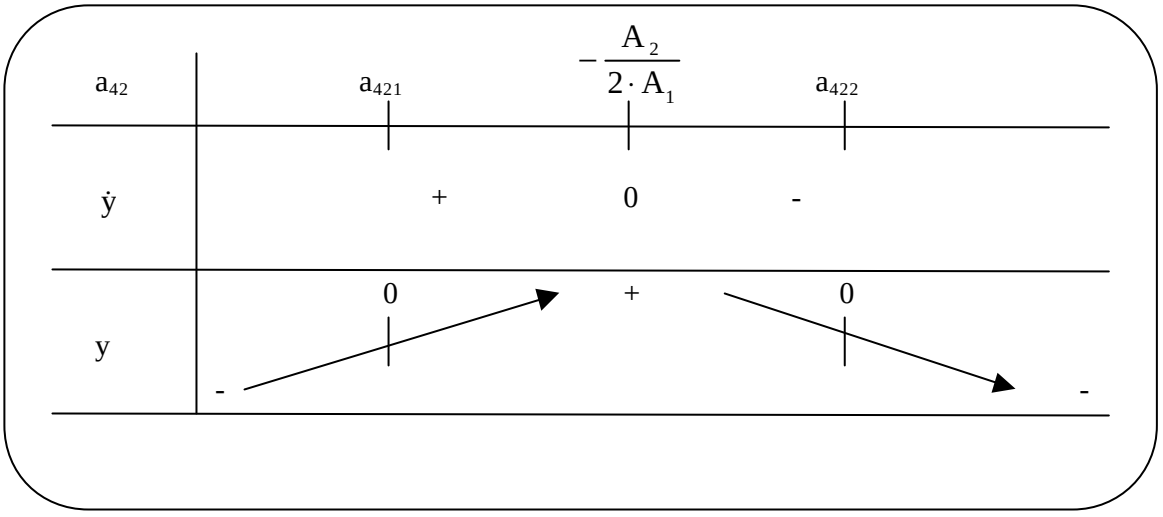

Figure 41. Sign of y

So the inequality of (A2.3) is fulfilled only if a_{42} belongs to the interval [a_{421} a_{422}].

In other words, the solution a_{420} of (A2.10) and (A2.12) must belong to the interval [a_{421} a_{422}] defined in (A2.17).	(A2.18)

Then the steady state that fulfil the equations system (A2.3) is :

$$X_0 = \begin{bmatrix} a_{410} \\ a_{420} \\ a_{430} \\ 0 \end{bmatrix} \qquad \text{(A2.19)}$$

If the solution a_{420} of (A2.10) and (A2.12) does not belong to $[a_{421} \quad a_{422}]$ defined in (A2.17), the steady state X_0 does not exist.

([3]) Remark : $A_1 < 0 \Leftrightarrow \left(1 - \frac{1}{C_{50}}\right) < 0$ as long as $q_d < \left(\alpha_{53} \cdot \mu_5 + \alpha_{15,1} \cdot k_{D15}\right) \cdot V$,

or $q_d < 2.25 \ \ l/h$, which is true in the case of the 25 litres prototype reactor.

5.3.5 Analysis of the set 4 of equations

Recall of set 4

$$\begin{aligned} &-\beta \cdot a_{41} + \beta \cdot a_{i41} + \alpha_{41} \cdot \mu_4 \cdot C_4 \cdot a_{43} + \alpha_{51} \cdot \mu_5 \cdot C_5 \cdot a_{53} = 0 \\ &-\beta \cdot a_{42} + \beta \cdot a_{i42} + \frac{1}{K} \cdot \alpha_{42} \cdot \mu_4 \cdot C_4 \cdot a_{43} + \frac{1}{K} \cdot \alpha_{52} \cdot \mu_5 \cdot C_5 \cdot a_{53} = 0 \\ &-\beta_S + \alpha_{43} \cdot \mu_4 \cdot C_4 + \alpha_{11,1} \cdot k_{D11} < 0 \quad \text{to have} \quad a_{43} = 0 \quad \text{at infinite} \\ &-\beta_S + \alpha_{53} \cdot \mu_5 \cdot C_5 + \alpha_{15,1} \cdot k_{D15} = 0 \end{aligned} \qquad \text{(A2.4)}$$

The way to solve this set 4 is quite similar to the one of set 3.

As $a_{43} = 0$, (A2.4) can be simplified into :

$$-\beta \cdot a_{41} + \beta \cdot a_{i41} + \alpha_{51} \cdot \mu_5 \cdot C_5 \cdot a_{53} = 0$$

$$-\beta \cdot a_{42} + \beta \cdot a_{i42} + \frac{1}{K} \cdot \alpha_{52} \cdot \mu_5 \cdot C_5 \cdot a_{53} = 0$$

$$-\beta_S + \alpha_{53} \cdot \mu_5 \cdot C_5 + \alpha_{15,1} \cdot k_{D15} = 0$$

From the 2 first equations, one of the variables a_{41} and a_{42} can be expressed in function of the other :

$$a_{42} = \frac{\alpha_{52}}{\alpha_{51}} \cdot \frac{1}{K} \cdot \left(a_{41} - a_{i41}\right) + a_{i42}$$

$$a_{41} = K \frac{\alpha_{51}}{\alpha_{52}} \cdot \left(a_{42} - a_{i42}\right) + a_{i41}$$

When these variables are replaced into the expression of C_5 of the third equation, one obtains a second order equation where a_{41} or a_{42} is the unknown (see relations (A2.20) and (A2.24) hereafter). So the system (A2.4) has 2 mathematical roots. Then the problem is to determine if these 2 roots are physical solutions. As for (A2.3) it is possible to check that (A2.4) has only one positive solution.

1. Expression of a_{410} :

a_{410} is a solution of the second order equation where a_{41} is the unknown :

$$
\begin{aligned}
&A_1 \cdot a_{41}^2 + A_2 \cdot a_{41} + A_3 = 0 \\
&\text{with} \qquad A_1 = \left(1 - \frac{1}{C_{50}}\right) \cdot K_\alpha \\
&\qquad\qquad A_2 = \left(1 - \frac{1}{C_{50}}\right) \cdot \left(a_{i42} - K_\alpha \cdot a_{i41}\right) + k_{S51} \cdot K_\alpha + k_{S52} \\
&\qquad\qquad A_3 = k_{S51} \cdot \left(a_{i42} - K_\alpha \cdot a_{i41} + k_{S52}\right) \\
&\qquad\qquad \frac{1}{C_{50}} = \frac{\alpha_{53} \cdot \mu_5}{\beta_S - \alpha_{15,1} \cdot k_{D15}} \\
&\qquad\qquad K_\alpha = \frac{\alpha_{52}}{\alpha_{51}} \cdot \frac{1}{K}
\end{aligned}
\qquad \text{(A2.20)}
$$

Given $\Delta = A_2^2 - 4 \cdot A_1 \cdot A_3$

if $\Delta \geq 0$, the roots are: $a'_{410} = \dfrac{-A_2 + \sqrt{\Delta}}{2 \cdot A_1}$ and $a_{410} = \dfrac{-A_2 - \sqrt{\Delta}}{2 \cdot A_1}$ (A2.21)

with $a'_{410} < a_{410}$ because $A_1 < 0$ (see section A2.2 Remark ([3])).

There is only one positive root a_{410} as long as $\dfrac{A_3}{A_1} < 0 \quad \Leftrightarrow \quad A_3 > 0$

$$
\begin{aligned}
&\Leftrightarrow a_{i42} \geq a_{i42m} \\
&\text{with} \qquad a_{i42m} = \frac{\alpha_{52}}{\alpha_{51}} \cdot \frac{1}{K} \cdot a_{i41} - k_{S52}
\end{aligned}
\qquad \text{(A2.22)}
$$

When $a_{i42} < a_{i42m}$, there are 2 positive roots as the sign of A_2 is positive $\Leftrightarrow -\dfrac{A_2}{A_1} > 0$.

Moreover it is impossible to determine the sign of a_{420} when it is computed from:

$$a_{420} = \frac{\alpha_{52}}{\alpha_{51}} \cdot \frac{1}{K} \cdot \left(a_{410} - a_{i41}\right) + a_{i42} \qquad \text{(A2.23)}$$

It is why it is preferable to extract a_{42} from the following second order equation (A2.24).

2. Expression of a_{420} :

a_{420} is a solution of the second order equation where a_{42} is the unknown :

$$
\begin{aligned}
&A_1 \cdot a_{42}^2 + A_2 \cdot a_{42} + A_3 = 0 \\
&\text{with} \qquad A_1 = \left(1 - \frac{1}{C_{50}}\right) \cdot K_\alpha \\
&\qquad\qquad A_2 = \left(1 - \frac{1}{C_{50}}\right) \cdot \left(a_{i41} - K_\alpha \cdot a_{i42}\right) + k_{S52} \cdot K_\alpha + k_{S51} \\
&\qquad\qquad A_3 = k_{S52} \cdot \left(a_{i41} - K_\alpha \cdot a_{i42} + k_{S51}\right) \\
&\qquad\qquad \frac{1}{C_{50}} = \frac{\alpha_{53} \cdot \mu_5}{\beta_S - \alpha_{15,1} \cdot k_{D15}} \\
&\qquad\qquad K_\alpha = \frac{\alpha_{51}}{\alpha_{52}} \cdot K
\end{aligned}
\qquad \text{(A2.24)}
$$

Given $\Delta = A_2^2 - 4 \cdot A_1 \cdot A_3$

if $\Delta \geq 0$, the roots are: $a'_{420} = \frac{-A_2 + \sqrt{\Delta}}{2 \cdot A_1}$ and $a_{420} = \frac{-A_2 - \sqrt{\Delta}}{2 \cdot A_1}$ (A2.25)

with $a'_{420} < a_{420}$ because $A_1 < 0$.

There is only one positive root a_{420} as long as $\frac{A_3}{A_1} < 0 \quad \Leftrightarrow \quad A_3 > 0$

$\Leftrightarrow a_{i42} \leq a_{i42M}$

with $a_{i42M} = \frac{\alpha_{52}}{\alpha_{51}} \cdot \frac{1}{K} \cdot (a_{i41} + k_{S51})$ (A2.26)

When $a_{i42} > a_{i42M}$, it is not easy to know if the roots are positive or negative because the sign of $\frac{A_2}{A_1}$ cannot be determined.

The lack of determination is cancelled in next section.

3. How to compute a_{410} and a_{420}

The previous results are gathered in Figure 42.

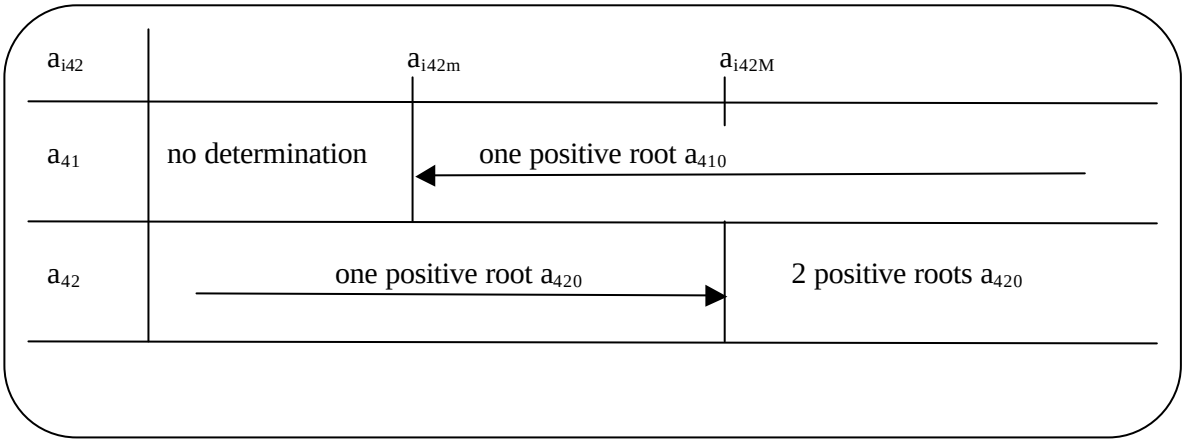

Figure 42. Domain of existence of only one positive root for a_{41} and a_{42}

This figure is the same as Fout! Verwijzingsbron niet gevonden. **but the numerical value of the milestones are different**

So to be sure to get the only one positive solution, it is sufficient to compute :

- a_{410} of (A2.21) when a_{i42} is such that : $a_{i42} \geq a_{i42m}$ or $a_{i42} \geq a_{i42M}$
- a_{420} of (A2.25) when a_{i42} is such that : $a_{i42} < a_{i42M}$

When a_{410} is computed by (A2.21), a_{420} is computed by :

$$a_{420} = \frac{\alpha_{52}}{\alpha_{51}} \cdot \frac{1}{K} \cdot (a_{410} - a_{i41}) + a_{i42} \quad \text{(A2.27)}$$

When a_{420} is computed by (A2.25), a_{410} is computed by :

$$a_{410} = K \frac{\alpha_{51}}{\alpha_{52}} \cdot (a_{420} - a_{i42}) + a_{i41} \quad \text{(A2.28)}$$

The expression of BioSugar2 concentration is :

$$a_{530} = \frac{\beta}{\alpha_{51} \cdot \mu_5 \cdot C_{50}} \cdot (a_{410} - a_{i41}) \qquad \text{(A2.29)}$$

4. Taking into account the negative derivative of BioSugar concentration

The objective is now to look for the implications of the inequality (third equation of A2.4).

This inequality can be rewritten :

$$\frac{a_{41}}{k_{S41} + a_{41}} \cdot \frac{a_{42}}{k_{S42} + a_{42}} < C_{40}$$

$$\text{with} \quad C_{40} = \frac{\beta_S - \alpha_{11,1} \cdot k_{D11}}{\alpha_{43} \cdot \mu_4} \qquad \text{(A2.30)}$$

$$\text{Re call:} \quad \alpha_{43} > 0 \quad \text{and} \quad \alpha_{11,1} < 0$$

It implies :

$$y > 0$$

$$\text{with} \quad y = A_1 \cdot a_{42}^2 + A_2 \cdot a_{42} + A_3$$

$$A_1 = \left(1 - \frac{1}{C_{40}}\right) \cdot K_\alpha$$

$$A_2 = \left(1 - \frac{1}{C_{40}}\right) \cdot (a_{i41} - K_\alpha \cdot a_{i42}) + k_{S42} \cdot K_\alpha + k_{S41} \qquad \text{(A2.31)}$$

$$A_3 = k_{S42} \cdot (a_{i41} - K_\alpha \cdot a_{i42} + k_{S41})$$

$$\frac{1}{C_{40}} = \frac{\alpha_{43} \cdot \mu_4}{\beta_S - \alpha_{11,1} \cdot k_{D11}}$$

$$K_\alpha = \frac{\alpha_{51}}{\alpha_{52}} \cdot K$$

Given $\Delta = A_2^2 - 4 \cdot A_1 \cdot A_3$

if $\Delta \geq 0$, the roots of 'y = 0' are: $a_{421} = \frac{-A_2 + \sqrt{\Delta}}{2 \cdot A_1}$ and $a_{422} = \frac{-A_2 - \sqrt{\Delta}}{2 \cdot A_1}$ (A2.32)

with $a_{421} < a_{422}$ because $A_1 < 0$ ([3]).

The derivative of y is : $\dot{y} = 2 \cdot A_1 \cdot a_{42} + A_2$

Figure A2.4 shows that 'y' is positive for a_{42} belonging to the interval [a_{421} a_{422}].

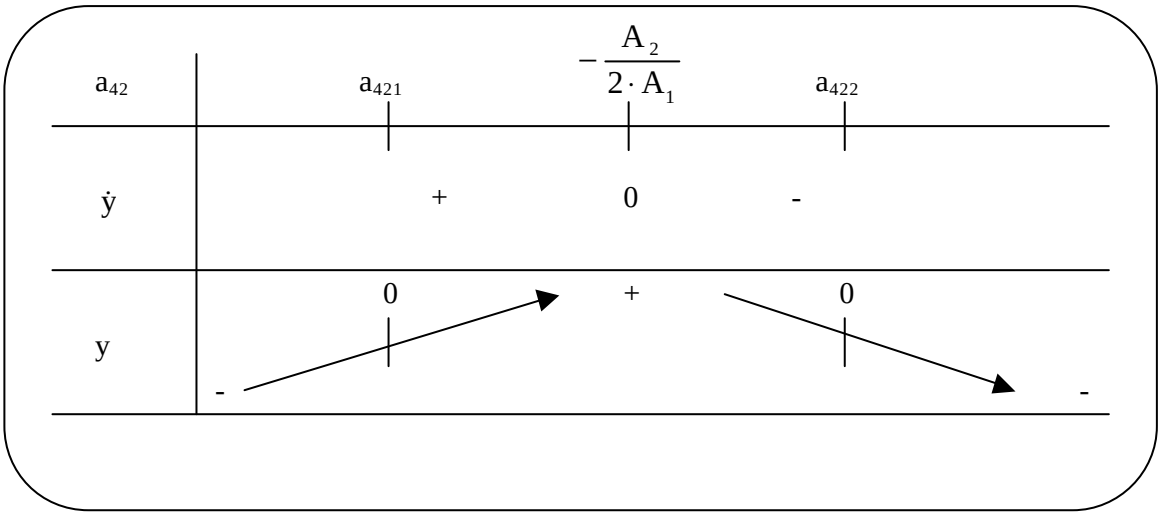

Figure 43. Sign of y

This figure is the same as Figure 41 but the numerical value of the milestones are different

So the inequality of (A2.4) is fulfilled only if a_{42} belongs to the interval [a_{421} a_{422}].

In other words, the solution a_{420} of (A2.23) and (A2.25) must belong to the interval [a_{421} a_{422}] defined in (A2.32). (A2.33)

Then the steady state that fulfil the equations system (A2.4) is :

$$X_0 = \begin{bmatrix} a_{410} \\ a_{420} \\ 0 \\ a_{530} \end{bmatrix} \qquad \text{(A2.34)}$$

If the solution a_{420} of (A2.23) and (A2.25) does not belong to [a_{421} a_{422}] defined in (A2.32), the steady state X_0 does not exist.

5.3.6 Illustration

The aim is to illustrate the analytical computation of the steady state established in section A2.3 and A2.4 . The 2 examples are those of section 2.3 . One will see that the simulations lead to the same steady states.

The variables of a steady state are only the MonoSacch and NH3 concentrations at input of the sub-process (Table 21).

Table 21. MonoSacch and NH3 concentrations at input of the sub-process

	Simulation 1	**Simulation 2**
a_{i41} (g/l) :MonoSacch input	11.95	11.95
a_{i42} (g/l) :NH3 total form input	0.5622	$9.37\ 10^{-2}$

Looking for a steady state with a null BioSugar2 :

If such a steady state exists, it is a solution of the set 3 of equations : (A2.3).

The condition of existence is gathered in Table 22.

Table 22. Condition of existence of a steady state with a null BioSugar2

	Simulation 1	**Simulation 2**
a_{420} from (A2.10) or (A2.12) (g/l of NH3 total form)	$4.49352\ 10^{-1}$	$1.5954\ 10^{-3}$
Condition (A2.18) on a_{420} to fulfil $f_5<0$ (g/l of NH3 total form)	$a_{420} \in$ $[6.8812\ 10^{-3} \quad 4.49349\ 10^{-1}]$	$a_{420} \in$ $[0 \quad 6.8815\ 10^{-3}\ ]$
Is the condition satisfied ?	no	yes

Looking for a steady state with a null BioSugar :

If such a steady state exists, it is a solution of the set 4 of equations : (A2.4).

The condition of existence is gathered in Table 23.

Table 23. Condition of existence of a steady state with a null BioSugar

	Simulation 1	**Simulation 2**
Is the condition satisfied ?	no	yes
a_{420} from (A2.23) or (A2.25) (g/l of NH3 total form)	$4.5802\ 10^{-1}$	$6.8816\ 10^{-3}$
Condition (A2.33) on a_{420} to fulfil $f_4<0$ (g/l of NH3 total form)	$a_{420} \in$ $[1.5877\ 10^{-3} \quad 4.5803\ 10^{-3}\ ]$	$a_{420} \in$ $[0 \quad 1.5998\ 10^{-3}\ ]$
Is the condition satisfied ?	yes	no

Steady state :

Only one physical solution exists for each simulation.

<u>For simulation 1:</u>

the steady state is the solution of (A2.4) with a null BioSugar. The numerical value of the state X_0 is given by (A2.21) or (A2.28) for a_{410} and (A2.29) for a_{530} .

For simulation 2:

the steady state is the solution of (A2.3) with a null BioSugar2. The numerical value of the state X_0 is given by (A2.6) or (A2.13) for a_{410} and (A2.14) for a_{430} .

The numerical value of the steady state is gathered in Table 24.

Table 24. Value of the steady state of the sub-process ([E4], [E5], [E11] & [E15])

	Simulation 1	**Simulation 2**
a_{410} (g/l of MonoSacch)	$1.2806\ 10^{-5}$	2.1937
a_{420} (g/l of NH3 total form)	$4.5802\ 10^{-1}$	$1.5954\ 10^{-3}$
a_{430} (g/l of BioSugar)	0	$1.9284\ 10^{-1}$
a_{530} (g/l of BioSugar2)	$2.1805\ 10^{-1}$	0

In simulation 1, all the MonoSacch is removed from the medium. As long as NH3 is in enough quantity, MonoSacch is consumed until its concentration goes down the half saturation constant ($k_{S41}=10^{-2}$ g/l) of BioSugar growth. Then this biomass is disadvantaged versus BioSugar2 despite its high specific growth rate ($\mu_{M\_BioSugar} = 0.4\ h^{-1}$ and $\mu_{M\_BioSugar2} = 0.1\ h^{-1}$). On the contrary in simulation 2 where MonoSacch is no more limiting, the BioSugar2 growth is disadvantaged by its low specific growth rate.
The value of the steady state obtained by the analytical way above can be checked on the following Figure 44 and Figure 45 that are zooms during the last 500 hours of simulation when the process is reaching its steady state.

Checking the stability of the steady state :

The question arises whether the biomass that is going to zero could grow after an injection of the same biomass into the reactor. Simulations show that the steady state is stable.
In simulation 1, when the steady state is reached (BioSugar=0), an addition of BioSugar is done. Figure 46 shows that the added biomass disappears because its growth is not sufficient compared to its decay.
In the same way, in simulation 2, when the steady state is reached (BioSugar2=0), an addition of BioSugar2 is done. Figure 47 shows that the added biomass disappears also for the same reason.

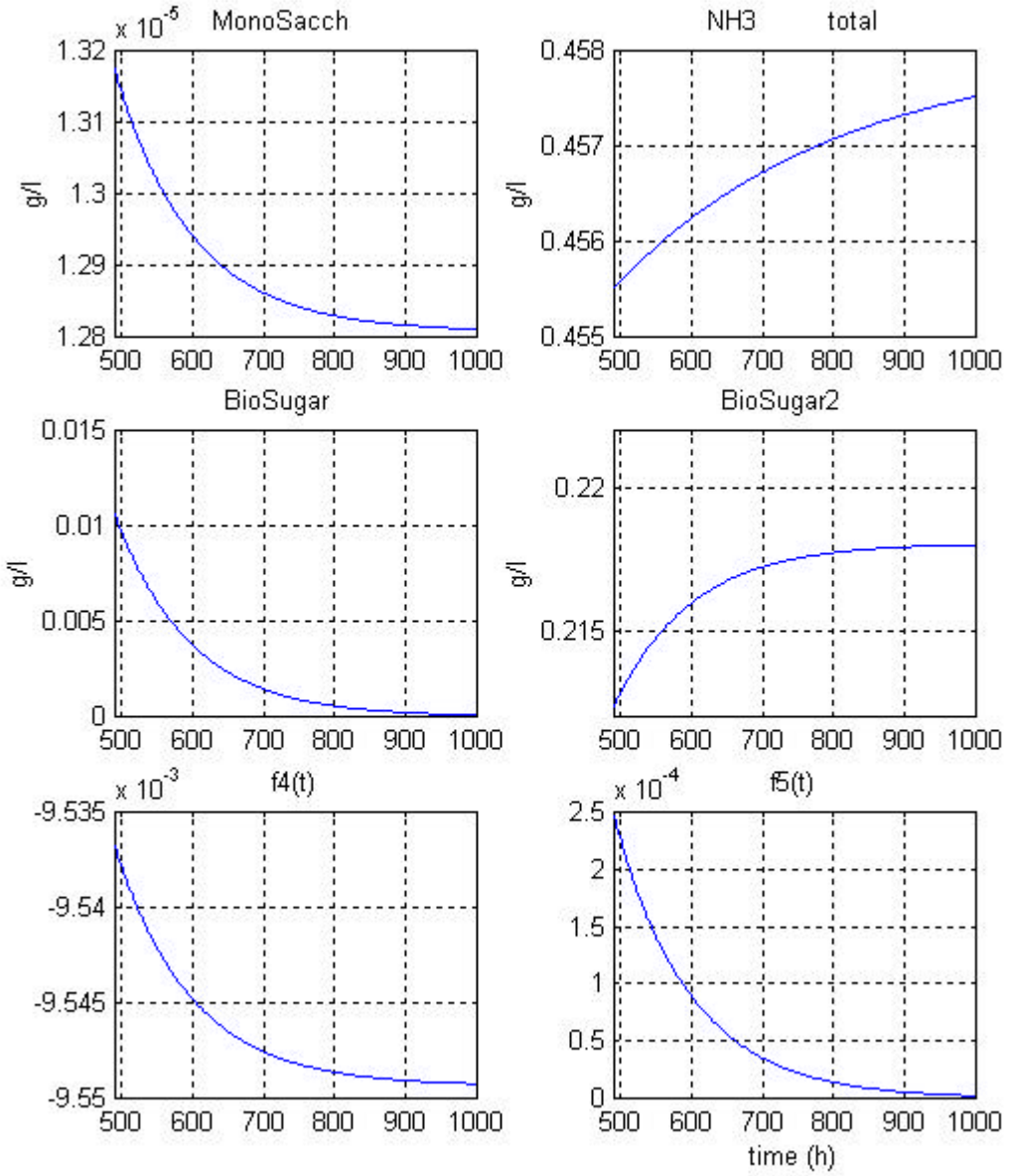

Figure 44. Simulation 1; Evolution function of time expressed in hour.

NH3 is 'high' compared to MonoSacch
Inputs: 0.562 g/l of NH3 total form and 11.95 g/l of MonoSacch

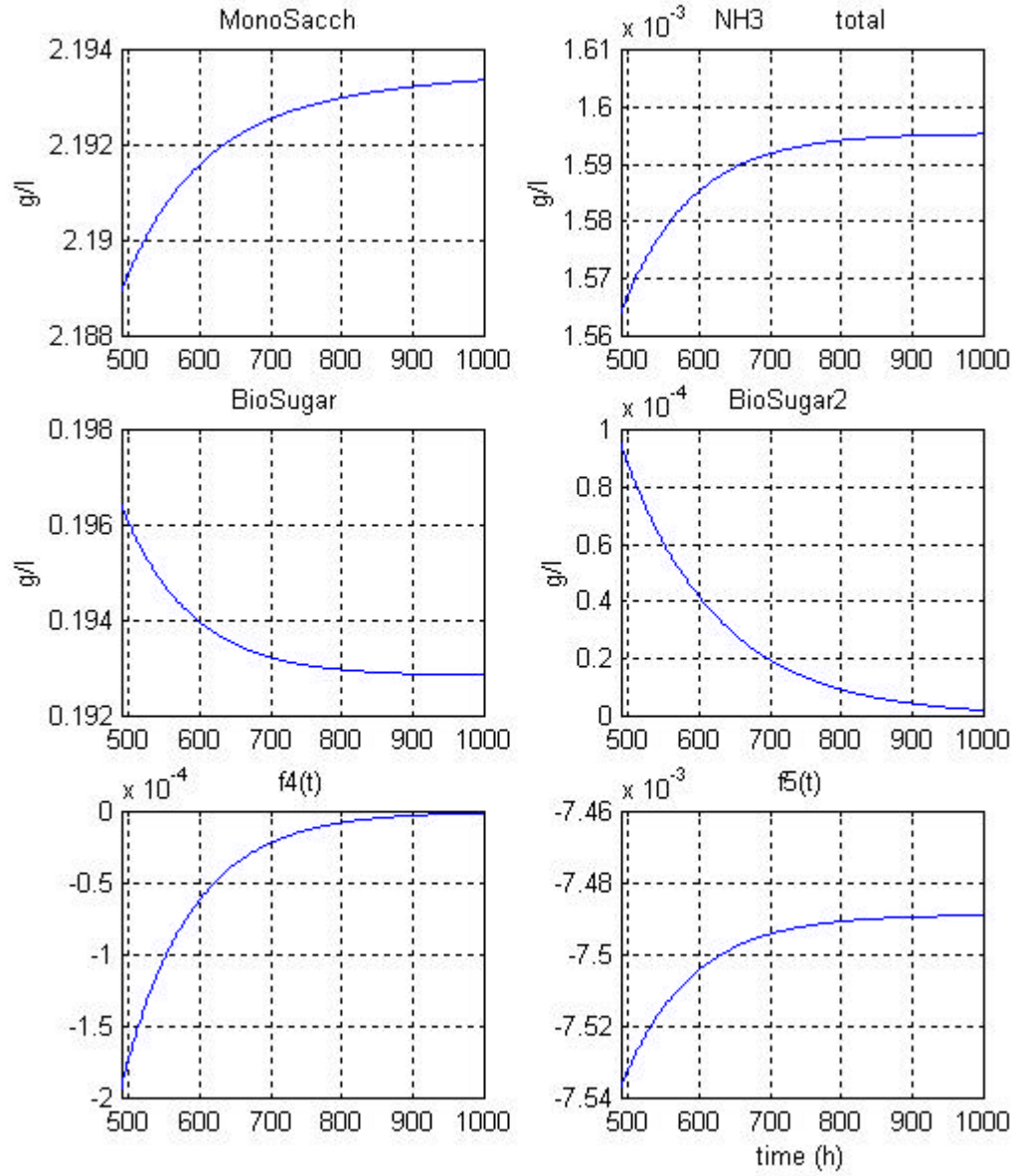

Figure 45. Simulation 2; Evolution function of time expressed in hour.

NH3 is 'low' compared to MonoSacch
Inputs: 9.37 10^{-2} g/l of NH3 total form and 11.95 g/l of MonoSacch

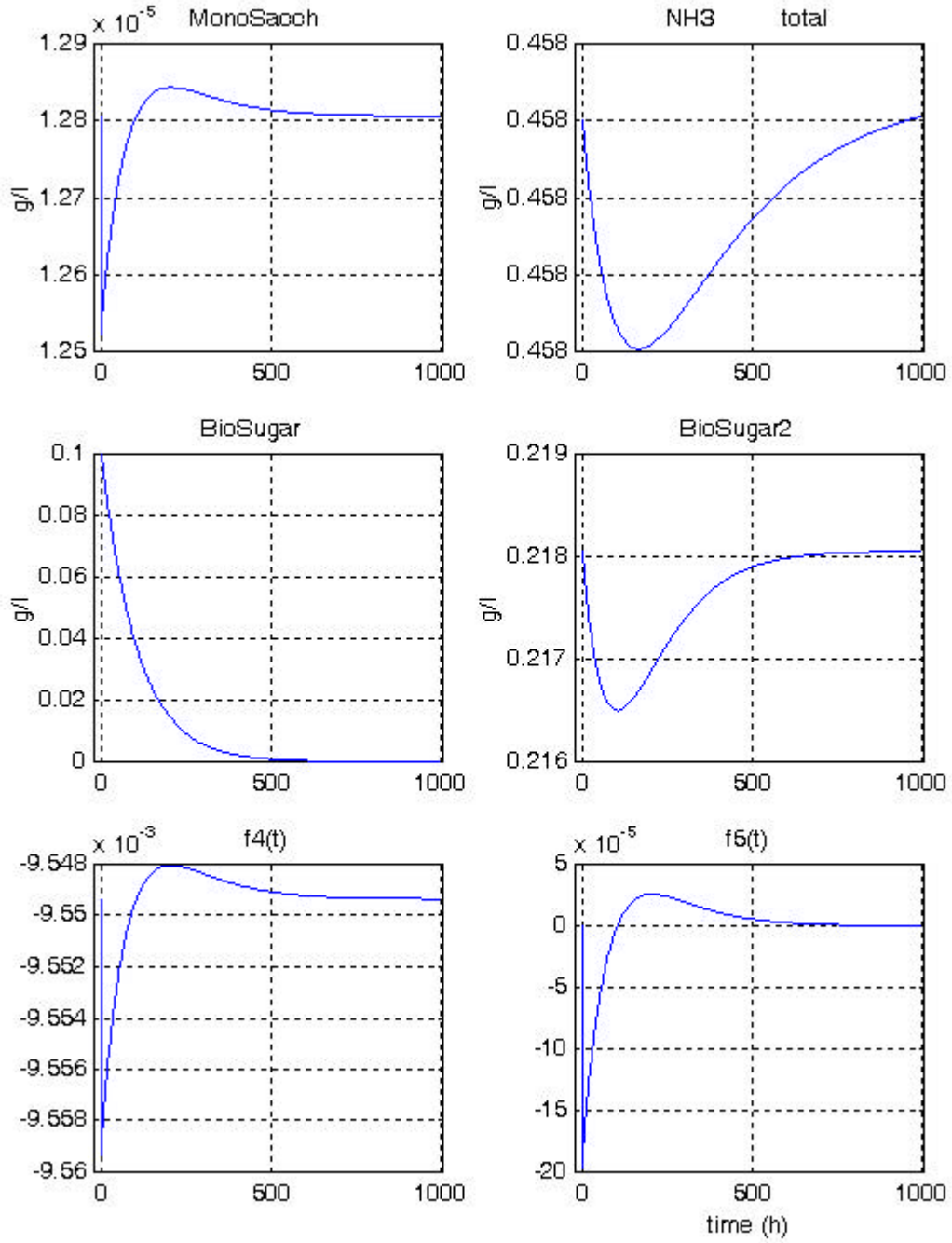

Figure 46. Simulation 1; Evolution function of time expressed in hour.

NH3 is 'high' compared to MonoSacch
Inputs: 0.562 g/l of NH3 total form and 11.95 g/l of MonoSacch
Initial state is steady state for MonoSacch, NH3 and BioSugar2 with initial addition of BioSugar (0.1 g/l).
Þ the process comes to its steady state where BioSugar = 0 (f_4 remains <0).

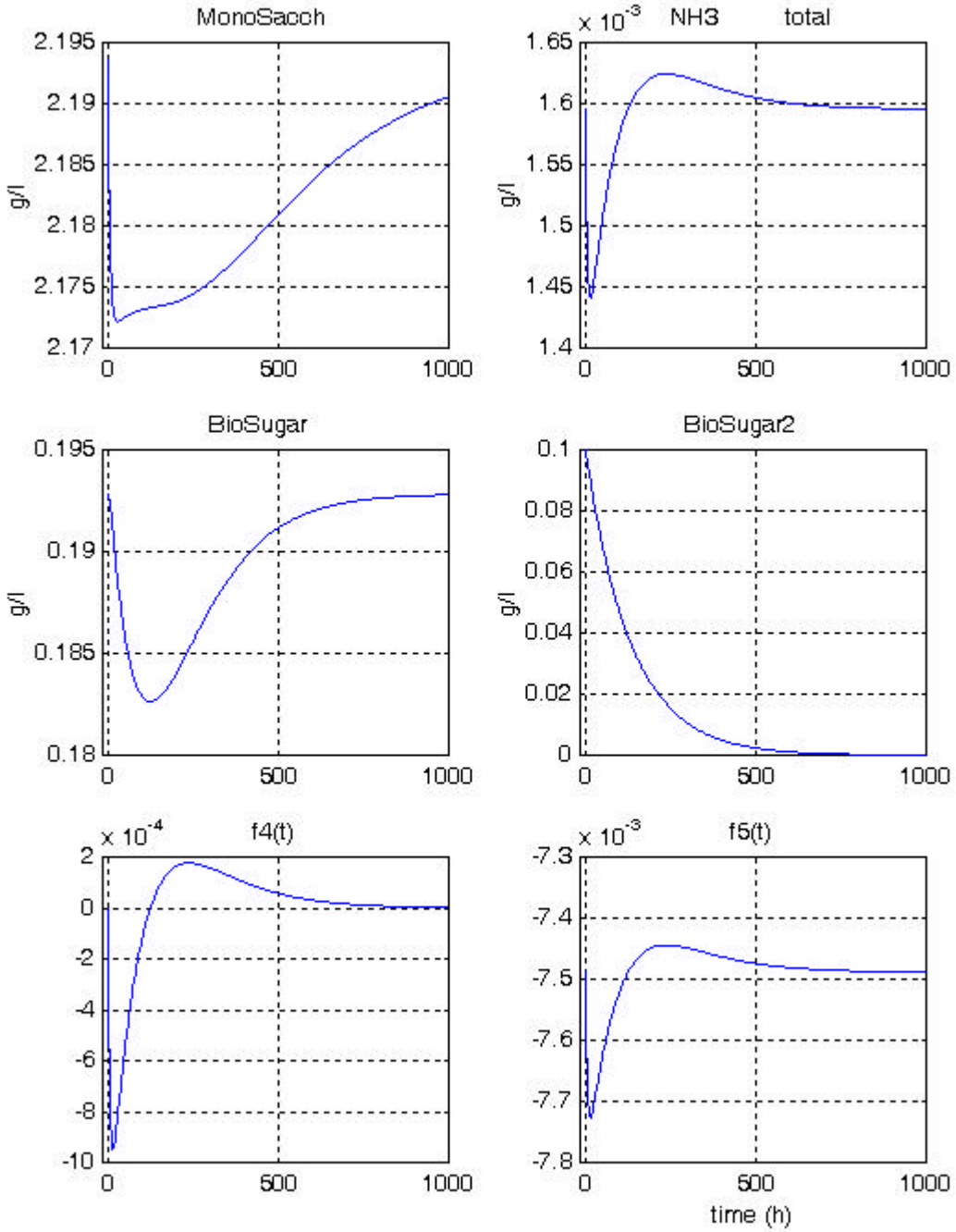

Figure 47. Simulation 2; Evolution function of time expressed in hour.

NH3 is 'low' compared to MonoSacch
Inputs: 9.37 10^{-2} g/l of NH3 total form and 11.95 g/l of MonoSacch
Initial state is steady state for MonoSacch, NH3 and BioSugar with initial addition of BioSugar2 (0.1 g/l).
Þ the process comes to its steady state where BioSugar2 = 0 (f_5 remains <0).

5.4 RESPONSE TIMES OF THE WHOLE PROCESS (REACTIONS [E 1] to [E 16])

The response times are estimated by simulations of input steps around the standard steady state point defined in the LGCB model on 30 July 2004.

Steady state.
This point, detailed in Table 25, is obtained by simulation on a long run so that the value are converging and constant (of course, when the drain flow rate is null, the variables 'BioDead' and 'SolidInert' are integrative and cannot be constant; but their slope are constant).

Table 25. Steady state of the standard process on 30 July 2004 (expressed in g/l of total form)

Faeces	: 6.249600e-002
Wheat	: 1.249920e-001
Potato	: 1.249920e-001
Salad	: 1.249920e-001
AA	: 2.023983e+000
PA	: 6.184313e-001
BA	: 5.622085e+000
VA	: 2.453633e-001
CA	: 2.736799e-001
NH3	: 4.565270e-001
CO2	: 9.568548e-001
MonoSacch	: 1.281152e-005
OMProt	: 4.696153e-002
OMLip	: 6.260298e-005
OMCarb	: 1.684421e-001
OMFibre	: 8.293469e-001
AminoA	: 5.004300e-004
BioSugar	: 0.000000e-000
BioSugar2	: 2.180547e-001
BioAA	: 1.139552e-001
BioLCFA	: 5.354000e-002
SolubleInert	: 3.100355e+000

The approximation explained in the introduction can be justified here. This approximation concerns the fact that the consumption of NH3 by reaction [E 7] was neglected when considering the sub-process defined by the reactions [E 4], [E 5], [E 11] & [E 15].
One can note here (**Fout! Verwijzingsbron niet gevonden.**) that the sub-process and the whole process have nearly same steady state : the biggest difference is for NH3 precisely and the distance is less than 0.5 %. So the approximation done in section 2 (study of the sub-process) is perfectly justified.

Table 26. Comparison of the steady states of the sub-process and whole process

State component	Values at steady state of the sub-process (copy of Figure 43)	Values at steady state of the whole process (copy of Table 25)
MonoSacch (g/l)	$1.2806\ 10^{-5}$	$1.281152\ 10^{-5}$
NH3 (g/l of total form)	$4.5802\ 10^{-1}$	$4.565270\ 10^{-1}$
BioSugar (g/l)	0	0
BioSugar2 (g/l)	$2.1805\ 10^{-1}$	$2.180547\ 10^{-1}$

Response times.
The response times are measured from simulations of positive input step, plotted in the following figures and gathered in Table 27:

- Figure 48 to Figure 53: input flow rate step (10 % of the standard input value: qi0=0.07875 l/h;
- Figure 53 to Figure 59: drain flow rate step (step of 0.007875 l/h);
- Figure 59 to Figure 65 : input concentrations step (10 % of the standard input values).

Process excitation / Component	Input flow rate		Drain flow rate		Input concentrations	
	(hours)	(days)	(hours)	(days)	(hours)	(days)
Wastes (faeces, wheat, potato, salad)	15	0.625	15		15	
VFA (AA, PA, BA, VA, CA)	1000	40	1000	40	1000	40
NH3	1000	40	1500	60	1500	60
Mono_Sacch **OM_Lip** **OM_Carb** **OM_Fibre**	500	20	500	20	500	20
OM_Prot	30	1.25	30	1.25	30	1.25
Amino_A	500	20	500	20	500	20
Biomasses (BioSugar2, Bio_AA, Bio_LCFA)	500	20	500	20	500	20
SolubleInert	1000	40	1000	40	1000	40

Table 27. Response times (expressed in hours and days) of the outputs

for the different kinds of process excitation
and for the nominal simulated process of 30 July 2004 by LGCB.

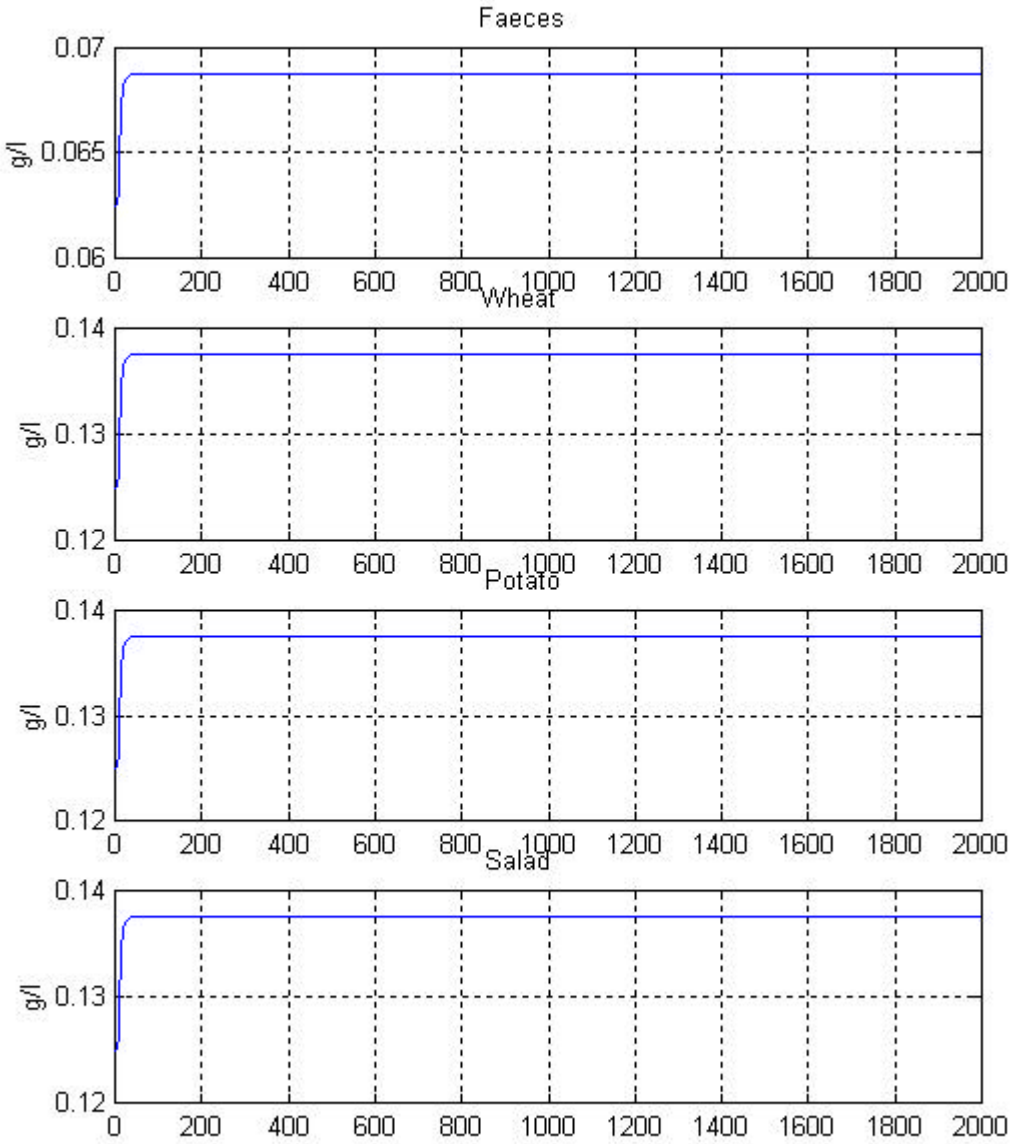

Figure 48. Input flow rate step

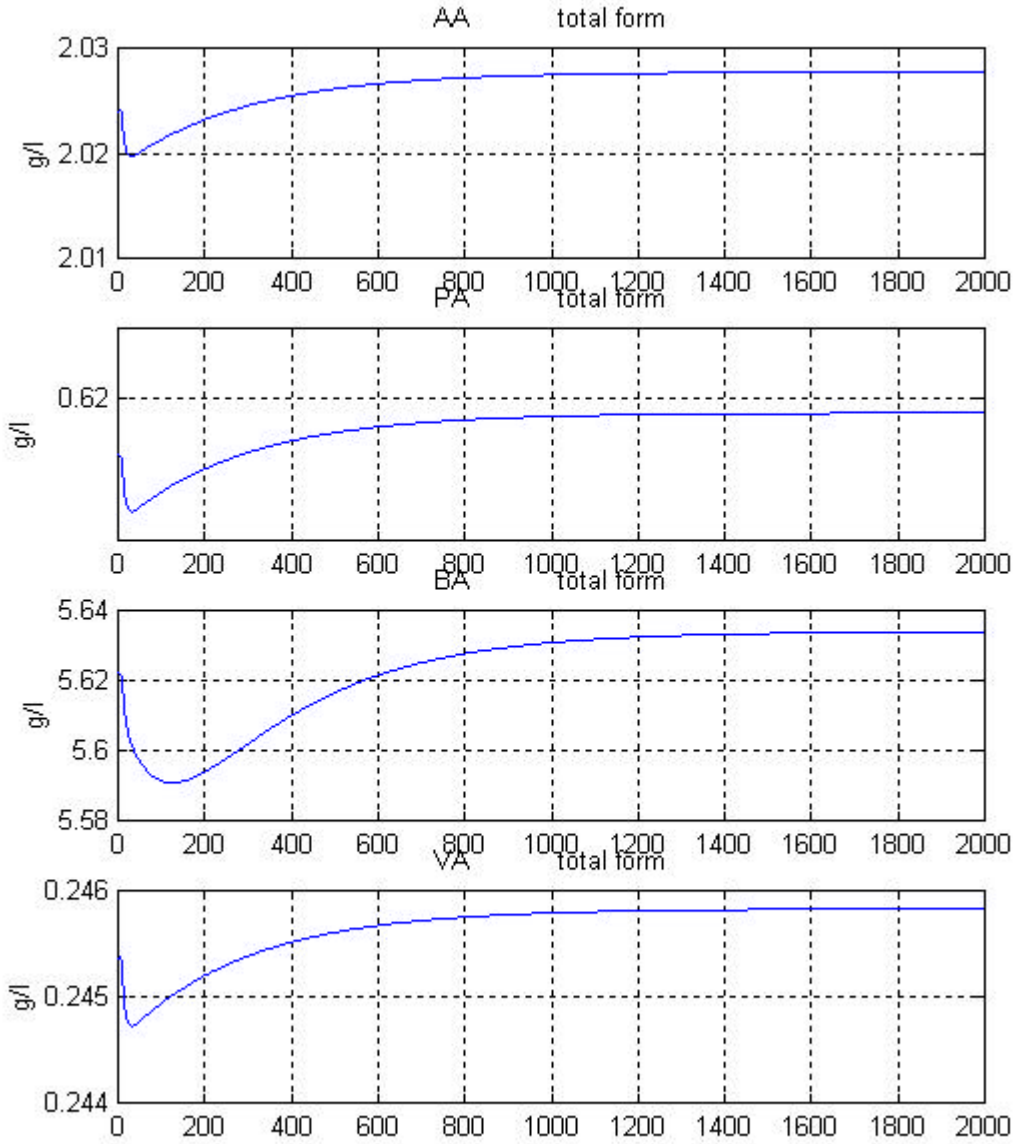

Figure 49. Input flow rate step

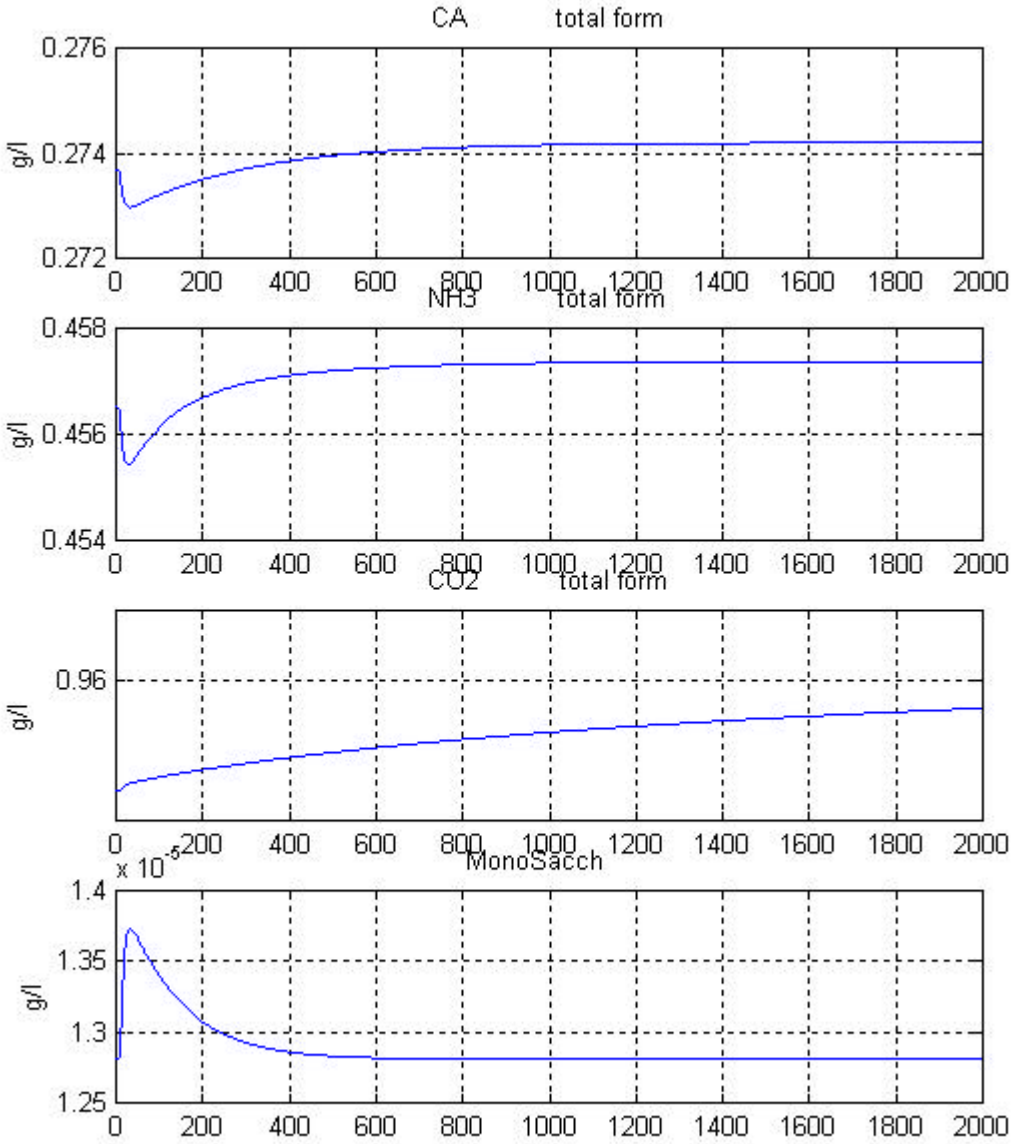

Figure 50. Input flow rate step

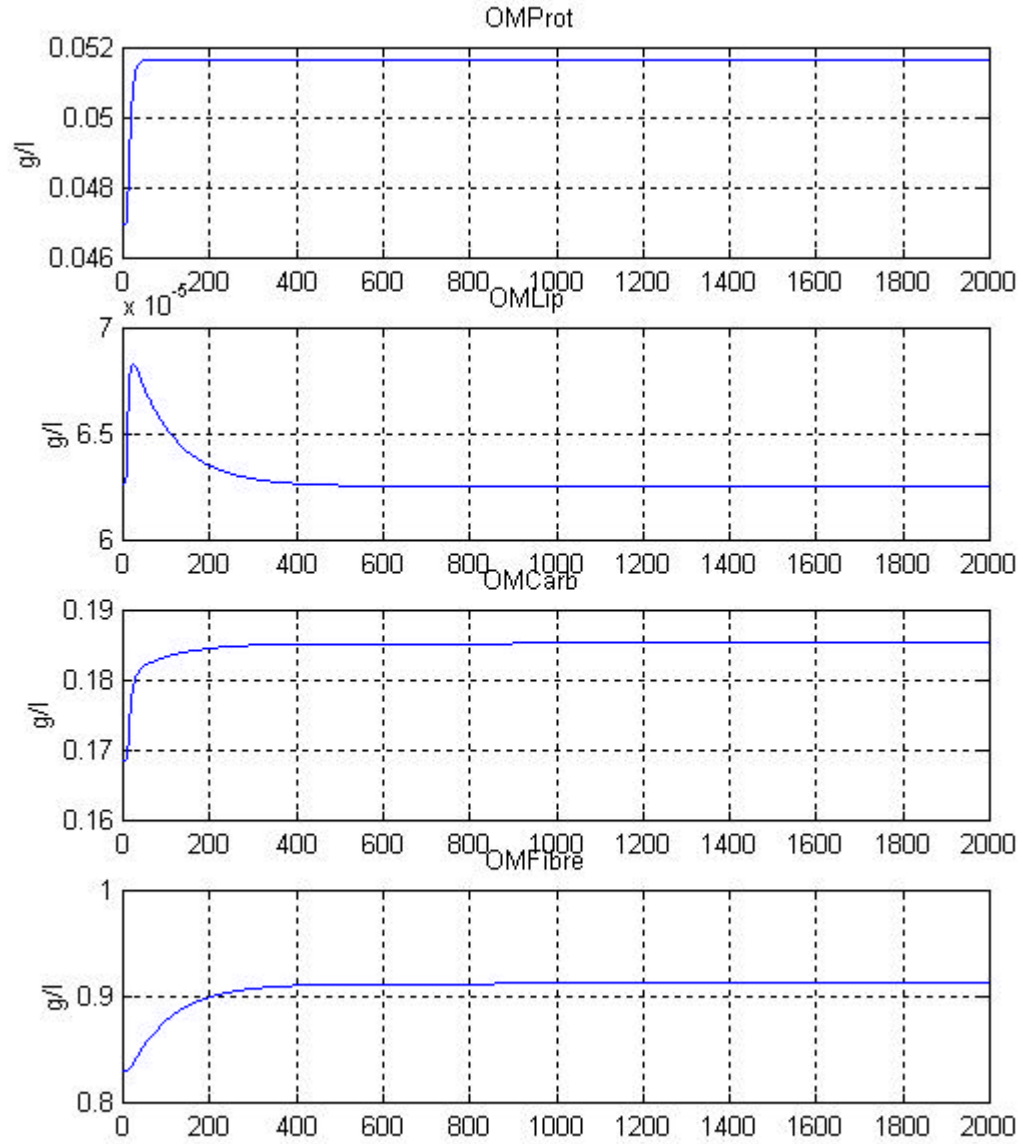

Figure 51. Input flow rate step

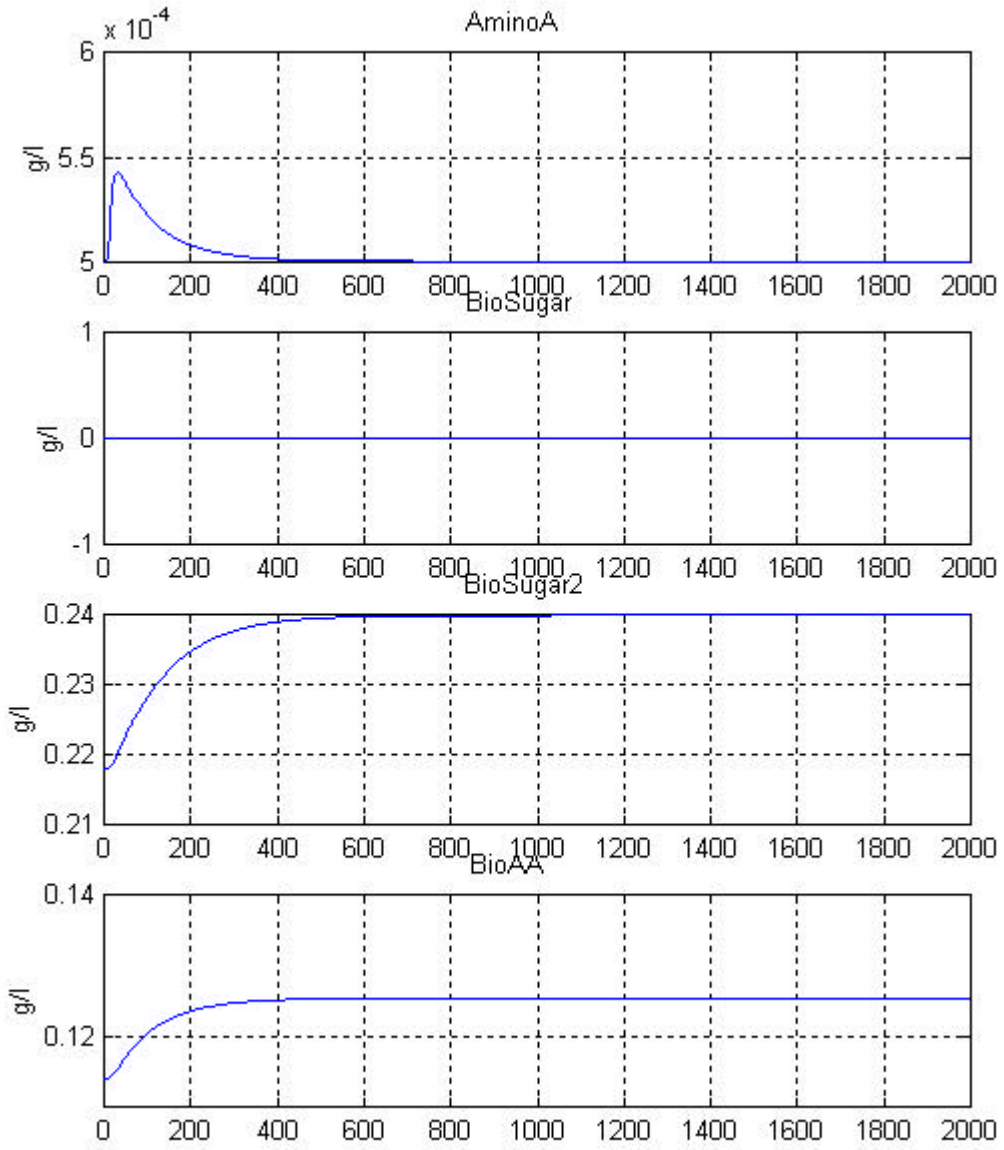

Figure 52. Input flow rate step

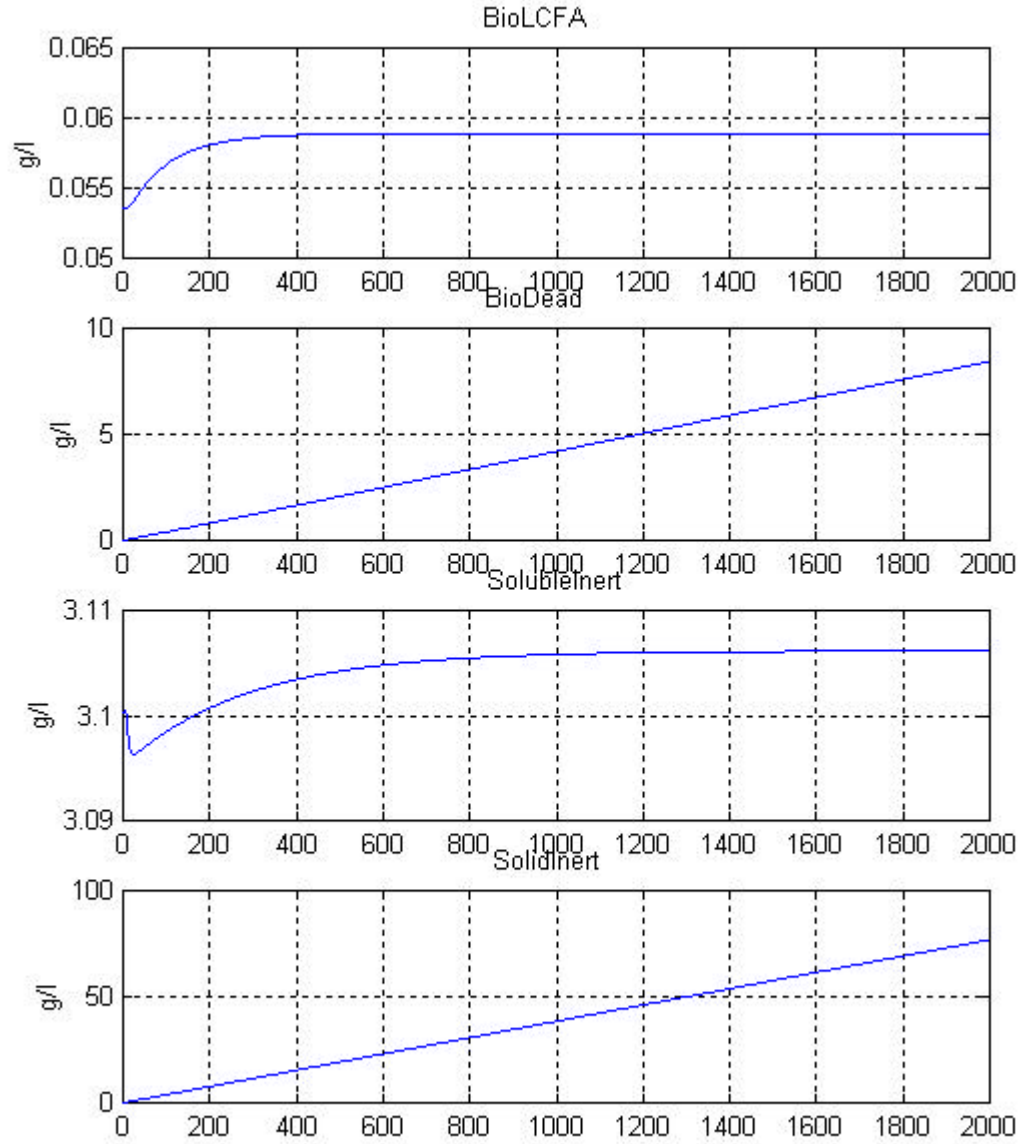

Figure 53. Input flow rate step

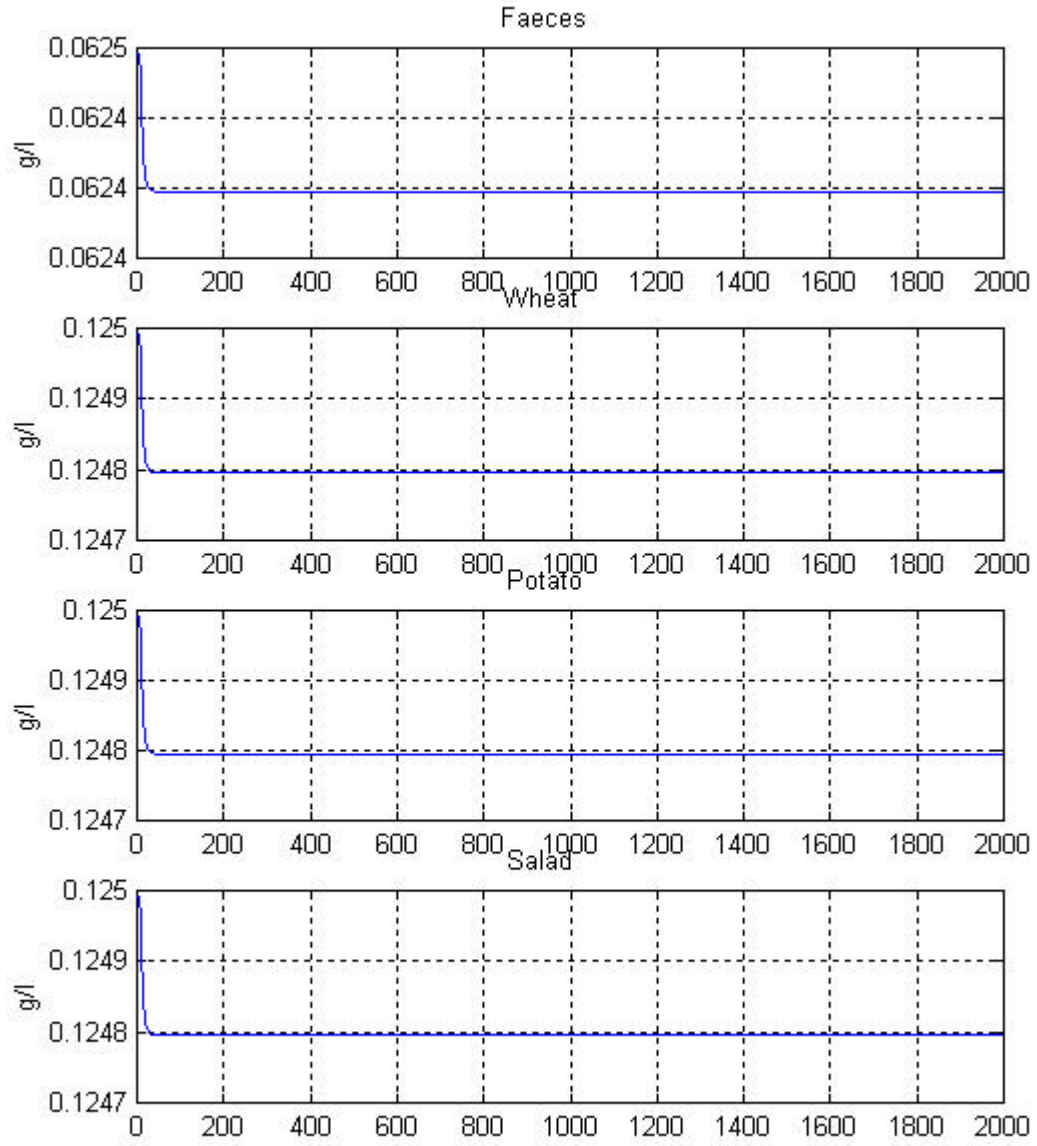

Figure 54. Drain flow rate step

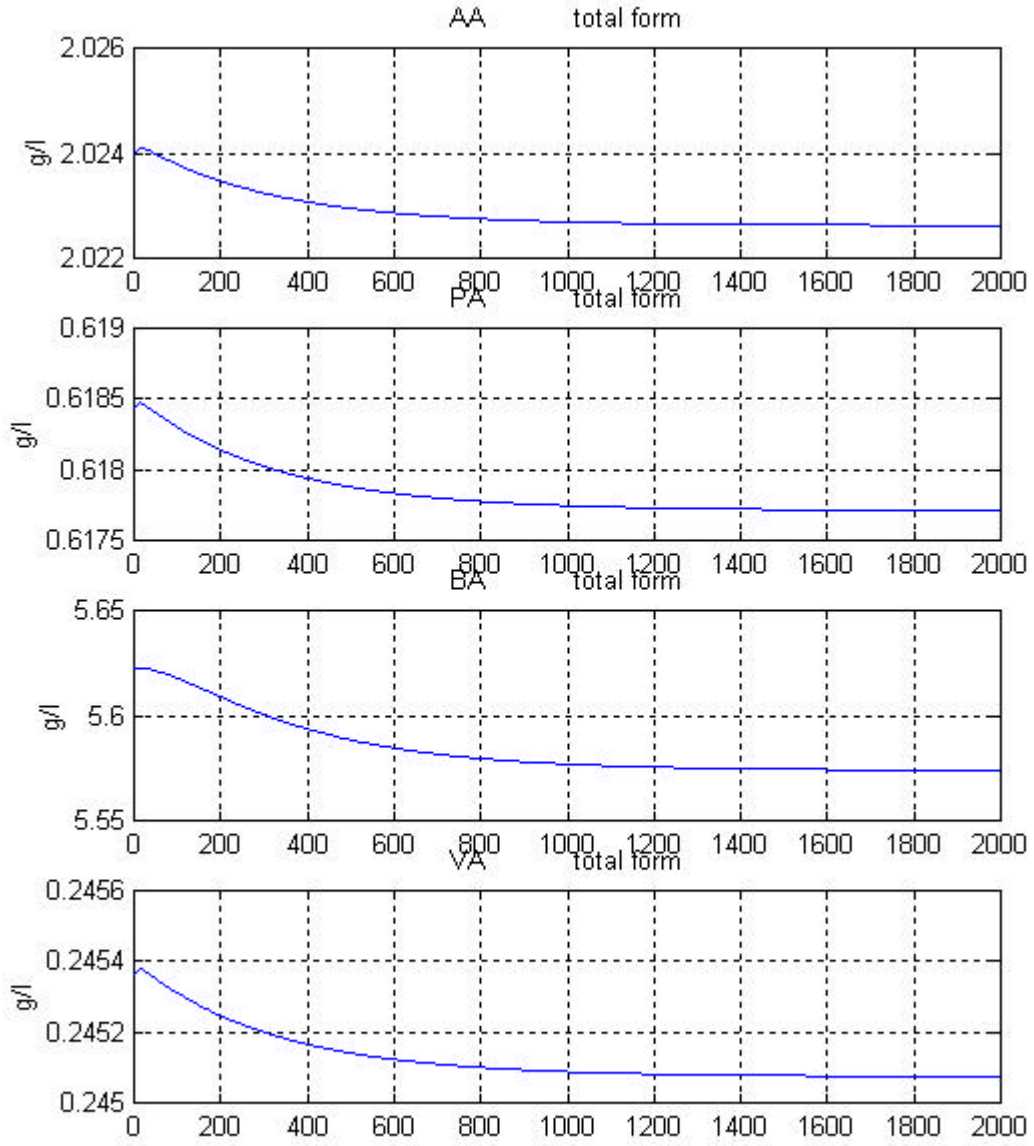

Figure 55. Drain flow rate step

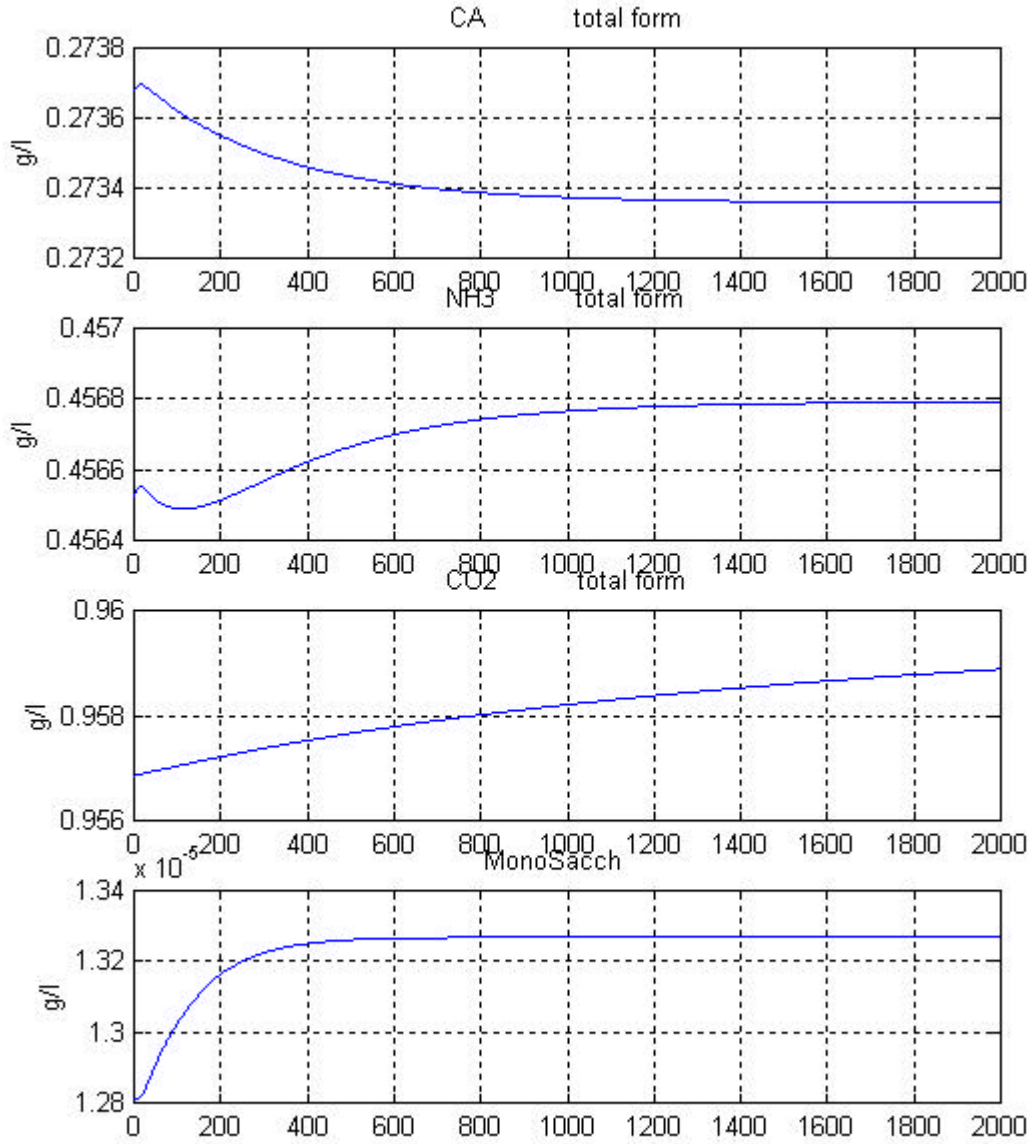

Figure 56. Drain flow rate step

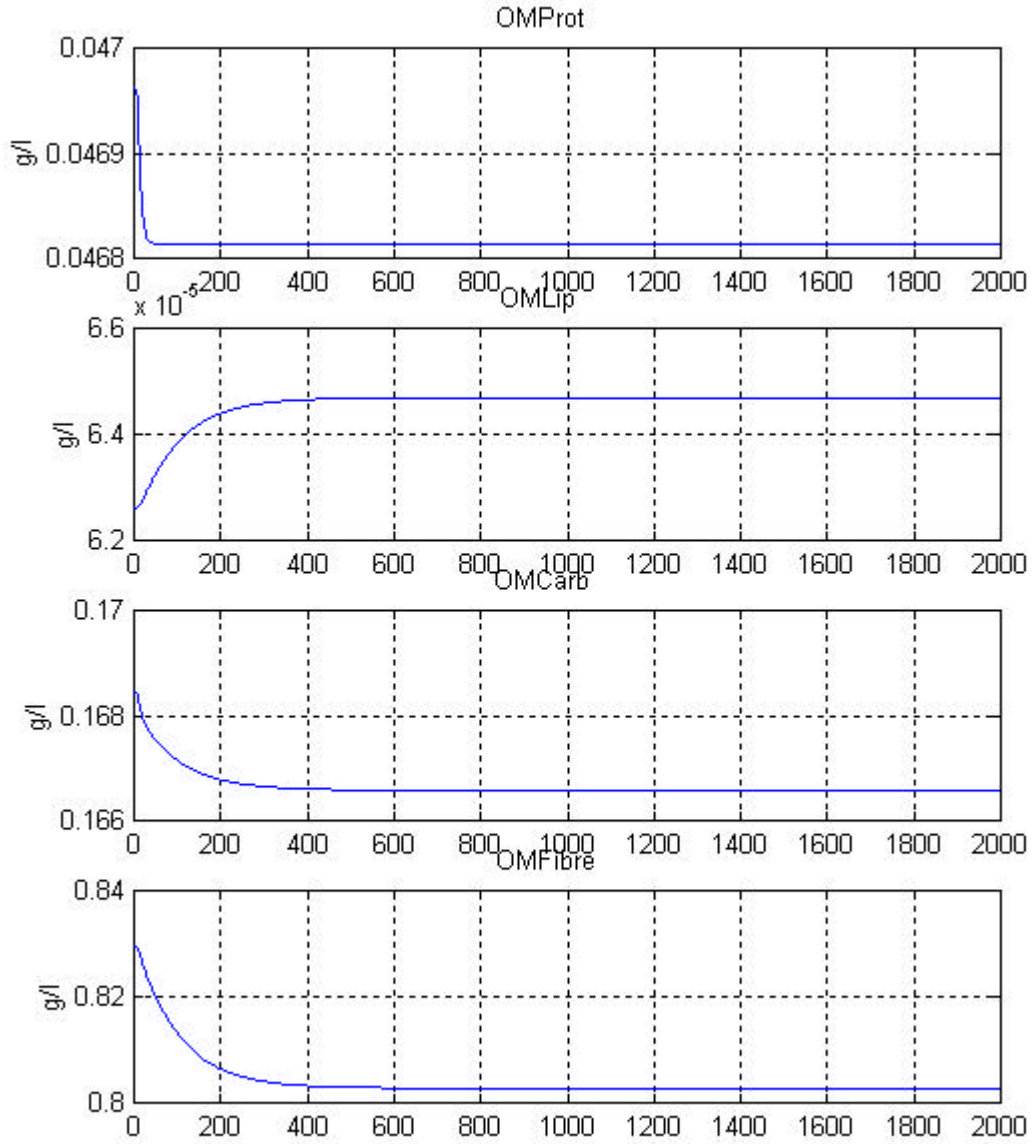

Figure 57. Drain flow rate step

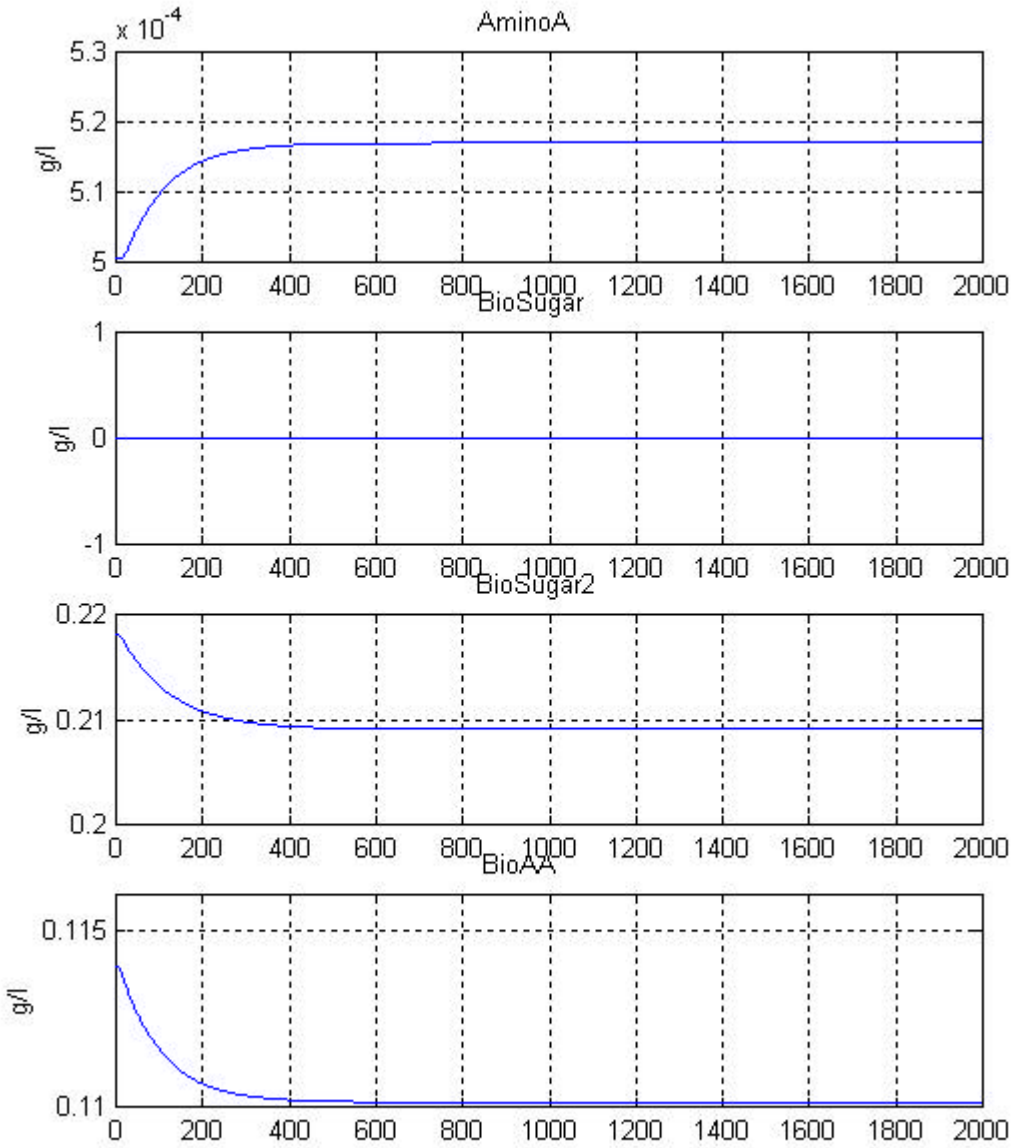

Figure 58. Drain flow rate step

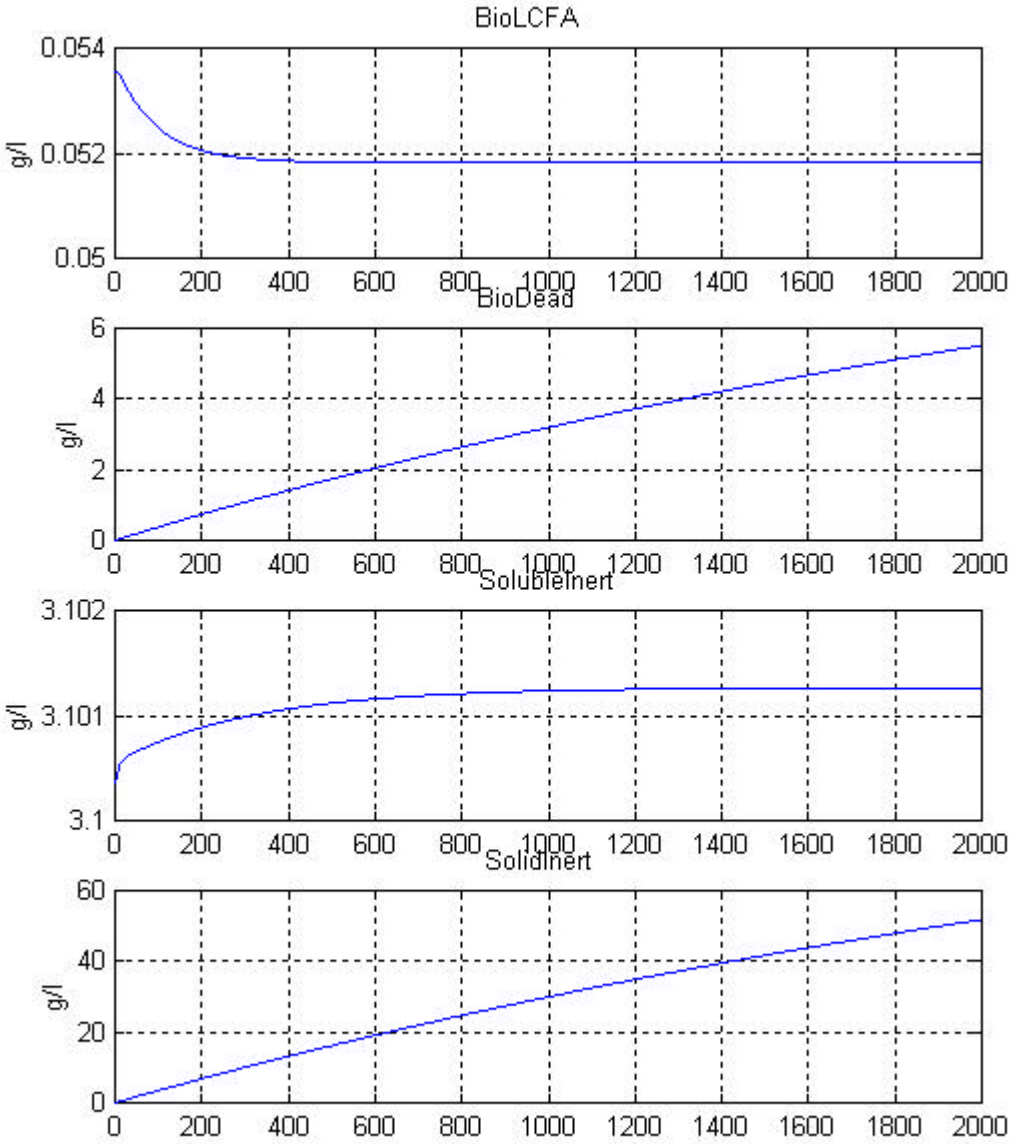

Figure 59. Drain flow rate step

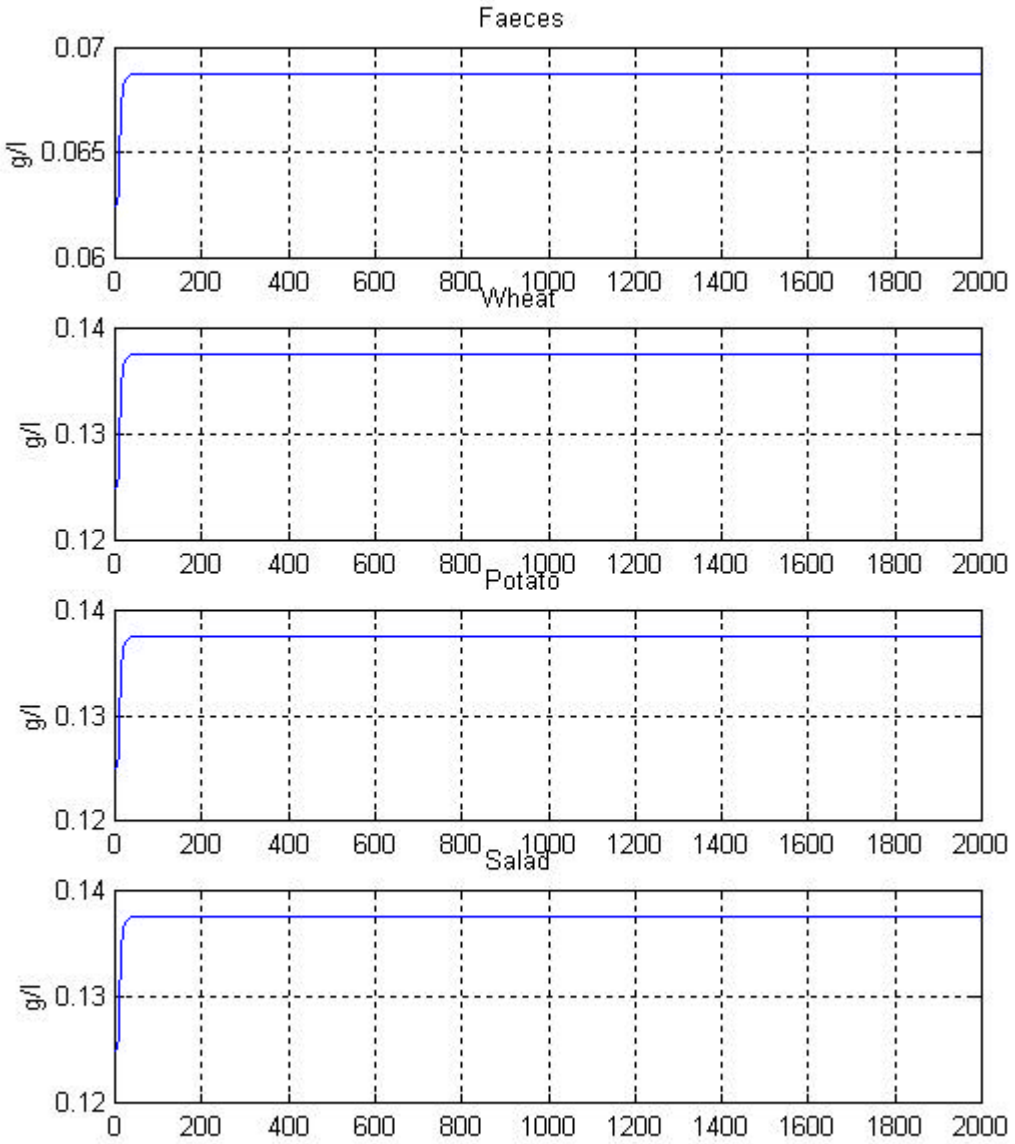

Figure 60. Input concentrations step

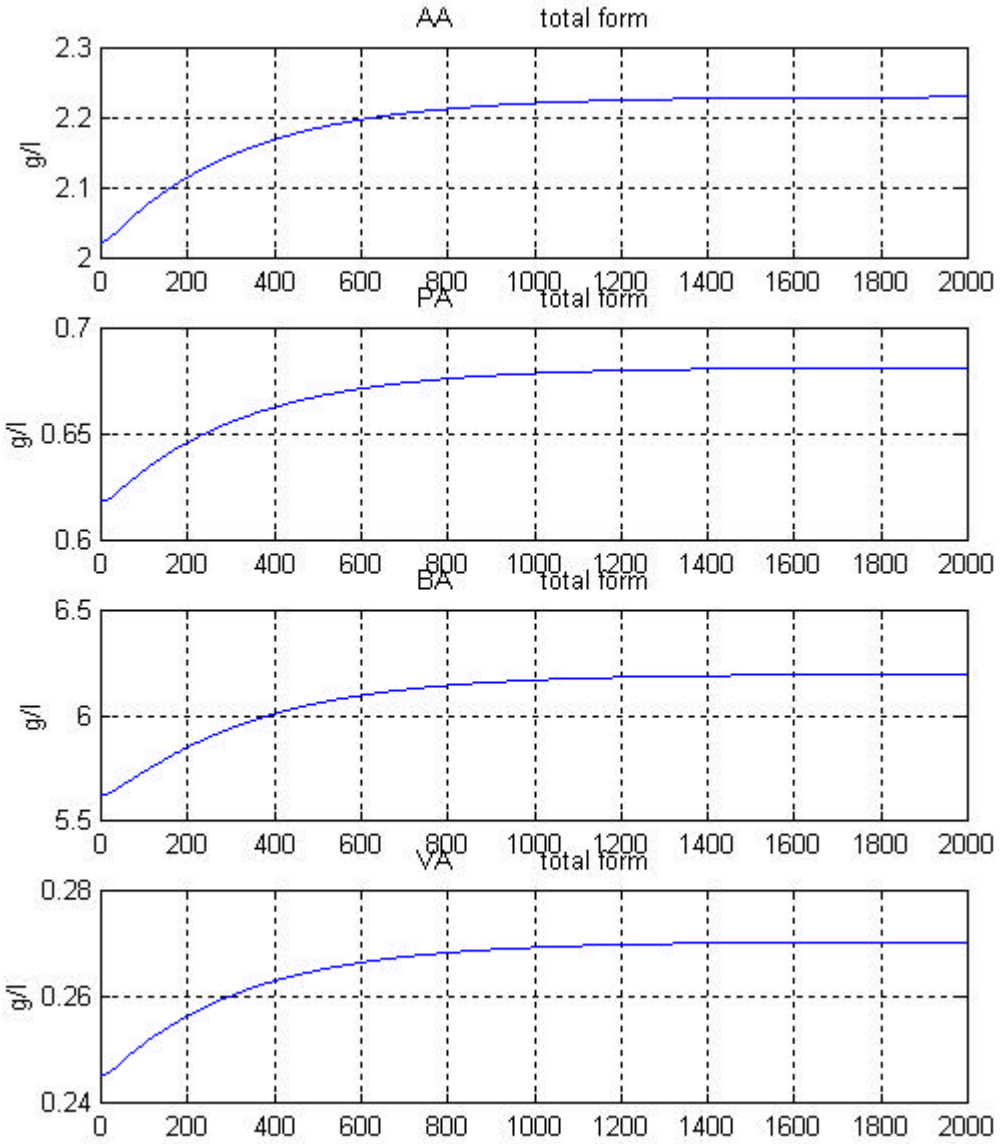

Figure 61. Input concentrations step

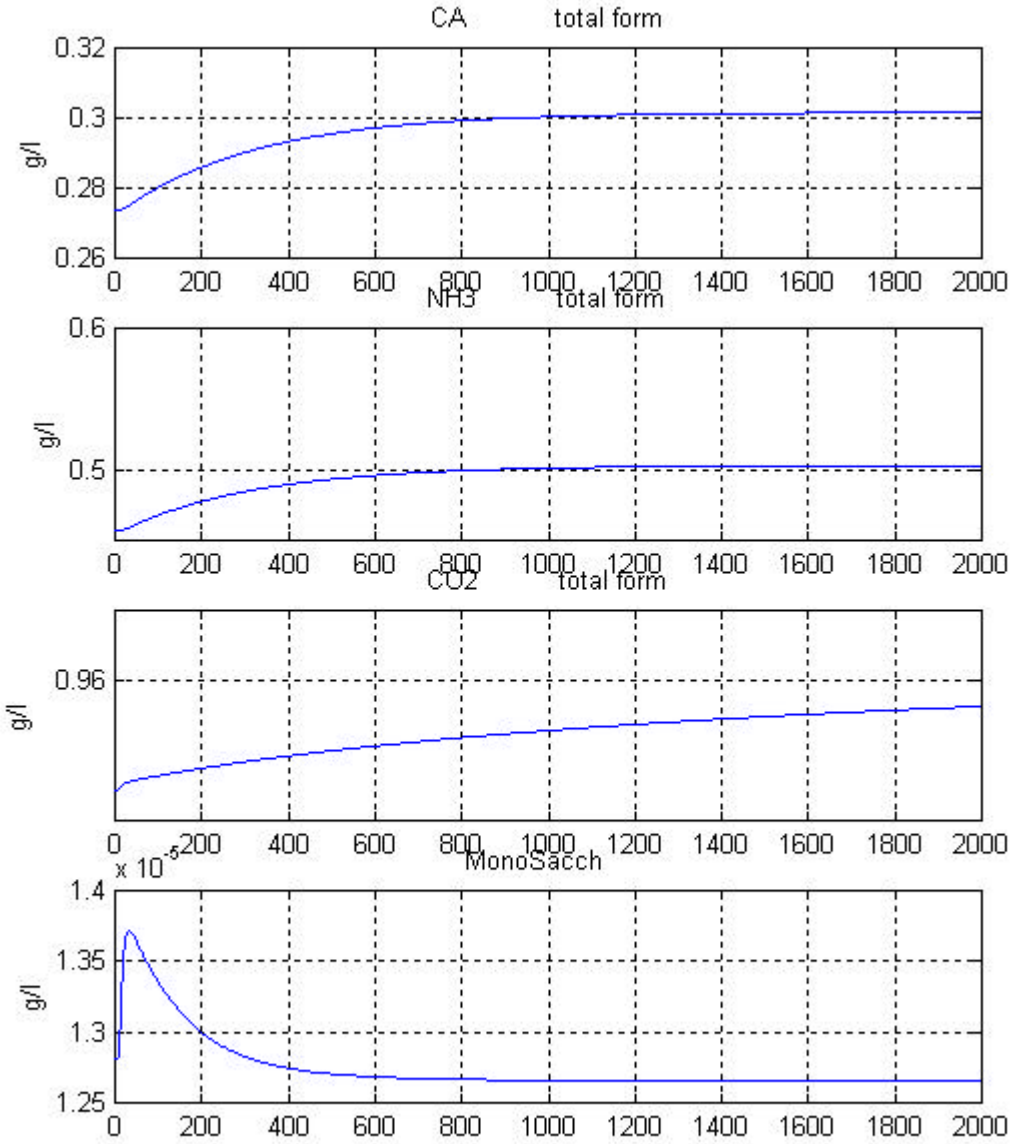

Figure 62. Input concentrations step

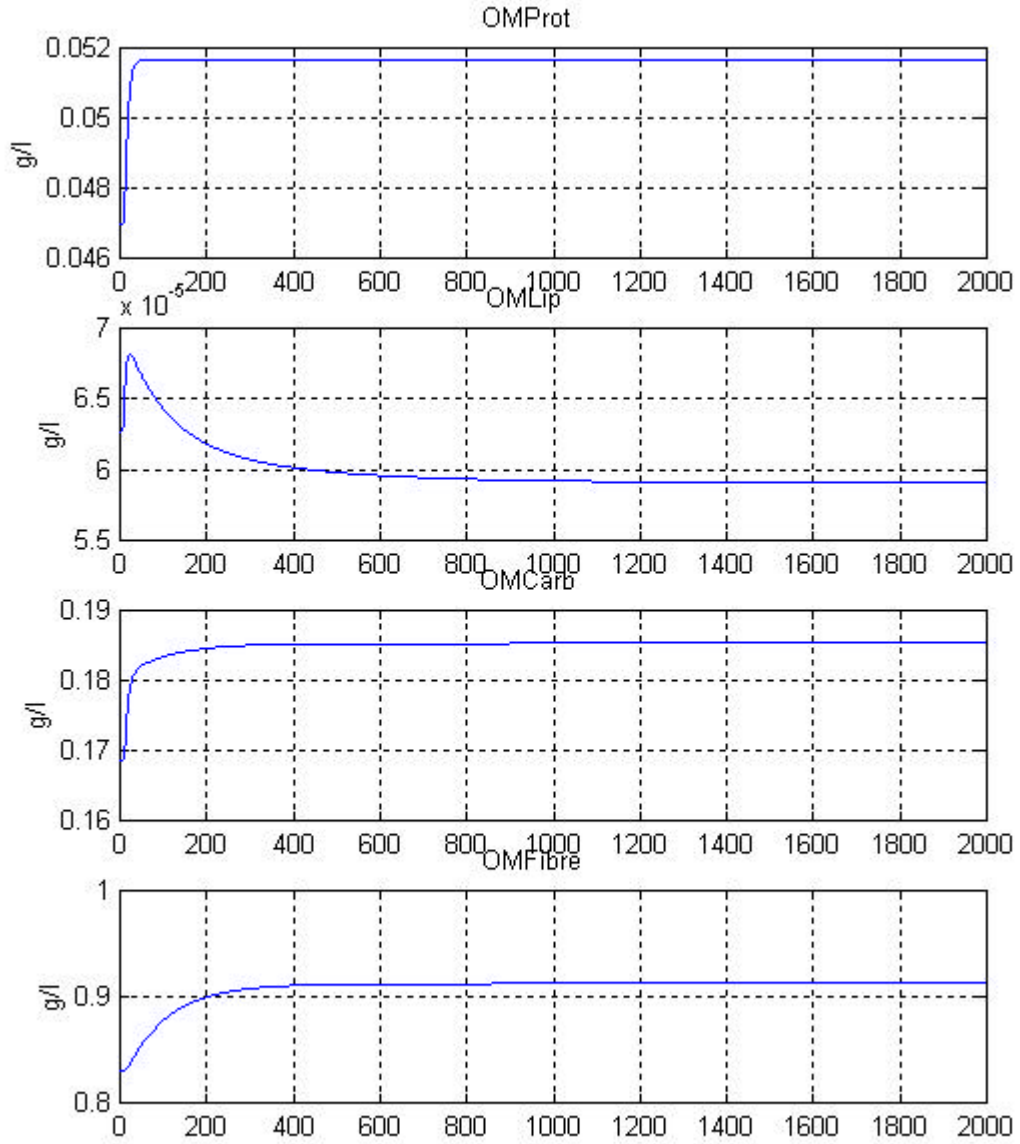

Figure 63. Input concentrations step

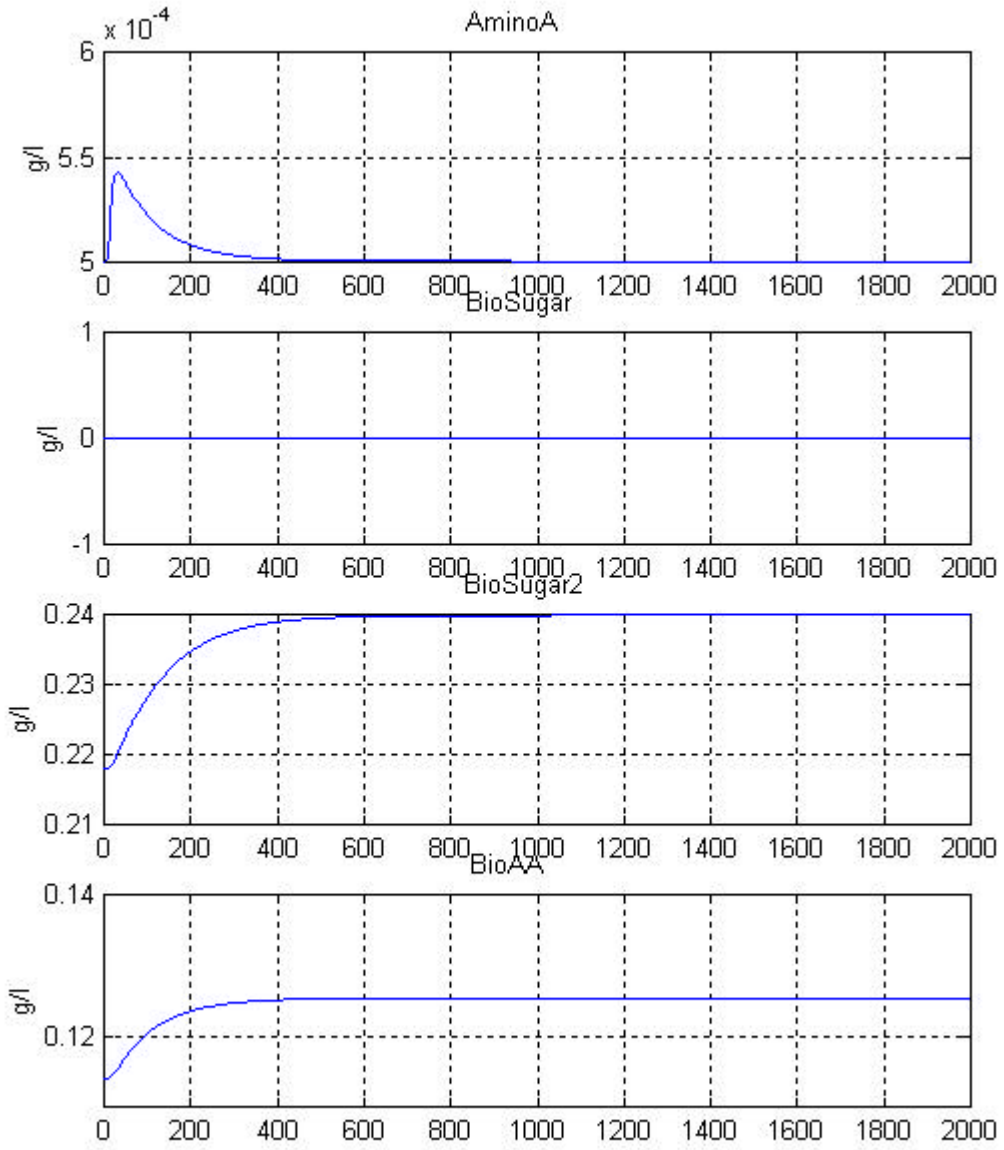

Figure 64. Input concentrations step

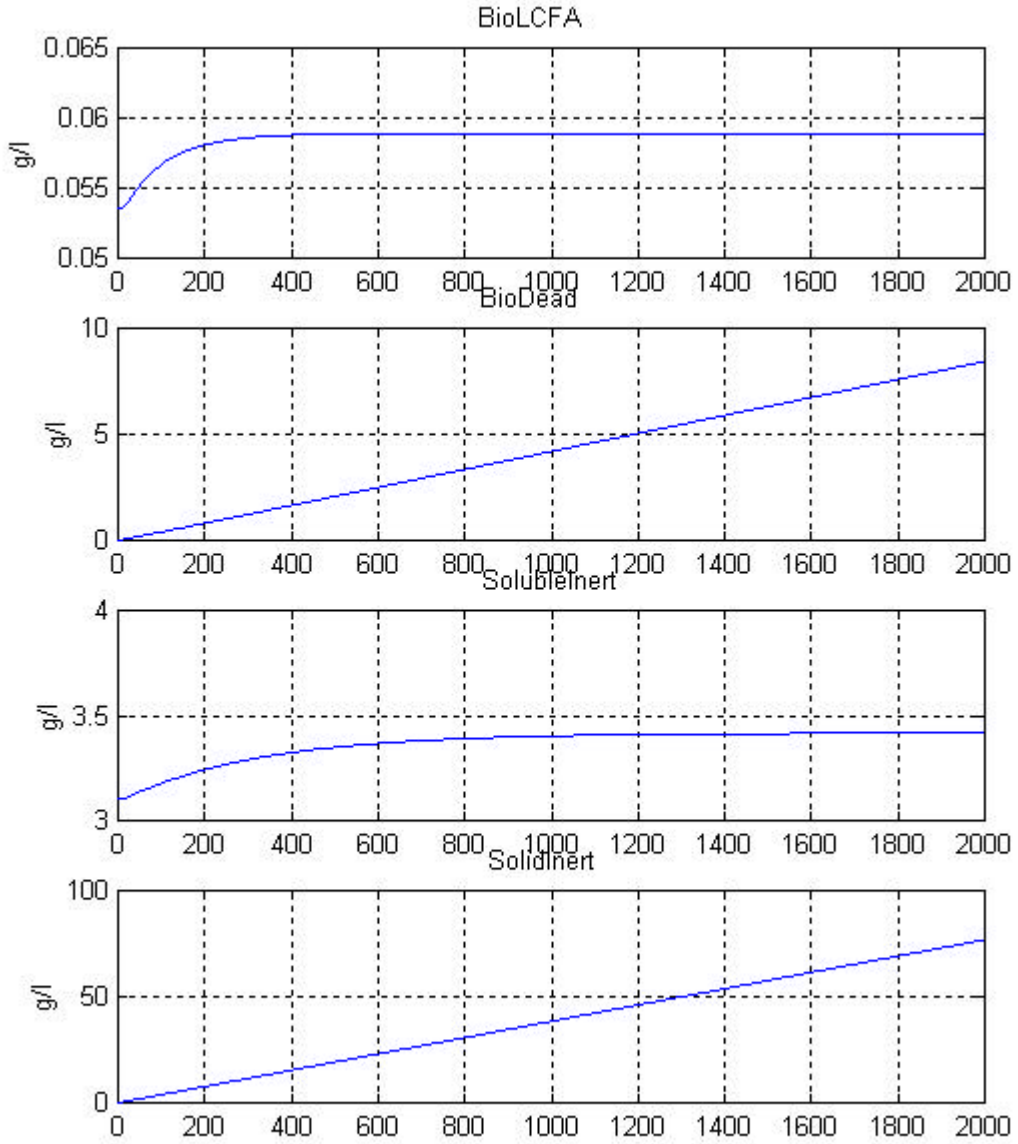

Figure 65. Input concentrations step

5.5 TOOL FOR THE OPTIMISATION OF THE SIMULATED PROCESS

The system of ODE's, describing the process, is programmed in the Matalb file 'process.m'. The integration is done by the solver defined in the Simulink window 'g_simpro'.
The physico-chemical parameters (stoechiometry, kinetics, acid/base dissociation constants, gas/liquid equilibrium constants, … are defined in the Matlab files 'i_sim_1.m' and 'i_physic.m'.
The initial state and the time variable inputs of the process are defined in 'i_sim.m'. This file contains also the numerical values of the simulation parameters (time range, tolerance, …), the characteristics and functioning conditions of the reactor (volumes, temperature, pH …).
In a practical way, when the simulation conditions are defined in 'i_sim.m', the simulator is called by launching 'g_simpro' in the Matalb working window.

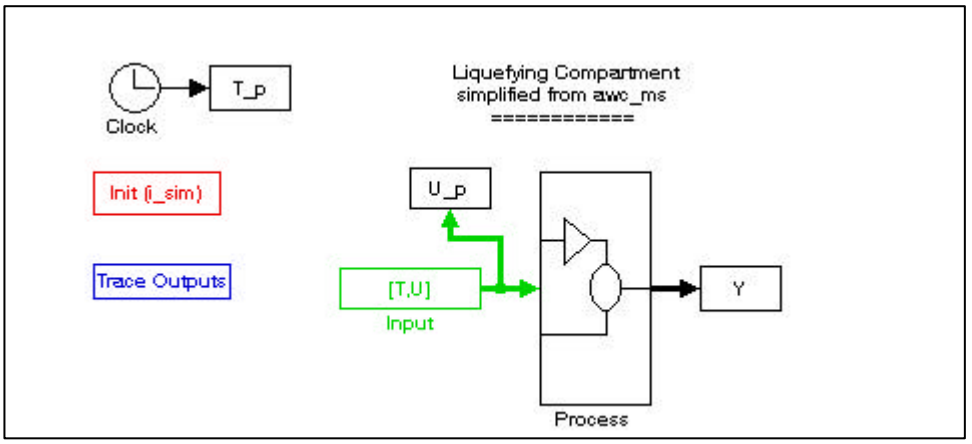

Figure 66. Simulink simulator

Then the initialisation is done by a double click on the red button 'Init (i_sim)'.
Then the simulation is launched in the menu 'Simulation/Start' of Simulink.
The results are plotted by a double-click on the blue button 'Trace Outputs'.

5.5.1 . Main programme.

```
%*****************************************************************
%       Process simplified from LGCB model                       *
%       Version 1.1     February 2005                            *
%                                                                *
%                                                                *
%       i_sim.m   Initialization of the simulation               *
%                                                                *
%*****************************************************************
%
% This file will be used for the optimisation study.
% The standard process is defined as the LGCB one on 30July2004 with the modifications
% justified in section 3 of TN1 .
% The initial std inputs are defined in table 3.1 of TN1 .
% The initial state is the steady state associated to these std inputs.
% The optimisation study will consist in modifying :
%  . the input consentrations (with a same factor for all the input
%    compounds in order to simulate a input conc. variation;
%  . the input liquid flow rate;
%  . the drain flow rate.
% Remark1 : as justified in TN3, the BioSugar biomass is null.
% Remark2 : if pb occurs with null biomass, use 'process.m' with 'ode45 Dormand-Prince'
%           or 'processNullBiomass.m' with 'ode15s', which is far quicker and
%           gives same results.

clear all
```

```
% Choice of a test
  typtst=0; titre='Std process at steady state';
  typstep=2; titre='Input concentrations step';
  typstep=3; titre='Drain flow rate step';
  typstep=1; titre='Input flow rate step';

% Simulation parameters
  tdeb=0; % (h) initial time of the simulation
  tfin=2000; % (h) final time of the simulation
  tmax=2; % (h) max step size of the solver
  dt=5; % (h) simulation period of the process inputs
  tolr=1e-6;  % normal tolerance for general case
  tola=1e-8;
  nbptx=200000;
% Simulation horizon
  T = [0:dt:tfin]';

% Physico-chemical parameters
  i_sim_1 % init parameters m.file

% System parameters
  NIcompounds=10; % Number of input concentrations
  NIflows=4; % Number of flow rates
  NE=NIcompounds+NIflows; % Dimension of the process input vector
  NX=NXcompounds+1; % Dimension of the process state vector (from 'i_sim_1.m')
                    % plus 1 : for the number of mole of the gas volume
  NS=NX; % Dimension of the process output vector

% Process inputs
  qi0=0.07875; % (l/h) initial input liquid flow rate
  qd0=0; % (l:h) initial drain flow rate
  qf0=qi0-qd0; % (l/h) initial filtrate flow rate (volume V can change)
  qo0=450; % (l/h) initial reactor outlet liquid flow rate (email EPAS)
  if qo0<qf0+qd0
    disp('Error on setting the reactor outlet liquid flow rate')
    break
  end
  % Initial concentration of input compounds
  % They are the conc. of the 'NIcompounds' first compounds of 'CompoundsName'
  ai0=zeros(NIcompounds,1);
  if typtst==0
    ai0(iFaeces)=3.968; % (g/l) data from 'awc_ms'
    ai0(iWheat)=7.936; % (g/l) data from 'awc_ms'
    ai0(iSalad)=7.936; % (g/l) data from 'awc_ms'
    ai0(iPotato)=7.936; % (g/l) data from 'awc_ms'
    ai0(iAA)=.091/Kdiss(iAA); % (g/l) data from 'awc_ms'; molecular form
    ai0(iPA)=.018/Kdiss(iPA); % (g/l) data from 'awc_ms'; molecular form
    ai0(iBA)=.021/Kdiss(iBA); % (g/l) data from 'awc_ms'; molecular form
    ai0(iVA)=.006/Kdiss(iVA); % (g/l) data from 'awc_ms'; molecular form
    ai0(iCA)=.007/Kdiss(iCA); % (g/l) data from 'awc_ms'; molecular form
    ai0(iNH3)=.025/Kdiss(iNH3); % (g/l) data from 'awc_ms'; molecular form
  end
  ai0=ai0./MassMol(1:NIcompounds); % (mol/l) unit requested by 'process.m'
  U0=[qi0; qd0; qf0; qo0; ai0]; % Initial inputs
  U=ones(size(T)) * U0'; % time process inputs

% Initial steady state obtained by simulation
  if 0
    % 1. Computation of the steady state
    % Arbitrary initial state
    % init of X0 (g/l of total form)
    X0=zeros(NX,1);
    X0(iBioSugar2)=1e-3;
    X0(iBioAA)=1e-3;
    X0(iBioLCFA)=1e-3;
    X0(1:NX-1)=X0(1:NX-1)./MassMol./Kdiss;  %  (mol/l  =  unit  requested  by  'process.m');
molecular form
    % Arbitrary nN2
    nN2=VG/VMol*273/Temp; % VG full of N2 at starting the simulation
    [T_p,X,Y,Xss]=stesta(U0);
    % Display
    disp('Displaying the steady state (g/l of total form)')
    disp('-----------------------------------------------')
    for jj=1:NXcompounds
      texte=[CompoundsName(jj,:),' : 'num2str(Xss(jj)*MassMol(jj)*Kdiss(jj),'%15.6e')];
      disp(texte)
    end
```

```
    % Plotting to check the steady state
    t_sim
    Xss(iBioSugar)=0; % to be sure the BioSugar is null
    eval(['save Xsteady',num2str(typtst),' Xss'])
  else
    % 2. Loading the previously computated steady state
     eval(['load Xsteady',num2str(typtst)]) % (mol/l of molecular form = unit requested by
'process.m')
    nN2=VG/VMol*273/Temp; % gas volume full of N2 at starting the simulation
  end
  X0=Xss';

  % Arbitrary init of BioDead, SolidInert and number of mole of produced CO2 gas
  X0(iBioDead)=0;
  X0(iSolidInert)=0;
  if 0 % 0 --> to let unchanged the steady state of CO2 gas
    if 1 % Init of CO2 G at thermodynamical equilibrium with L
      V_CO2=VG*X0(iCO2)/LG_CO2;
    else % Arbitrary init of CO2 G
      V_CO2=0; % Initial partial volume of CO2 in the gas volume at 'Temp' under 1 atmosphere
    end
    if V_CO2 > VG
      disp('Incorrect initial partial volume of CO2 in the gas volume')
      break
    end
    X0(NX)=V_CO2/VMol*273/Temp; %Initial number of mole of CO2 in the gas volume
    % Number of mole of N2 in the gas volume under 1 atmosphere
    nN2=(VG-V_CO2)/VMol*273/Temp; % The number of N2 is constant all along the simulation
  end

% Temporal inputs
  if typstep == 1
    kqi=1.1; % multiplicative factor of input flow
    t1=10;
    ind = find(T>=t1);
    U(ind,1)=kqi*qi0*ones(size(ind)); % (l/h) Step of input flow
  elseif typstep == 2
    iCompounds=NIflows+[iFaeces, iWheat, iSalad, iPotato, iAA, iPA, iBA, iVA, iCA, iNH3];
    kC=1.1; % multiplicative factor of input concentrations
    t1=10;
    ind = find(T>=t1);
    U(ind,iCompounds)=kC*U(ind,iCompounds); % (mol/l) Step of input concentrations
  elseif typstep == 3
    %kqd=1.1; % multiplicative factor of drain flow
    t1=10;
    ind = find(T>=t1);
    U(ind,2)=qd0+qi0/10*ones(size(ind)); % (l/h) Step of drain flow
  end

disp(' *** C1 simplified from LGCB model - End of initialization ***')
```

5.5.2 Parameters initialisation.

```
%************************************************************************
%       Process simplified from LGCB model                              *
%       Version 1.1     February 2005                                   *
%                                                                       *
%                                                                       *
%       i_sim_1.m   Initialization of parameters of the Compartment 1   *
%                                                                       *
%************************************************************************
% Building or loading the parameters
% ----------------------------------
%if 0
%  load Param_1
%else
  % 1. Name of the chemical compounds involved in the Liquefying compartment
  %    ---------------------------------------------------------------------
  % ATTENTION: The 'NIcompounds' first compounds are common to Input and State vectors
  CompoundsName=[
    'Faeces      '; %1
    'Wheat       '; %2
    'Potato      '; %3
    'Salad       '; %4
    'AA          '; %5
```

```
  'PA          '; %6
  'BA          '; %7
  'VA          '; %8
  'CA          '; %9
  'NH3         '; %10
  'CO2         '; %11
  'MonoSacch   '; %12
  'OMProt      '; %13
  'OMLip       '; %14
  'OMCarb      '; %15
  'OMFibre     '; %16
  'AminoA      '; %17
  'BioSugar    '; %18
  'BioSugar2   '; %19
  'BioAA       '; %20
  'BioLCFA     '; %21
  'BioDead     '; %22
  'SolubleInert'; %23
  'SolidInert  ']; %24
NXcompounds=size(CompoundsName,1); % Number of compounds in the state vector X
for ii=1:NXcompounds
  eval(['i',CompoundsName(ii,:),'=ii;'])
end

% 2. Name of the chemical reactions involved in the Liquefying compartment
%    ---------------------------------------------------------------------
ReactionsName=[
  'E1 ';
  'E2 ';
  'E3 ';
  'E4 ';
  'E5 ';
  'E6 ';
  'E7 ';
  'E8 ';
  'E9 ';
  'E10';
  'E11';
  'E12';
  'E13';
  'E15';
  'E16'];
NReactions=size(ReactionsName,1); % Number of reactions
for ii=1:NReactions
  eval(['i',ReactionsName(ii,:),'=ii;'])
end

% 3. Init stoechiometry matrix of the chemical reactions
%    -----------------------------------------------
% Source : 'equations_model.doc' on 16 July 2004 from LGCB (and 'awc_ms' when conflict)
% Each column of the matrix is the stoechiometry of a given reaction.
% There are 15 reactions (so 15 columns).
% Reaction [E14] is not simulated because 'BioHVFA' does not exist.
MS=zeros(NXcompounds,NReactions); % Init matrix

% Reaction [E1]; Hydrolysis; N order reaction
MS(iFaeces,iE1)=-1;
MS(iMonoSacch,iE1)=.00869;
MS(iOMProt,iE1)=.7654;
MS(iOMLip,iE1)=.1956;
MS(iSolubleInert,iE1)=.7828;

% Reaction [E8]; Hydrolysis; N order reaction
MS(iWheat,iE8)=-1;
MS(iOMProt,iE8)=.24574;
MS(iOMLip,iE8)=.058241;
MS(iOMCarb,iE8)=1.1141; % value of simulator 'awc_ms' and not of 'equations_model.doc'
MS(iOMFibre,iE8)=.04799;
MS(iSolidInert,iE8)=.60396;

% Reaction [E9]; Hydrolysis; N order reaction
MS(iPotato,iE9)=-1;
MS(iOMProt,iE9)=.30492;
MS(iOMLip,iE9)=.022854;
MS(iOMCarb,iE9)=2.0076; % value of simulator 'awc_ms' and not of 'equations_model.doc'
MS(iOMFibre,iE9)=.08344;
MS(iSolidInert,iE9)=.33315;
```

```
% Reaction [E10]; Hydrolysis; N order reaction
MS(iSalad,iE10)=-1;
MS(iOMProt,iE10)=.74077;
MS(iOMLip,iE10)=.18122;
MS(iOMCarb,iE10)=.56856; % value of simulator 'awc_ms' and not of 'equations_model.doc'
MS(iOMFibre,iE10)=.20033;
MS(iSolidInert,iE10)=.46094;

% Reaction [E2]; Carbohydrate hydrolysis; N order reaction
MS(iOMCarb,iE2)=-6;
MS(iMonoSacch,iE2)=1;

% Reaction [E4]; Acidogenesis; Monod/Pirt reaction
MS(iMonoSacch,iE4)=-1.091;
MS(iNH3,iE4)=-.1091;
MS(iBioSugar,iE4)=.1091;
MS(iAA,iE4)=.6667;
MS(iPA,iE4)=1.3333;
MS(iCO2,iE4)=.6667;

% Reaction [E5]; Acidogenesis; Monod/Pirt reaction
MS(iMonoSacch,iE5)=-1.0833;
MS(iNH3,iE5)=-.1;
MS(iBioSugar2,iE5)=.1;
MS(iBA,iE5)=1;
MS(iCO2,iE5)=2;

% Reaction [E3]; Acidogenesis; N order reaction
MS(iOMProt,iE3)=-1;
MS(iAminoA,iE3)=1;

% Reaction [E6]; Acidogenesis (amino-acids); Monod/Pirt reaction
MS(iAminoA,iE6)=-1;
MS(iBioAA,iE6)=.0241;
MS(iAA,iE6)=.16373;
MS(iPA,iE6)=.0612;
MS(iBA,iE6)=.019;
MS(iVA,iE6)=.0177;
MS(iCA,iE6)=.01734;
MS(iCO2,iE6)=.11816;
MS(iNH3,iE6)=.2489;

% Reaction [E7]; Acidogenesis (lipids); Monod/Pirt reaction
MS(iOMLip,iE7)=-.95;
MS(iNH3,iE7)=-.05;
MS(iBioLCFA,iE7)=.05;
MS(iAA,iE7)=.35;

% Reaction [E16]; Hydrolysis (fibre); N order reaction
MS(iOMFibre,iE16)=-1;
MS(iOMCarb,iE16)=3.9216;

% Reaction [E11]; Decay biomass
MS(iBioSugar,iE11)=-1;
MS(iBioDead,iE11)=1;

% Reaction [E12]; Decay biomass
MS(iBioAA,iE12)=-1;
MS(iBioDead,iE12)=1;

% Reaction [E13]; Decay biomass
MS(iBioLCFA,iE13)=-1;
MS(iBioDead,iE13)=1;

% Reaction [E15]; Decay biomass
MS(iBioSugar2,iE15)=-1;
MS(iBioDead,iE15)=1;

% 4. Init molar mass vector of the chemical compounds involved in the Liquefying compartment
%    ------------------------------------------------------------------------------------
Matom = [12; 1; 16; 14; 32; 31];  % C H O N S P atomik mass
% Composition matrix of the chemical compounds (atoms C H O N S P):
MSC=zeros(NXcompounds,6); % Init matrix
% Source : 'equations_model.doc' on 16 July 2004 from LGCB
% atom :                C         H         O         N         S         P
MSC(iCO2,:) =        [  1         0         2         0         0         0       ];
```

```
  MSC(iNH3,:) =        [  0         3         0         1         0         0       ];
  MSC(iAA,:)  =        [  2         4         2         0         0         0       ];
  MSC(iPA,:)  =        [  3         6         2         0         0         0       ];
  MSC(iBA,:)  =        [  4         8         2         0         0         0       ];
  MSC(iVA,:)  =        [  5        10         2         0         0         0       ];
  MSC(iCA,:)  =        [  6        12         2         0         0         0       ];
  MSC(iMonoSacch,:) =  [  6        12         6         0         0         0       ];
  MSC(iOMProt,:) =     [  1         1.56828    .3063     .2693     .00635    0       ];
  MSC(iOMLip,:)  =     [  1         2          .125      0         0         0       ];
  MSC(iOMCarb,:) =     [  1         1.6667     .8333     0         0         0       ];
  MSC(iOMFibre,:)=     [  0          0          0          0          0          0       ]; %
undefined
  MSC(iAminoA,:) =     [  1         1.98       .5122     .2693     .00635    0       ];
  MSC(iBioSugar,:)  =  [  5         7          2         1         0         0       ];
  MSC(iBioSugar2,:) =  [  5         7          2         1         0         0       ];
  MSC(iBioAA,:)     =  [  5         7          2         1         0         0       ];
  MSC(iBioLCFA,:)   =  [  5         7          2         1         0         0       ];
  MSC(iBioDead,:)   =  [  5         7          2         1         0         0       ];
  MSC(iFaeces,:)    =  [  0          0          0          0          0          0       ]; %
undefined
  MSC(iWheat,:)     =  [  0          0          0          0          0          0       ]; %
undefined
  MSC(iPotato,:)    =  [  0          0          0          0          0          0       ]; %
undefined
  MSC(iSalad,:)     =  [  0          0          0          0          0          0       ]; %
undefined
  MSC(iSolubleInert,:)=[  0          0          0          0          0          0       ]; %
undefined
  MSC(iSolidInert,:)  =[  0          0          0          0          0          0       ]; %
undefined

  % Checking the stoechiometry of all the reactions
  if 0
    % atom :              C         H         O         N         S         P
    MSC1 =              [  0         2         1         0         0         0       ]; % H2O
    % Reaction: E1 E2   E3     E4    E5 E6     E7      E8 E9 E10 E11 E12 E13 E14 E15 E16
    MS1  =     [0  -1.5 -.2057 .9939 .3 -.3482 -.68125 0  0  0   0   0   0   0   0   0]; % H2O
    disp('Visual checking of the stoechiometry of all the reactions')
    disp('------------------------------------------------------------')
    for ii=1:NReactions
      disp(['Reaction: ',ReactionsName(ii,:)])
      disp( '============')
      for jj=1:NXcompounds
        texte=[CompoundsName(jj,:),' : 'num2str(MS(jj,ii),'%15.6f')];
        disp(texte)
      end
      mass_balance=[[MS(:,ii);MS1(ii)]'*[MSC;MSC1]];
      if ~all(all(abs(mass_balance) < 5e-4 ))
        format short e
        disp('*=*=* Stoechiometry is unbalanced *=*=*')
        disp('            C            H            O            N            S            P')
        disp(mass_balance)
      end
      if ii<NReactions
        disp('Strike a key to check the stoechio of the next reaction')
        disp(' ')
        pause
      end
    end
  end

  MassMol=MSC*Matom; %  (g) molar mass
   MassMol(iOMFibre)      =100; % (g) molar mass from 'rapport P Patoux' on September 2004
(deduced from tables p.12)
  MassMol(iFaeces)      =100; % (g) molar mass from 'equations_model.doc' on 16 July 2004
  MassMol(iWheat)       =100; % (g) molar mass from 'equations_model.doc' on 16 July 2004
  MassMol(iPotato)      =100; % (g) molar mass from 'equations_model.doc' on 16 July 2004
  MassMol(iSalad)       =100; % (g) molar mass from 'equations_model.doc' on 16 July 2004
  MassMol(iSolubleInert)=100; % (g) molar mass from 'equations_model.doc' on 16 July 2004
  MassMol(iSolidInert)  =100; % (g) molar mass from 'equations_model.doc' on 16 July 2004

  % Checking the molar mass of the compounds
  if 0
    disp('Displaying the molar mass')
    disp('-------------------------')
      for jj=1:NXcompounds
        texte=[CompoundsName(jj,:),' : 'num2str(MassMol(jj),'%15.6f')];
```

```
        disp(texte)
      end
  end

  % 5. Kinetics parameters
  %    -------------------
  kNorder=zeros(1,NReactions); % Init of k of the N order kinetics
  kNorder(iE1)=.2/abs(MS(iFaeces,iE1)); % (h-1)
  kNorder(iE2)=.2/abs(MS(iOMCarb,iE2)); % (h-1)
  kNorder(iE3)=.2/abs(MS(iOMProt,iE3)); % (h-1)
  kNorder(iE8)=.2/abs(MS(iWheat,iE8)); % (h-1)
  kNorder(iE9)=.2/abs(MS(iPotato,iE9)); % (h-1)
  kNorder(iE10)=.2/abs(MS(iSalad,iE10)); % (h-1)
  kNorder(iE16)=.01/abs(MS(iOMFibre,iE16)); % (h-1)

  muM=zeros(1,NReactions); % Init of specific growth rate of the Monod/Pirt kinetics
  muM(iE4)=.4/abs(MS(iBioSugar,iE4)); % (h-1)
  muM(iE5)=.1/abs(MS(iBioSugar2,iE5)); % (h-1)
  muM(iE6)=.21/abs(MS(iBioAA,iE6)); % (h-1)
  muM(iE7)=.4/abs(MS(iBioLCFA,iE7)); % (h-1)

  kS=zeros(2,NReactions); % Init of kS of the Monod/Pirt kinetics
  kS(:,iE4)=[1e-4; 1e-2]./[MassMol(iNH3);MassMol(iMonoSacch)]; % (mol/l)
  kS(:,iE5)=[1e-4; 1e-4]./[MassMol(iNH3);MassMol(iMonoSacch)]; % (mol/l)
  kS(:,iE6)=[.01; 0]./MassMol(iAminoA); % (mol/l)
  kS(:,iE7)=[1e-3; 1e-3]./[MassMol(iNH3);MassMol(iOMLip)]; % (mol/l)

  kI=zeros(1,NReactions); % Init of kI of the Monod/Pirt kinetics
  kI(iE6)=.9/MassMol(iNH3); % (mol/l)

  kD=zeros(1,NReactions); % Init of kD of the biomass decay
  kD(iE11)=.01/abs(MS(iBioSugar,iE11)); % (h-1)
  kD(iE12)=.01/abs(MS(iBioAA,iE12)); % (h-1)
  kD(iE13)=.01/abs(MS(iBioLCFA,iE13)); % (h-1)
  kD(iE15)=.01/abs(MS(iBioSugar2,iE15)); % (h-1)

  % 6. Reactor parameters
  % ---------------------
  VT=27; % (l) Total volume of the reactor
  VL=25; % (l) Liquid volume
  VG=VT-VL;  % (l) Gas volume
  if VG < 0
    disp('Error on volume of gas')
    break
  end
  Temp = 273+55; % K ('awc_ms' on 30 July 2004)
  pH = 5.6;      % 'awc_ms' on 30 July 2004

  % 7. Physico-chemical equilibrium
  %    ----------------------------
  [kpart,Ka] = i_physic(Temp,pH);
  % 7.1. Partition coefficients
   kpartN = kpart([6,4,7:end],1);    % NH3 CO2 AA PA BA VA CA (computed only to check the
values)
  % Remarks concerning the partition coefficient of the compounds :
  % The highest value of the partition coefficients is for CO2 (kpart=3082).
  % The other values are much lower (<21).
  % ==> only CO2 is assumed to be a biphasic compound (present in gas & liquid phases)
  LG_CO2=1000/18/kpart(4); %Liquid/gas thermodynamical equilibrium coefficient for CO2

  % 7.2. Dissociation coefficients
  % for CO2:
  KCO2 = Ka(1,1)/(10^(-pH))*(1+Ka(2,1)/(10^(-pH))); % [HCO3-]+[CO3--] = KCO2 * [CO2]solvated
  % dissociation vector for all the compounds
  Kdiss=ones(NXcompounds,1); % Init to 1 for all the state components
  % Remarks concerning the form (molecular/ionic) of the compounds :
  % Rem1: [NH4+]=(Kdiss-1)*[NH3]solvated with Kdis=619 means that nearly all amonia is under
NH4+ form
  % Rem2: [VFA-]=(Kdiss-1)[VFA] with Kdiss=6 means the ionic form is greater than
  % the molecular form but not enough to neglect the molecular form (in fact,
  % the molecular form cannot be neglected because it is the reactive form).
  % Rem3: [HCO3-]+[CO3--]=KCO2*[CO2]solvated with KCO2=0.21 means the ionic form
  % cannot be neglected against the molecular form.
  % ==> with the present simulator, the Acid/Base dissociation must be taken into account
  Kdiss(iCO2)=1+KCO2;
  Kdiss(iNH3)=1+(10^(-pH))/Ka(3);
  Kdiss(iAA)=1+Ka(5)/(10^(-pH));
```

```
  Kdiss(iPA)=1+Ka(6)/(10^(-pH));
  Kdiss(iBA)=1+Ka(7)/(10^(-pH));
  Kdiss(iVA)=1+Ka(8)/(10^(-pH));
  Kdiss(iCA)=1+Ka(9)/(10^(-pH));

  % 8. Gas/liquid transfer parameters
  % ----------------------------
  KLa = 10;    % from 'awc_ms'

  % 9. Indices of compounds for 'process.m'
  indL=[iAA, iPA, iBA, iVA, iCA, iNH3, iCO2, iMonoSacch, ...
        iAminoA, iSolubleInert]; % indices of Liquid compounds (=soluble compounds)
  indS=[iFaeces, iWheat, iPotato, iSalad, iOMProt, iOMLip, iOMCarb, iOMFibre, ...
         iBioSugar, iBioSugar2, iBioAA, iBioLCFA, iBioDead, iSolidInert]; % indices of Solid
compounds
  %indB=[]; % indices of Biomasses

  % 10. Molat volume
  VMol=22.414; % Molar volume at 273 K and 1 atm

  % Saving parameters
  %for ii=1:NXcompounds
  %  eval(['clear i',CompoundsName(ii,:)]) % clear indices
  %end
  %save Param_1
%end
```

5.5.3 Process simulator.

```
%************************************************************************
%       Process simplified from LGCB model for Liquefying Compartment      *
%       Version 1.1     January 2005                                       *
%                                                                          *
%                                                                          *
%       process.m : Computation of the derivative vector and output vector *
%                                                                          *
%************************************************************************

function [sys,x0]=process(tn,x,u,flag, ...
                          X0, NE, NS, NX, NIflows, NIcompounds, NXcompounds, ...
                          NReactions, MS, MassMol, VL, muM, kNorder, ...
                           kS, kI, kD, Kdiss, KLa, LG_CO2, nN2, ...
                          indL, indS, CompoundsName, ReactionsName)


% PROCESS        S-Function for simulation of a simplified Liquefying Compartment
%
% Synopsis
%       [sys,x0]=process(tn,x,u,flag,X0, ...)
%
% Parameters
%       X0      initial state vector
%       For the other parameters, see in file 'i_sim.m'
%
% State vector x
%       Length of the state vector : NX
%       x(1:NX-1) : concentration of the compounds (liquid and solid) in the reactor
%       x(NX)     : number of mole of CO2 gas produced at top of the reactor
% Inputs
%       The input vector is composed of
%       . input liquid flow rate
%       . drain flow rate
%       . filtrate liquid flow rate
%       . reactor outlet liquid flow rate
%       . the concentration of the wastes in the input liquid;
%                           of AA, PA, BA, VA, CA and NH3 in the input liquid.
%
% Outputs
%       The output vector is equal to the state vector

x0=[]; % to be Matlab 5.3 compliant
%> Sizes array and Initial conditions ----------------------------------------
if flag==0,
   sys = [
        NX   % continuous states
        0    % discrete states
```

```
        NS   % outputs
        NE   % inputs
        0    % discontinuous ...
        0    % direct feedthrough
        ];
   x0 = [X0];

%> Continuous state (computation of derivatives) ------------------------------
elseif abs(flag)==1,
  % Init
    for ii=1:NXcompounds
      eval(['i',CompoundsName(ii,:),'=ii;']) % Index of compounds in state vector 'x'
    end
    for ii=1:NReactions
      eval(['i',ReactionsName(ii,:),'=ii;'])
    end

  % The concentrations cannot be negative
    ind = find(x<0);
    x(ind) = zeros(size(ind));

    % Splitting the input vector 'u'
    qi=u(1); % (l/h) input liquid flow rate
    qd=u(2); % (l/h) drain flow rate
    qf=u(3); % (l/h) filtrate flow rate
    qo=u(4); % (l/h) reactor outlet flow rate
    ai=zeros(NX-1,1); % init concentration of the input liquid
    ai(1:NIcompounds)=u(NIflows+[1:NIcompounds]); % (mol/l) concentration of the input liquid

    % Reactions rates
    % 1. Corrective terms of biomasses growth (Monod/Pirt model terms)
    C=zeros(NReactions,1); % Init corrective terms
    C(iE4)=muM(iE4)*x(iNH3)/(kS(1,iE4)+x(iNH3))*x(iMonoSacch)/(kS(2,iE4)+x(iMonoSacch));
    C(iE5)=muM(iE5)*x(iNH3)/(kS(1,iE5)+x(iNH3))*x(iMonoSacch)/(kS(2,iE5)+x(iMonoSacch));
    C(iE6)=muM(iE6)*x(iAminoA)/(kS(1,iE6)+x(iAminoA))/(1+x(iNH3)/kI(iE6));
    C(iE7)=muM(iE7)*x(iNH3)/(kS(1,iE7)+x(iNH3))*x(iOMLip)/(kS(2,iE7)+x(iOMLip));
    % 2. Chemical kinetics. Conc. are in mol/l.
    Rr=zeros(NReactions,1); % Reactions kinetics init
    Rr(iE1)=kNorder(iE1)*x(iFaeces); % Reaction [E1]; Hydrolysis; N order reaction
    Rr(iE2)=kNorder(iE2)*x(iOMCarb); % Reaction [E2]; Hydrolysis; N order reaction
    Rr(iE3)=kNorder(iE3)*x(iOMProt); % Reaction [E3]; Hydrolysis; N order reaction
    Rr(iE8)=kNorder(iE8)*x(iWheat); % Reaction [E8]; Hydrolysis; N order reaction
    Rr(iE9)=kNorder(iE9)*x(iPotato); % Reaction [E9]; Hydrolysis; N order reaction
    Rr(iE10)=kNorder(iE10)*x(iSalad); % Reaction [E10]; Hydrolysis; N order reaction
    Rr(iE16)=kNorder(iE16)*x(iOMFibre); % Reaction [E16]; Hydrolysis; N order reaction
    Rr(iE4)=C(iE4)*x(iBioSugar);% Reaction [E4]; Acidogenesis; Monod/Pirt
    Rr(iE5)=C(iE5)*x(iBioSugar2);% Reaction [E5]; Acidogenesis; Monod/Pirt
    Rr(iE6)=C(iE6)*x(iBioAA);% Reaction [E6]; Acidogenesis; Monod/Pirt
    Rr(iE7)=C(iE7)*x(iBioLCFA);% Reaction [E7]; Acidogenesis; Monod/Pirt
    Rr(iE11)=kD(iE11)*x(iBioSugar); % Reaction [E11]; Biomass decay
    Rr(iE12)=kD(iE12)*x(iBioAA); % Reaction [E12]; Biomass decay
    Rr(iE13)=kD(iE13)*x(iBioLCFA); % Reaction [E13]; Biomass decay
    Rr(iE15)=kD(iE15)*x(iBioSugar2); % Reaction [E15]; Biomass decay
    % Variation rates of each compounds for all the reactions
    Ar=zeros(NXcompounds,1); % Init variation rate
    for jj=1:NXcompounds
      Ar(jj)=MS(jj,:)*Rr;
    end
    Ar=Ar./Kdiss; % Taking into account the acid/base dissociation for concerned compounds

    % State derivative
    sys=zeros(NX,1);
    betaL=qi/VL;
    betaS=qd*qo/(qo+qd-qi)/VL;
    % 1. State derivative of the Liquid compounds (compounds soluble in liquid phase)
    % 1.1. Monophasic compounds
    sys(indL)=betaL*(ai(indL)-x(indL)) + Ar(indL);
    % 1.2. Biphasic compound (compound in gas & liquid phases): CO2
    fmCO2=x(NX)/(x(NX)+nN2); % molar fraction of CO2 in the gas phase (CO2 + N2)
    gradCO2=fmCO2*LG_CO2-x(iCO2); % Condition of positive flux (from gas to liquid)
    if (x(end)<=0 & gradCO2>0)
      phi=0;
      tn_phi=[tn, phi]
    else
      phi=KLa*gradCO2;
    end
    sys(iCO2)=sys(iCO2)+phi/Kdiss(iCO2);
```

```
    % 2. State derivative of the solid compound
    sys(indS)=-betaS*x(indS)+betaL*ai(indS)+Ar(indS);
    %% 3. State derivative of biomasses
    %sys(indB)=( -betaS+MS(indB,[iE4,iE5,iE6,iE7])*C([iE4,iE5,iE6,iE7])+ ...
    %  MS(indB,[iE11,iE15,iE12,iE13])*kD([iE11,iE15,iE12,iE13])').*x(indB);
    % 3. State derivative of the number of mole of gas
    sys(NX)=-phi*VL;

    %> Outputs ----------------------------------------------------------------
elseif flag==3,
  % The concentrations cannot be negative (if they were ==> problem to analyse)
    %ind = find(x<0);
    %if ~isempty(ind)
    %  disp(['Negative concentration in process at time t=',num2str(tn),' hour'])
    %  keyboard
    %end

    sys=x;
%> ------------------------------------------------------------------------
else
   sys = [];
end
```

5.5.4 Steady state simulation.

```
%*****************************************************************
%       Process simplified from LGCB model                       *
%       Version 1       February 2005                            *
%                                                                *
%                                                                *
%       stesta.m   Numerical comptutation of the steady state    *
%                                                                *
%*****************************************************************
function [T_p,X,Y,Xss]=stesta(U0)

% init solver parameters
tolr=1e-6;  % normal tolerance for general case
tola=1e-8;
tmax=2; % (h) max step size of the solver

% Specific rebuilding of the inputs for steady state
tdeb=0;
tfin=2000;
T=[tdeb tfin]';

% Init constant process inputs
U=ones(size(T)) * U0'; % time process inputs
ut = [T U];

%tic
options = simset('Solver','ode15s','RelTol',tolr,'AbsTol',tola,'MaxStep',tmax);
[T_p,X,Y] = sim('g_process',[tdeb tfin],options,ut);
%toc

Xss=X(end,:); % The last point is assumed to be steady state (to be checked by plotting)
```

5.5.5 Plotting.

```
% Plotting simulation of the process
% ==================================
%close all
doc = 2;        % 1 for 'ppt' file; 2 for 'doc' file
trait = .5;
if doc == 1, trait = 2; end

  biphasic=zeros(NXcompounds,1);
  biphasic([iAA,iPA,iBA,iVA,iCA,iNH3,iCO2])=ones(7,1);

% Plotting the outputs expressed in g/l of total form
if 1
  fen2tr
  jj=0;
  for ii=1:NXcompounds
    jj=jj+1;
    if jj>=5,
```

```
      jj=1;
      fen2tr
    end
    subplot(4,1,jj)
    plot(T_p, Y(:,ii)*MassMol(ii)*Kdiss(ii)),grid
    if biphasic(ii)
      title([CompoundsName(ii,:),' total form']), ylabel('g/l')
    else
      title([CompoundsName(ii,:)]), ylabel('g/l')
    end
    if jj==4
      if doc==0, trtitre(gcf,titre), end
    end
  end

  if 0
  fen2tr
  subplot(4,1,1)
  plot(T_p, Y(:,NXcompounds+1)),grid
  title('Number of mol of CO2 gas'), ylabel('mol')

  subplot(4,1,2)
  plot(T_p(1:end-1), diff(Y(:,NXcompounds+1))./diff(T_p)),grid
  title('Production rate of CO2 gas'), ylabel('mol/h')

  subplot(4,1,3)
  plot(T, U(:,1),T, U(:,2),'--'), grid
  title('Input flow rate(b-)    Drain flow rate(g--)'),ylabel('l/h')

  TotalSolid=Y(:,indS)*MassMol(indS); % 'indS' : defined in 'i_sim_1.m'
  subplot(414)
  plot(T_p, TotalSolid, T_p, Y(:,iSolidInert)*MassMol(iSolidInert), '--'), grid
  title('Total Solid (-)  SolidInert(--)'), ylabel('g/l')

  if doc==0, trtitre(gcf,titre), end
  end

% Plotting the outputs expressed in g/l of molecular and ionic forms
else
  fen2tr
  jj=0;
  for ii=1:NXcompounds
    jj=jj+1;
    if jj>=5,
      jj=1;
      fen2tr
    end
    subplot(4,1,jj)
    if biphasic(ii)
      plot(T_p, Y(:,ii)*MassMol(ii),T_p, Y(:,ii)*MassMol(ii)*(Kdiss(ii)-1),'--'),grid
      title([CompoundsName(ii,:),'molecular (-)   ionic(--)']), ylabel('g/l')
    else
      plot(T_p, Y(:,ii)*MassMol(ii)),grid
      title([CompoundsName(ii,:)]), ylabel('g/l')
    end
    if jj==4
      trtitre(gcf,titre)
    end
  end

  fen2tr
  subplot(4,1,1)
  plot(T_p, Y(:,NXcompounds+1)),grid
  title('Number of mol of CO2 gas'), ylabel('mol')

  subplot(4,1,2)
  plot(T_p(1:end-1), diff(Y(:,NXcompounds+1))./diff(T_p)),grid
  title('Production rate of CO2 gas'), ylabel('mol/h')

  subplot(4,1,3)
  plot(T, U(:,1),T, U(:,2),'--'), grid
  title('Input flow rate(b-)    Drain flow rate(g--)'),ylabel('l/h')

  TotalSolid=Y(:,indS)*MassMol(indS); % 'indS' : defined in 'i_sim_1.m'
  subplot(414)
  plot(T_p, TotalSolid, T_p, Y(:,iSolidInert)*MassMol(iSolidInert), '--'), grid
  title('Total Solid (-)  SolidInert(--)'), ylabel('g/l')
```

```
  trtitre(gcf,titre)

  if 0
    fen2tr
    subplot(4,1,1)
    plot(T_p, U_p(:,NIflows+iAA)*MassMol(iAA)*Kdiss(iAA),'o'), grid
    title('Total AA input conc.'),ylabel('g/l')

    subplot(4,1,2)
    plot(T_p, U_p(:,NIflows+iNH3)*MassMol(iNH3)*Kdiss(iNH3),'o'), grid
    title('Total NH3 input conc.'),ylabel('g/l')
  end
end
```