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TECHNICAL NOTE 74.2

Anaerobic Waste Compartment modelling and simulation toolbox
-AWC_MS -

AWC toolbox improvement
Variable pressure and volumes bioreactor modelling and simulation

Version 1
Issue 1

L. Poughon

Document change log

Version	Issue	Date	Observations
0	0	July 2003	Draft version
1	0	August 2003	Final version 1 AWC_MS version 1.1
1	1	January 2005	Version 1 – Revision 1 AWC_MS version 1.1

Content

I <u>Introduction</u>

In the continuation of the technical note 74.1, the present work completes the Anaerobic Waste Compartment Modelling and Simulation toolbox (AWC_MS).

A more complex hydrodynamic model was developed and added into the toolbox. Some modifications and corrections were also made to improve the toolbox.
The resulting AWC_MS MatLab™ toolbox is released as version 1.1.

The new hydrodynamic model added in the toolbox allows to simulate a reactor operated in gas and liquid fed-batch conditions with variable liquid/gas volume and variable pressure. A set of tests was performed, some of them being presented in this work in order to check the reliability of the model.

II **Modelling of a bioreactor with variable pressure and liquid volume**

In the previous AWC_MS release (version 1.0), there is only one kind of process: a simple chemostat reactor with constant liquid (and gas) volume and constant pressure. In fact for most of the experiments currently performed on the anaerobic controlled reactors:
- the reactor is often operated in fed-batch for liquid and gas
- the gas production is released by an over-pressure valve
- pH is a variable which evolves during the process

Then in order to complete the AWC_MS toolbox, a second model was developed. In this model:
- input gas and liquid flows rates may be different of the output flows
- gas and liquid volumes may be variables
- pressure may be variable during the simulation
- pH and Ec are also considered as variables, but at this time we don't have a reliable model for predicting the evolution of pH or Ec during a simulation

II.1 Mathematical model of the reactor

In the model of this reactor (figure 1), several variables are introduced:
- the liquid input flow rate
- the liquid output flow rate
- the gas input flow rate
- the gas output flow rate
- the liquid volume
- the gas pressure
- the pH
- the Ec
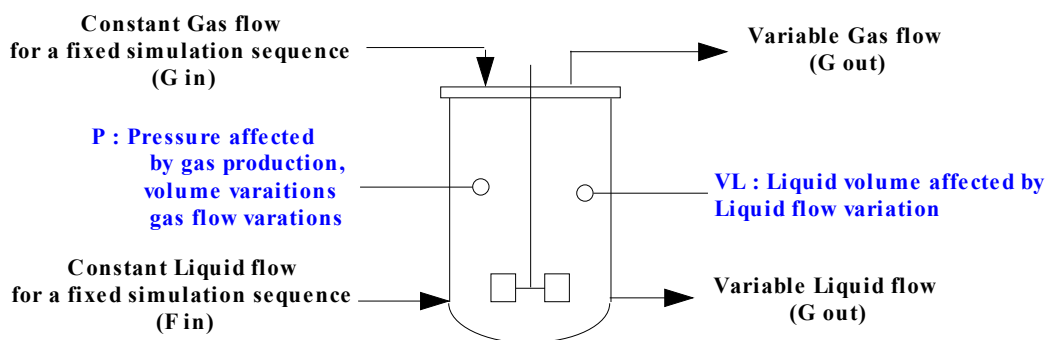
Figure 1 : Principles of the reactor with variable pressure and volume.

The expressions of mass balance equations on the reactor are greatly affected by introducing pressure and liquid volume as function of time. Moreover, as some variables are linked together, it is necessary to fix in the model, which variables are dependent to the other ones, which are controlled and which are manipulated.

For example, liquid input flow rate, liquid output flow rate and liquid volume are linked together and can not evolve independently. In this 3 variables it must be chosen which one is calculated from the other.

For this reason, the control mode for liquid volume and pressure must be fixed.

For liquid volume there are two options:

1 – no control of the volume. In such a case, the liquid input flow rate **and** the liquid output flow rate **are fixed**. The volume in the reactor evolves depending on the differences between the two flow rates. At this time variations due to water evaporation and metabolic water production are not taken into account. When critical values (liquid volume=0 or liquid volume=reactor volume) are reached, the volume value is frozen and variations are reported to the liquid output flow (as in option 2)

2 – control of volume at an objective value. In this case, only the liquid input flow rate is fixed. The liquid output flow rate **is first fixed to the initial value but is manipulated** (automatically recalculated) **when the volume reaches the maximum or minimum (V=0 Liter) values**. When the maximal value is reached, the output flow rate is manipulated in order to maintain this maximum volume.

For the gas pressure there are also two options :

1 – control of pressure by a valve. In such a case, **there is no output gas flow rate**. The pressure can increase to reach a maximal value for which the valve opens. Then the pressure falls to the reference pressure while excess gas is rejected.

2 – pressure is kept constant. This corresponds to the situation used for the previous chemostat modelling (TN 74.1). In this case, the gas output flow rate is manipulated in order to maintain the reactor pressure constant.

For the mathematical expressions detailed in the next chapters, the notations used are reported in the following table.

Notations
Si refers to the compound i
V_L and V_G : respectively liquid and gas reactor volumes (l)
Vout : cumulative volume of gas produced in Nl (T=0°C, P=1atm)
F_{in} : the input liquid flow rate (l.h^{-1})
F_{out} : the output liquid flow rate (l.h^{-1})
G_{in} : the input gas flow rate (l.h^{-1})
G_{out} the output gas flow rate (l.h^{-1})
P :gas pressure in reactor (Pa)
P_{out} output gas pressure (Pa)
Pref : reference pressure (Pa)
$P_{overpress}$: Pressure for opening valve (Pa)
$n\|_{overpress}$: gas lost by opened valve (mol)
$n_{Si}\|_G$: moles of gas Si in the reactor (mol)

$C_{Si}^{in}\big|_L$ and $C_{Si}^{in}\big|_G$: respectively the liquid and gas input concentration of Si (g/l)

$C_{Si}\big|_L$ and $C_{Si}\big|_G$: respectively the liquid and gas reactor/output concentration of Si (g/l)

$\phi_{Si}\big|_{GL}$: gas liquid transfer rate (g.l^{-1}.h^{-1})

$\phi_{Si}\big|_{Reac}$: Liquid reactions rate for Si (g.l^{-1}.h^{-1})   ; $\phi_{Si}\big|_{Reac} = \sum r_{Si}$, $\phi_{Si}\big|_{Reac}$ is the sum of all the reaction

rates r_{Si} (biological and acid-base) of compound Si

II.2 Expression of the liquid volume variation $\dfrac{dV_L}{dt}$

As explained previously, there is two options for managing the liquid volume, what implies two algorithms for the calculation of $\dfrac{dV_L}{dt}$:

Volume control	Relations used for in volume variation
No (ranging between 0 and reactor volume)	$\dfrac{dV_L}{dt} = \sum F_{in} - F_{out}$ $\dfrac{dF_{out}}{dt} = \begin{cases} 0 & \text{while } 0.1\%\,V_{reactor} < V_L < 99.9\%\,V_{reactor} \\ \dfrac{dV_{Lt}}{dt}.3600 & \text{in other cases} \end{cases}$
Yes (ranging between 0 and a maximum volume)	$\dfrac{dV_L}{dt} = \sum F_{in} - F_{out}$ $\dfrac{dF_{out}}{dt} = \begin{cases} 0 & \text{while } 0.1\%\,V_{reactor} < V_L < V_{max} \\ \dfrac{dV_{Lt}}{dt}.3600 & \text{in other cases} \end{cases}$

Table 1: Expressions of the liquid volume variation $\dfrac{dV_L}{dt}$

The variation of liquid volume is only calculated from the difference between input and output flows. The output liquid flow rate $\dfrac{dF_{out}}{dt}$ is manipulated in order to maintain the liquid volume in the correct range. The input flow rate is not manipulated. It is important to keep in mind that volume variation due to evaporation or metabolic water production/consumption is not taken into account. 3600 is an arbitrary value characterising the response time for changes in flow rates.

II.3 Expression of the gas pressure variation $\dfrac{dP}{dt}$

The calculation of the gas pressure variation is more complicated than for the liquid volume as it requires to manipulate the open/close sequence of an over-pressure valve.
It is not possible to manage directly the pressure. We manage only the quantity of matter (moles of gas) released when the valve is open. The variation of the pressure is a consequence of the variation of the quantity of moles inside the reactor. Then instead of pressure we can manipulate two variables (table 2):

- $n\big|_{overpress}$: the moles of gas released by the pressure valve
- Gout: the gas output flow rate.

Pressure control	Expressions of pressure variation
Over-pressure valve Manipulated varaible : n_overpress	$\dfrac{dn\big\|_{overpress}}{dt} = \begin{cases} 0 & \text{while } P < \text{P\_overpress} \\ 3600 * \dfrac{(\text{P\_open - P\_ref}).\text{Vg}}{R.T}\, e^{(-3600*(t-t\_open))} & \text{when valve is open} \end{cases}$ $\dfrac{dG_{out}}{dt} = 0$ $\dfrac{dV_{g\_prod}}{dt} = \dfrac{dn\big\|_{overpress}}{dt}.R.T_{ou}t.P_{out}$ $\dfrac{dP}{dt} = \sum \dfrac{dPi}{dt} + \dfrac{dPinert}{dt}$
Constant pressure Manipulated variable :G_{out}	$\dfrac{dn\_overpress}{dt} = 0$ $\dfrac{dG_{out}}{dt} = \dfrac{R.T_{out}}{P_{out}}.\left[-V_L \sum_{Si} \dfrac{\phi_{Si}\big\|_{GL}}{M_{Si}} + KLa * \dfrac{(P - P\_\text{ref})Vg}{R.T} \right].3600$ $\dfrac{dV_{g\_prod}}{dt} = G_{out}$ $\dfrac{dP}{dt} = \sum \dfrac{dPi}{dt} + \dfrac{dPinert}{dt}$

Table 2: Expressions related to the gas pressure variation $\dfrac{dP}{dt}$. t_{open} and P_{open} are respectively the time and the pressure at which the valve is opened.

The variation of the total pressure is taken as the sum of the variation of partial pressure of gas compounds. It is important to notice that all compounds of the gas phase are not necessarily listed or considered (i.e. the sum of the gas fractions of the compounds listed in the model can be lower than 1). Then it is necessary to consider both in input gas flow rate and in the reactor gas phase, that a part of the gas is composed of inert compounds, not involved in reactions and phases exchange phenomena.

The variation of partial gas pressure is calculated from the perfect gas law:

$$\frac{dPi}{dt} = \frac{R.T}{Vg}.\left[\frac{dn_{Si}\big|_G}{dt} + \frac{n_{Si}\big|_G}{Vg}.dVg \right]$$

Where $n_{Si}\big|_G$ is the quantity of mole of i in the reactor gas phase, and then :

$$\frac{dn_{Si}\big|_G}{dt} = y_i.\frac{dn\_tot\big|_G}{dt}$$

For the inert part of the gas, the same relations are used :

$$\frac{dPinert}{dt} = \frac{R.T}{Vg}.\left[\frac{dn\_inert}{dt} + \frac{n\_inert}{Vg}.dVg \right]$$

with

$$n\_inert = (1 - \sum y_{Si}).\frac{P.V}{R.T}$$

and

$$
\begin{cases}
\dfrac{dn\_inert}{dt} = (1 - \sum y_{Si}\big|_{in}).Gmol_{in} - \dfrac{dn\big|_{overpress}}{dt} + \sum \dfrac{dn_{Si}\big|_{G}}{dt} & \text{for over pressure control} \\[3mm]
\dfrac{dn\_inert}{dt} = (1 - \sum y_{Si}\big|_{in}).Gmol_{in} - (1 - \sum y_{Si}\big|_{out}).Gmol_{out} & \text{for constant pressure control}
\end{cases}
$$

II.4 The liquid phase
The following relation calculates the variation of concentrations in the liquid phase:

$$\frac{dC_{Si}\big|_{L}}{dt} = \frac{1}{V_{L}}\left[\sum F_{in}.C_{Si}^{in}\big|_{L} - F_{out}.C_{Si}\big|_{L} + V_{L}.\phi_{Si}\big|_{GL} + V_{L}.\phi_{Si}\big|_{Reac} - C_{Si}\big|_{L}.\frac{dV_{L}}{dt}\right]$$

II.5 The gas phase
The following relation calculates the variation of concentrations in the gas phase:

$$\frac{dC_{Si}\big|_{G}}{dt} = \frac{1}{V_{G}}\left[\frac{dn_{Si}\big|_{G}}{dt}M_{Si} - C_{Si}\big|_{G}.\frac{dV_{G}}{dt}\right]$$

with

$$
\begin{cases}
\dfrac{dn_{Si}\big|_{G}}{dt} = \dfrac{C_{Si}\big|_{G}}{R.T}\dfrac{1}{M_{Si}}Gmol_{in} - y_{Si}\dfrac{dn\big|_{overpress}}{dt} - \dfrac{V_{L}}{M_{Si}}.\phi_{Si}\big|_{GL} & \text{for control by overpressure} \\[3mm]
\dfrac{dn_{Si}\big|_{G}}{dt} = \dfrac{C_{Si}\big|_{G}}{R.T}\dfrac{1}{M_{Si}}Gmol_{in} - y_{Si}Gmol_{out} - \dfrac{V_{L}}{M_{Si}}.\phi_{Si}\big|_{GL} & \text{for constant pressure control}
\end{cases}
$$

II.6 Implementation of the process in AWC_MS toolbox
In order to implement the model detailed above as a new process model in the AWC_MS toolbox, new scripts and functions were written and some functions of the toolbox were modified in order to take into account the addition of a new process model. These modifications are implemented as a new **version 1.1** for the toolbox.

II.6.1 Modification of the toolbox architecture, new scripts and functions
A scheme of the architecture of the toolbox is given in figure 2. This figure is slightly modified (circled elements) from the toolbox version 1.0 by addition of the menu for the new process model and the addition of the mathematical model itself.
The toolbox is now composed of 63 scripts and functions, the new files added being listed in table 3.

AWC_MS toolbox Version 1.1

Structure of the toolbox composed of 63 scripts and functions

Main Windows interface of AWC_MS

awc_ms.m
Main Interface window
Initialisation of global variables

awc_ms_bg.m
Main interface background

awc.jpg

awc_ms_menu.m
Main interface menus

awc_alert.m
Alert Window
Called for signaling missing script or error

Files managment

Load process or Simulation

ld_data.m
load a process parameters
return main window

Save process

sv_data.m
Save a process parameters
return main window

Save results text format

sv_simul.m
Save results as ASCII text file
return main window

Save all (process +simulations) matlab format

sv_simul2.m
Save current matlab workspace
return main window

Reset

reini_toolbox.m
Clear all and restart AWC_MS
return main window

Compounds

Definition

compound_def.m
Define compounds and some properties

check_compound.m
check and record *DATA_corp*
return main window
(Check(1)=1)

calc_compounds.m
windows size managment

Equilibria Properties

compound_prop.m
Equilibria properties and Filtration Properties

check_compound_p.m
Check and record *DATA_corp2*
return main window
(Check(1)=2)

Réactions/Kinetics

awc_reac.m
Window for reactions management

reac_awc.jpg

Step enzym
reac 1.1 to 1.10

model_bioenzym.m
Window Interface for *DATA_reac1_xx* data capture

data_reac_selector.m
Load existing data for the selected reaction

check_reac.m
Check and record *DATA_reacX_XX*
End -submenu **(Check(2)=1)**

Step acido
reac 2.1 to 2.10

model1_monod.m
Window Interface for *DATA_reac2_xx* data capture

data_reac_selector.m
Load existing data for the selected reaction

check_reac.m
Check and record *DATA_reacX_XX*
End -submenu **(Check(2)=1)**

Step aceto
reac 3.1 to 3.10

model1_monod.m
Window Interface for *DATA_reac3_xx* data capture

data_reac_selector.m
Load existing data for the selected reaction

check_reac.m
Check and record *DATA_reacX_XX*
End -submenu **(Check(2)=1)**

Step acet-meth
reac 4.1 to 4.10

model1_monod.m
Window Interface for *DATA_reac4_xx* data capture

data_reac_selector.m
Load existing data for the selected reaction

check_reac.m
Check and record *DATA_reacX_XX*
End -submenu **(Check(2)=1)**

Step methano
reac 5.1 to 5.10 — — — Same as above

other reac
reac 6.1 to 6.10
decomposition — — Same as above
decay — — Same as above

quit
return main window

AWC Process

awc basic

awc_process_base.m
Interface window for simple continuous/batch chemostat with FU

process_awc.jpg

calc_process.m
Calculation of linked variables (flow rates)

check_process_base.m
Check and record *DATA_process*
return main window **(Check(3)=1)**

awc advanced

awc_process.m
Interface window for continuous/batch chemostat with FU with volume/pressure variation

process_awc.jpg

calc_process.m
Calculation of linked variables (flow rates)

check_process.m
Check and record *DATA_process*
return main window **(Check(3)=1)**

Simulations

Initialise

ini_proc.m
Interface for capture of initial conditions

calc_ini.m
changes in input flow (daily - continuous...)

check_ini.m
Check and record *DATA_ini*
return main window **(Check(4)=1)**

simulation

simul.m
Interface for time initialisation and simulation options

simul_start..m
selection of simulation and check validity

simul_compute_base.m or **simul_compute.m**
Initialise DATA for ODE solvers and store results

calc_achase.m
Acid/base equilibria

conversion.m
conversion gas fraction--> concentration

calc_rate.m
Reaction rate calculation

conversion2.m conversion3.m c_to_frac.m
conversion concentration ->fraction gaz

INTEGRATION ODE

ode15s.m or ode45/m

syst_xxx.m
Process differential equations system

Csat_12.m Csat_1.m
Gas/liquid equilibria relations

r_xxx.m
Reaction rates models

r_achase.m
Acid/base pseudo reaction rate model

SIMULATION BLOCK

END SIMULATION
Return Main interface

ranging

ranging.m
Interface for time initialisation and simulation optionsfor a ranged simulation

SIMULATION BLOCK

Sequential

Interface for time initialisation and simulation optionsfor a sequential simulation

SIMULATION BLOCK

Results

concentrations

graph_out.m
Interactive plotting of concentrations of compounds

graph_change.m
Load data to plot

graphe_trace.m
Plot graphs

process

graph_process.m
Interactive plotting of process variable parameters

graph_p_change.m
Load data to plot

graphe_p_trace.m
Plot graphs

ranging plot 3D

graph_3D.m
Interactive plotting of 3D ranged results

graph_3D_change.m
Load data to plot
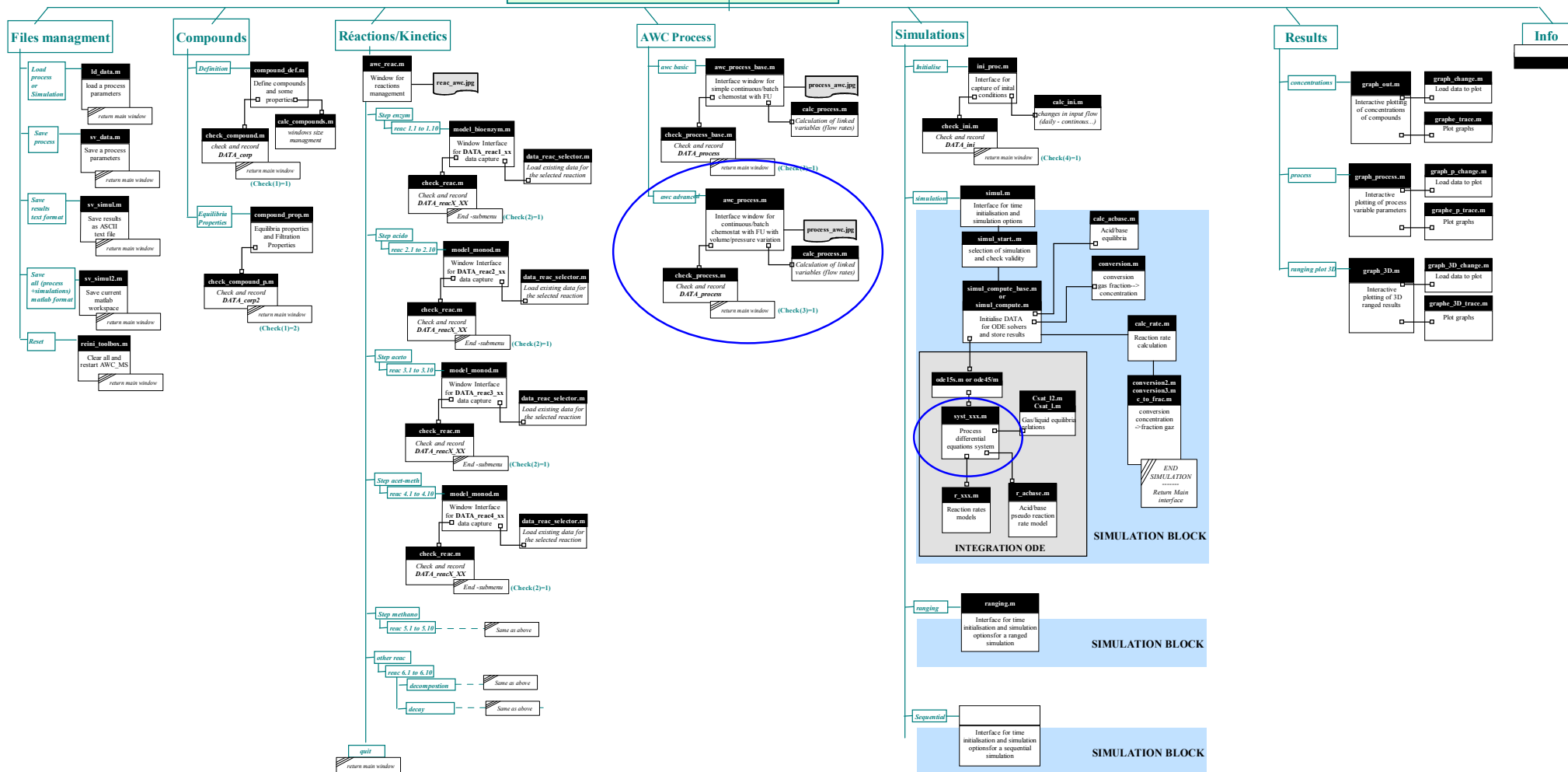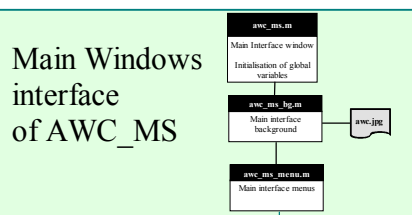
graphe_3D_trace.m
Plot graphs

Info

Figure 2 : architecture and dependencies of scripts and functions (files) in AWC_MS 1.1.
Circled elements concern parts of the toolbox changed/implemented from version 1.0

Script/function name		Function in AWC_MS	Called by….
Awc_process.m	S	Interface for data capture of the process parameters (advanced process)	awc_ms_menu.m
Calc_process2.m	F	Calculation of some dependant parameters for the process 2 (advanced process)	Awc_process.m
Check_process.m	S	Check and store valid parameters for the advanced process	Awc_process.m
Conversion3.m	F	Final conversion gas concentration to gas fraction (pressure is a variable parameter)	Simul_compute.m
Simul_compute.m	S	Initialisation of computation for the advanced process	simul_start.m
Syst_awc.m	F	Compute the ODE system to solve for the process which is simulated	ODE solvers Simul_base.m

Table 3 : new files added to the AWC_MS toolbox. S is for scripts; F is for functions

II.6.2 Interface for the new hydrodynamic model

In the process menu of the AWC_MS windows is added the element "AWC advanced process". Selecting this item open a new window interface (figure 3) for managing the parameters of the model for a bioreactor with variable pressure and volume as detailed in the previous section.

The process is composed of a biological reactor, which can be operated in continuous, batch and fed-batch. In this process 2 parameters can be managed:

- The liquid volume can be
    - controlled to limit its value to a fixed maximum
    - not controlled (in the limits of the empty reactor to the full filled reactor)

- The pressure can be controlled
    - to a constant fixed value (output flow rate is variable)
    - by an over-pressure valve which open at a fixed pressure

The Filtration Unit (FU) is modelled only as a separation unit, characterised by the separating capability for each compound (defined in the compound definition GUI). The modelling of this unit was already detailed in TN 74.1.

The picture of the GUI window (figure 3) used to capture the operating parameters of the system is a schematic representation of the process. Some of the parameters listed are not actually used in the model, but have been integrated in the interface for a possible future us. The parameters involved in the AWC advanced process model are:
- The total volume of the reactor
- The liquid volume of the reactor at simulation start-up
- The control option for the liquid volume
- The maximum liquid volume (when liquid volume is controled)
- The pH at start-up (for acid/base equilibria calculation)
- *The control option for pH (unused in calculation)*
- *The reference pH when controled (unused in calculation)*
- *The EC value (unused in calculations – only indicative value)*

- A k_La value (used for all compounds in gas/liquid equilibrium calculations)
- The input liquid flow rate (l/h)
- The gas input flow rate (in N.L/h – T=0°C ; P=1atm)
- The reactor temperature (important for gas calculation in PV=nRT relations)
- *The stirring rate (unused – only indicative value)*
- The condensor factor (applied only on vaporised liquid in gas)
- The input liquid flow rate on the FU (also the reactor liquid output)
- The output liquid flow rate on the FU (permeate flow rate in l/h)
- The drain flow rate from the recycling flow (FU retentate)
- The reactor reference pressure. This is the pressure at the start-up and the pressure which is reaches after opening of the over-pressure valve.
- The maximum pressure for which the over-pressure valve is calibrated
- The control option for the pressure
- The output pressure and the output temperature. It must be noticed that gas volume and flow rate at the output are given for this pressure and this temperature
- *Gas sink rate (h^{-1}) would be used for calculation of gas leakage (unused in current model)*
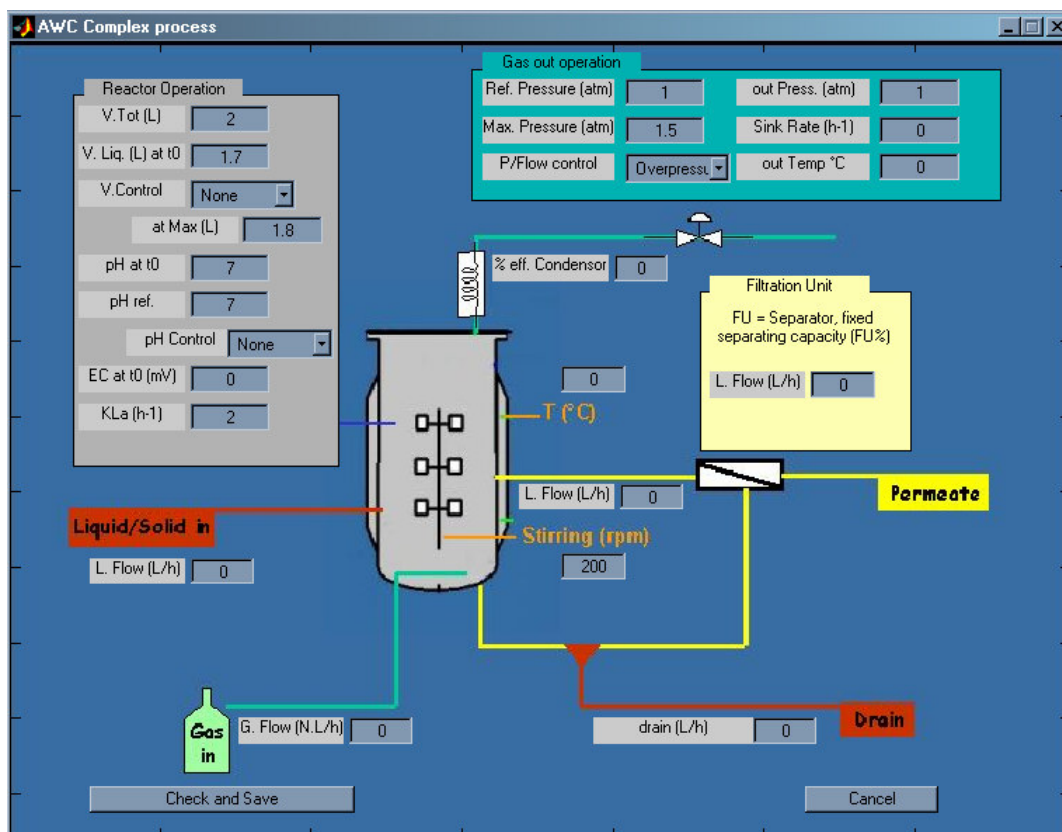
Figure 3: Window interface for the data capture of parameter of the bioreactor with variable pressure and volume

II.6.3 Computing and results

Computing of the model with AWC_MS toolbox is done as described in TN 74.1 :
- first, the liquid concentration and the gas fraction of compounds must be initialised;
- then, the type of simulation is chosen (sub-menu "standard simulation" or "ranging parameter simulation"). At the present time in the ranging parameter simulation only reactor volume and liquid input flow rate can be selected, but it is possible to add other parameters such as reference pressure, maximum pressure….

The simulation is performed as detailed in TN 74.1. Nevertheless it is important to keep in mind the changes reported in the following section III.

The results are displayed by the menu "Results". As several process parameters are computed during the simulation, they are considered as simulation results like the compounds concentrations or gas fractions. The "process operating conditions" sub-menu can display these parameters. The process variables evolving in time, which can be displayed, are:
- the liquid volume
- the pH
- the Ec
- the pressure
- the liquid input flow rate (for the reactor)
- the liquid output flow rate (for the reactor)
- the gas input flow rate (for the reactor)
- the gas output flow rate (for the reactor)
- the FU liquid output flow rate (permeate)
- the drain flow rate (retentate)
- the total volume of gas at the output of the reactor

II.6.4 Tests of the model
The model proposed can be computed with several combinations of operating conditions. It was then necessary to check the ability of the toolbox to compute the model for several possible combinations. Some tests (simulations) were then performed (table 5) and the results analysed in order to check the reliability of the computations.

The system used for the tests of the reactor with variable volume and pressure model is a simple water+O_2 system. No biological, enzymatic or chemical reactions are considered. But the gas/liquid equilibrium for oxygen is taken into account (ki(1atm,25°C)=42720). The objective of the tests is to check the reliability of the model for controlling and taking into account the pressure, the volumes and the gas and liquid flow rates variation during a simulation. It must be kept in mind that if the gas phase is not completely composed of oxygen, the remaining fraction is assumed to be an inert gas (no reaction and no phase transfer).

Several operating variables are kept constant for all the tests performed. They are reported in the following table 4. The other operating conditions are changed to perform the tests (table 5).

Reactor total volume : 2 litres
Reactor Liquid volume (t0) : 1.7 litre
PH : 7 (useless in tests)
EC : 0 (useless in test)
$K_La = 2h^{-1}$
Temperatures : all set to 0°C
Reactor reference pressure : 1 atm
Output pressure : 1 atm
Stirring rate : 200rpm (useless in test)

Table 4: Fixed operating conditions for the different tests

Test N°	Pressure	Liquid Volume	Liquid Flow in	Liquid flow out	Gas Flow in	O₂ liquid at t0	O₂ gas fraction at t0	Observations
1	OP 1.5->1	NC	0	0	0	1 g/l	1	
2	OP 1.5->1	NC	0	0	0	0 g/l	1	
3	OP 1.5->1	NC	0	0	0	1 g/l	0	
4	OP 1.5->1	NC	0	0	0.1NL/h	0 g/l	1	Input of inert gas
5	OP 1.5->1	NC until t₀+4h FO (1.9L) at t=4h	0 0.1 l/h at t=4h	0	0	0 g/l	1	Two step simulation (t₀; then t₀+4h)
6	OP 1.5 >1	FO at 1.8L	0.1 l/h	0	0.1NL/h	0 g/l	1	Input of inert gas
7	OP 1.5 >1	NC	0 0.1 l/h at t=4h	0	0	0 g/l	1	Two step simulation (t₀; then t₀+4h) **TEST IS LONG**
8	OP 1.5 >1	FO at 1.9L	0.1 l/h	0	0.01NL/h	0 g/l	1	Input of inert gas Low gas flow rate
9	OP 1.5 >1	FO at 1.9L	0.1 l/h	0.1 l/h	0.01NL/h	0 g/l	1	Input of inert gas Low gas flow rate
10	CP (1atm)	FO at 1.9L	0	0	0.01NL/h	0	1	

Table 5: Overview of the tests performed
OP Pm->Pr: overpressure, valve is opened for pressure Pm to reach reference pressure Pr
CP (Pr): constant pressure in the reactor (output flow is adapted in order to maintain the reference Pr pressure value)
NC : not controlled
FO (Vm): liquid flow out controlled when the maximum volume Vm is reached

II.6.4.1 Test 1 : Gas overpressure due to gas production from the liquid phase

In order to simulate the gas production by the liquid phase with the over-simplified system used to perform the tests, the liquid is over-saturated by the dissolved gas at $t_0=0$ (1g/l). This is of course abnormal and impossible conditions. The gas phase is pure O_2 ($y_{O2}=1$). The dissolved gas (here O_2) is then transferred to the gas phase, until equilibrium is reached between the two phases, what leads to increase the gas pressure. The system is closed (no gas or liquid input/output), and the volumes in the reactor are constant. The pressure is controlled by the over-pressure valve which open when pressure reaches 1.5 atm.

The variation of the O2 gas fraction are the result of precision of the numeric computation and are of the order of 10^{-10} (i.e. negligible).

When the pressure variations (increase and decrease) are rapid, the model has some difficulties to reach accurately the maximal and the reference pressure (figure c). We check here the gas/liquid equilibrium law and the functioning of the over-pressure valve.
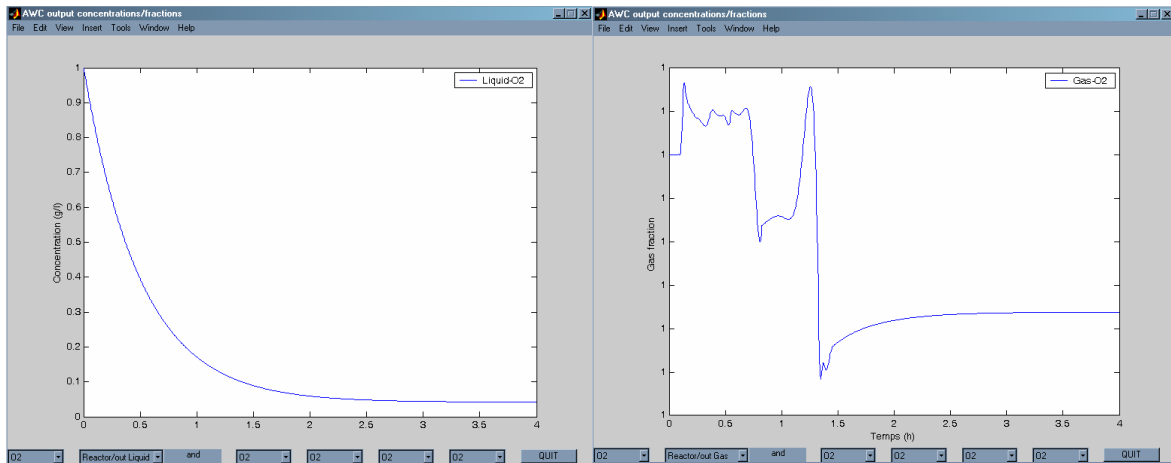
a) O_2 liquid concentration

b) O_2 gas fraction
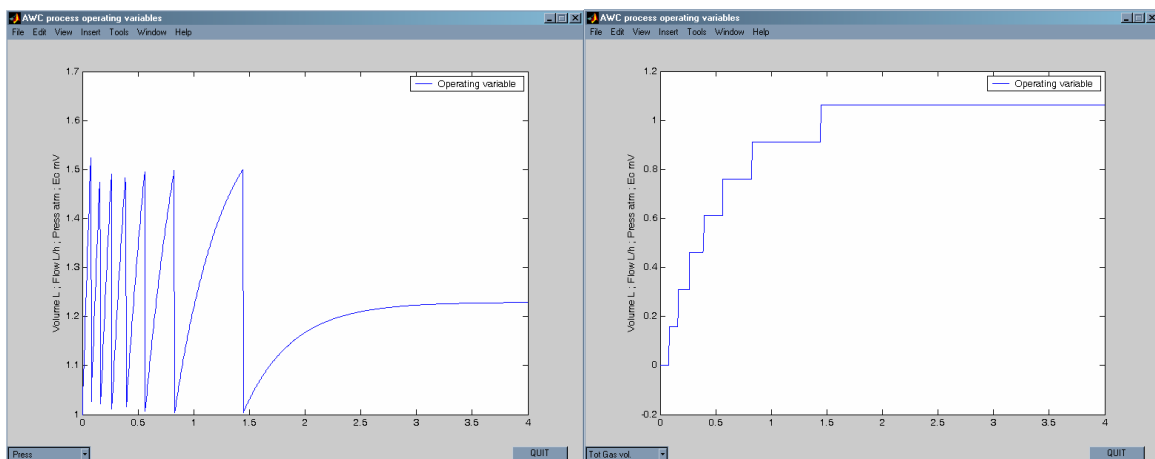
c) Gas pressure in reactor

d) Cumulative volume of gas produced

II.6.4.2 Test 2 : Gas liquid equilibrium and pressure decrease

In this simulation, the conditions are the same as for the test 1, except the O_2 concentration in the liquid phase at t0, which is set to 0g/l. This test checks the decrease of pressure due to gas transfer to the liquid phase (figure c). In principle the gas fraction is unchanged. In figure b, it is observed small variations of the gas fraction around 1. These variations are related to the numeric calculation precision and are in the present example of an order of magnitude of 10^{-10} (negligible).
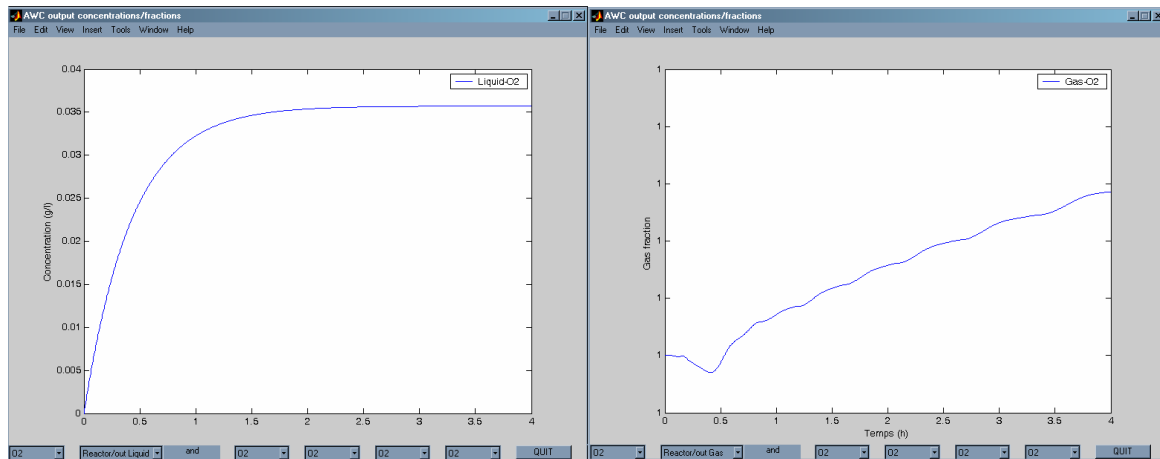
a) O_2 liquid concentration   b) O_2 gas fraction
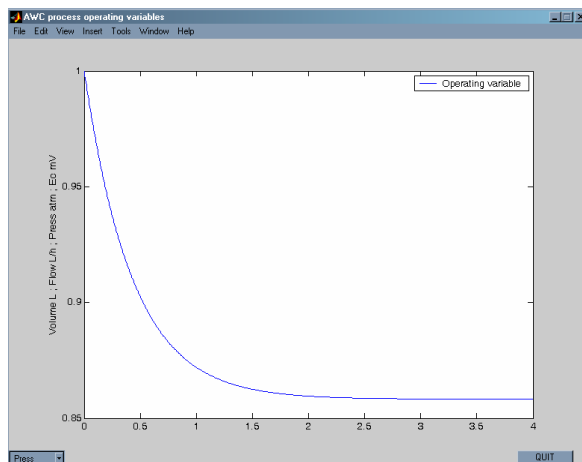
c) Gas pressure in reactor

II.6.4.3 Test 3 : Gas liquid equilibrium and pressure increase
With this test we check the ability to have an increase of the pressure (gas produced form the liquid phase as in test 1), associated to the opening of the valve when maximum pressure is reached, and to a change in the reactor gas composition due to the gas production. For this test, the conditions at $t_0=0$ are then the same as for test 1, except that gas in the reactor is an inert gas at t_0.
The equilibrium between gas and liquid is reached, and the overpressure system works also. We observed the same problem as for test 1 when pressure variations are too rapid (figure c).

With this test we check the reliability of the model to manage the inert part for the gas phase (figure b).
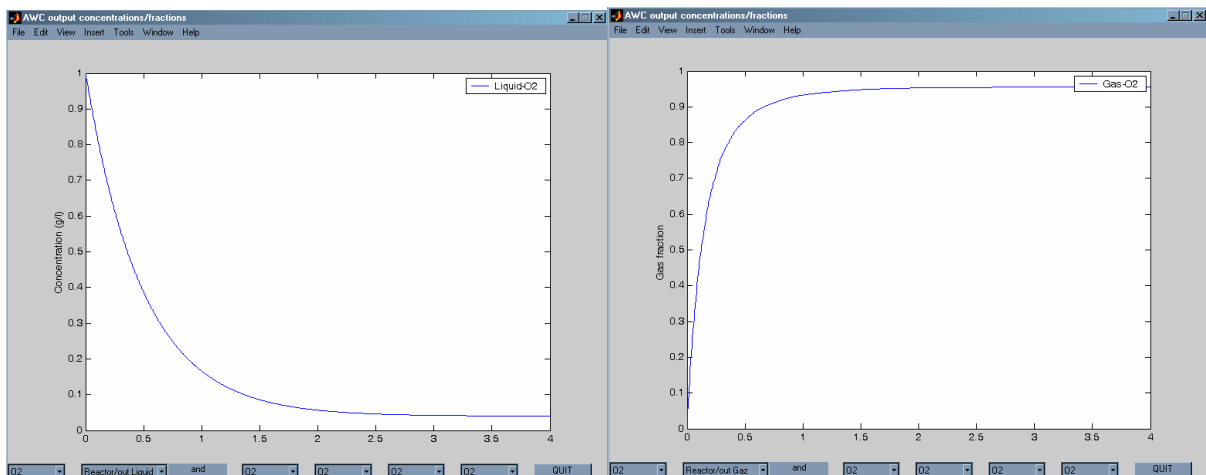
a) O_2 liquid concentration   b) O_2 gas fraction
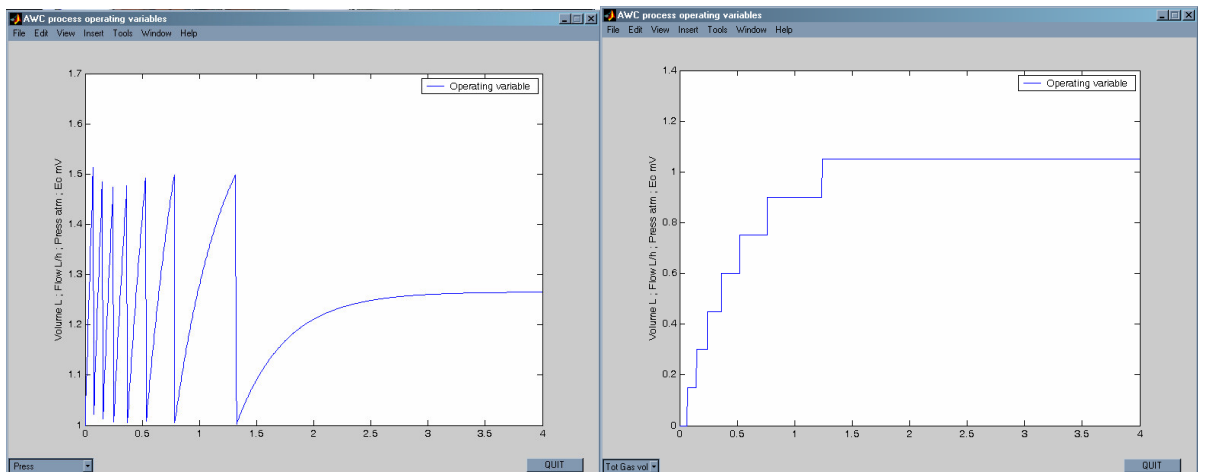
c) Gas pressure in reactor   d) Cumulative volume of gas produced

II.6.4.4 Test 4 : Gas overpressure due to constant input flow rate of an inert gas

With this test is checked the response to an increase of pressure due to a gas input, without a gas output. The initial (t0) conditions are taken as for the test 2, with a gas phase composed of oxygen only and a liquid phase free of oxygen. The input gas flow rate is set to 0.1NL/h of inert gas.

After the liquid/gas equilibrium a constant increase/decrease of the pressure is observed, in the range of the reference and maximum pressures given. It can be checked that the steps in volume production correspond to the 0.1NL/h of input (figure d). The increase of pressure is slow enough to have a good accuracy for the opening/closing periods for the valve (figure c).

These increases are also slow enough to allow the equilibrium between the gas and the liquid phases, then in figure a) it can be observed the crenelling of the curve due to the variation of the dissolved O2 saturation concentration. The gas used in the input is an inert gas, it is observed that O_2 in the gas phase is progressively replaced by the inert (figure b).
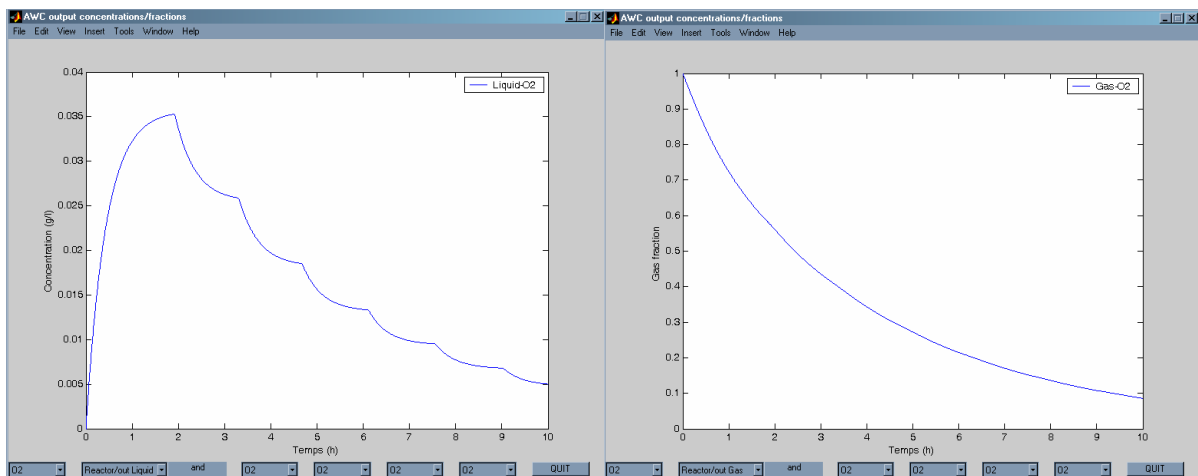
a) O_2 liquid concentration   b) O_2 gas fraction
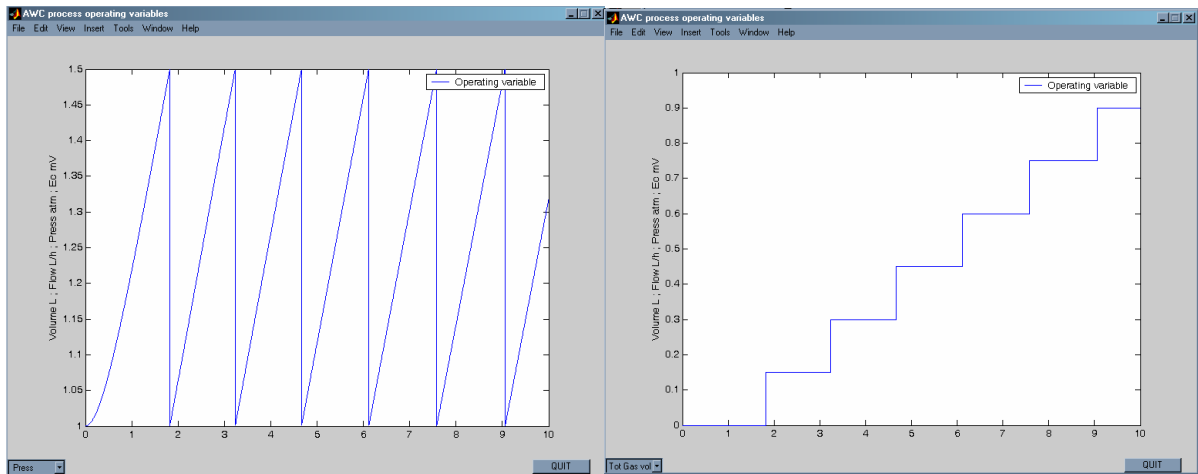
c) Gas pressure in reactor   d) Cumulative volume of gas produced

II.6.4.5 Test 5 : Continuing test 2 with the addition of a liquid input

With this test we check both the response of the model to sequential simulation and the effect of liquid volume variation to the pressure. Both pressure and liquid volume are controlled. The first part of the simulation (t=0 to t=4h) corresponds to test 2. At t=4h (black line in figures), the liquid flow rate is set to 0.1 l/h. It can be observed in figure a, the effect of the pressure (gas fraction remains equal to 1, see figure b) on dissolved concentration of O_2.

Figures e) and c) show respectively the increase of the liquid volume during about 1 hour (there is no liquid output), and the increase of pressure due to the reduction of the gas volume in the reactor. After one hour the volume reaches its maximum and an output liquid flow is generated to maintain this maximum volume (figure g). This output flow rate is equal to the input flow rate.

In figures a) and c) the decrease after t=6hours is the result of the O_2 leakage by the way of dissolved O_2 in the liquid flow (input liquid flow is assumed free of O_2)

As previously, the variation of the O_2 gas fraction is only the result of the numeric precision of computations (figure b).

This test shows that the model is reliable for simultaneous liquid volume control and over-pressure control.
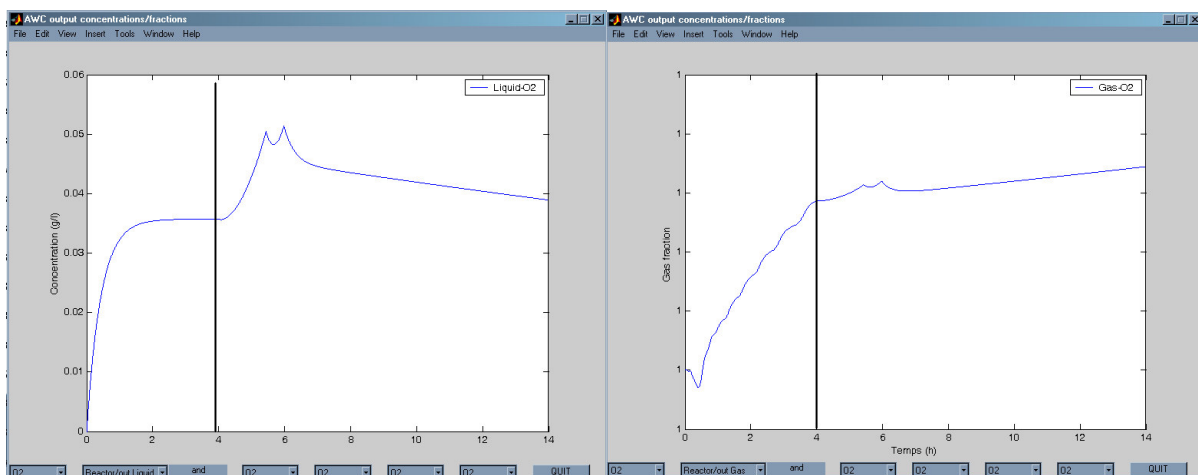
a) O_2 liquid concentration   b) O_2 gas fraction
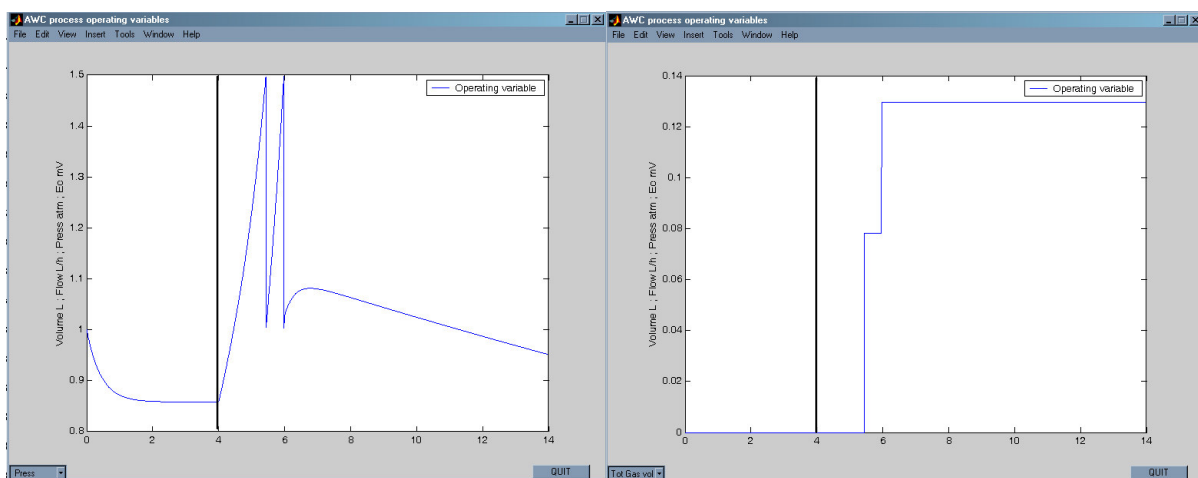
c) Gas pressure in reactor   d) Cumulative volume of gas produced
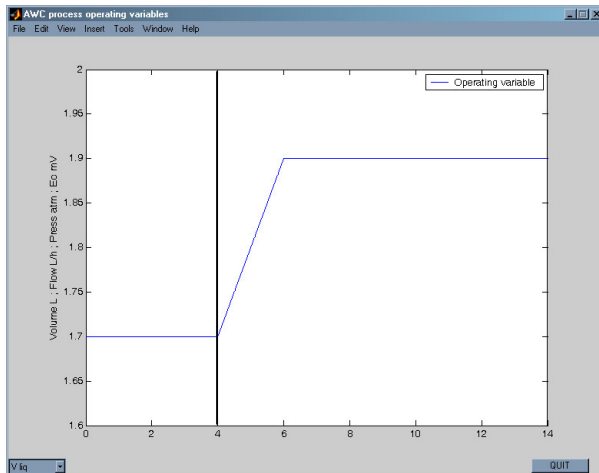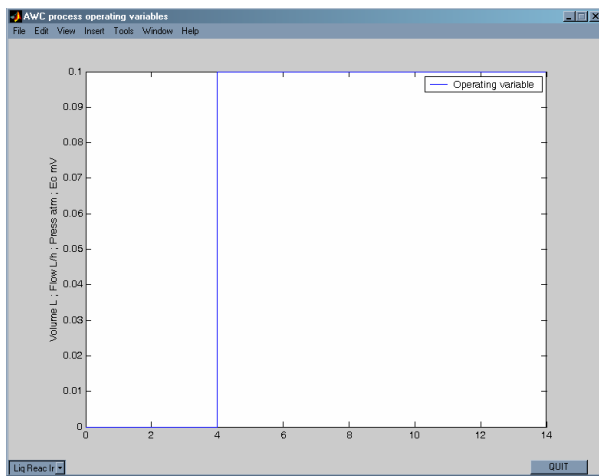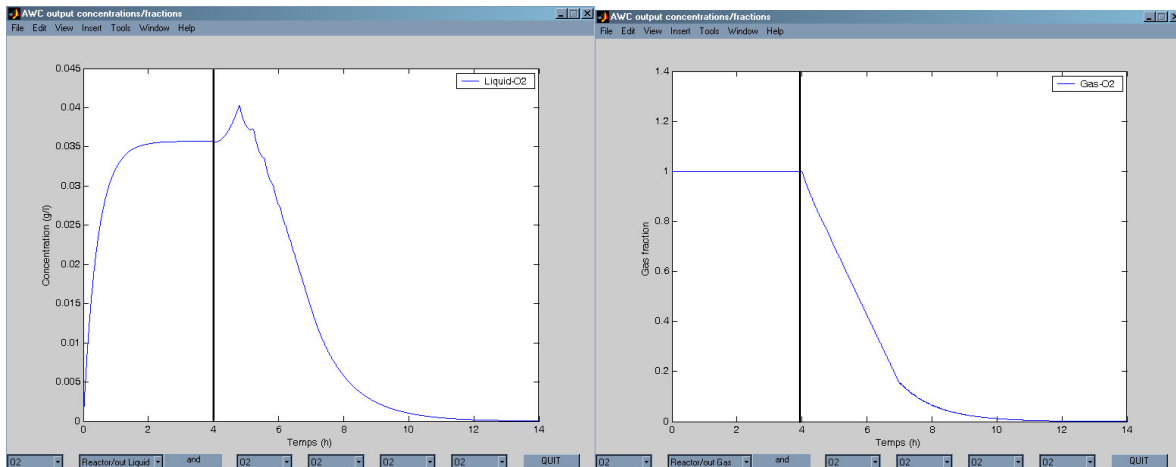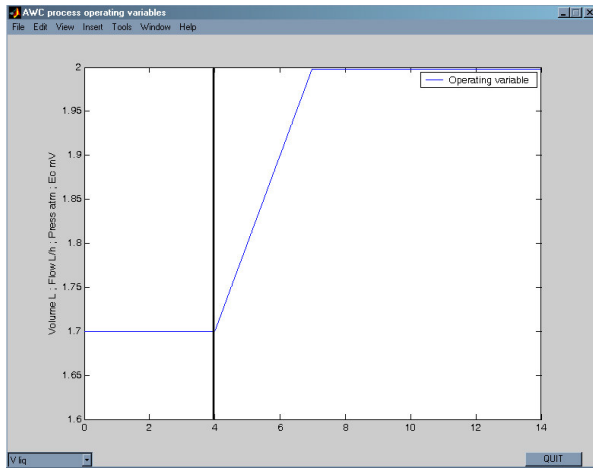
e) Liquid volume
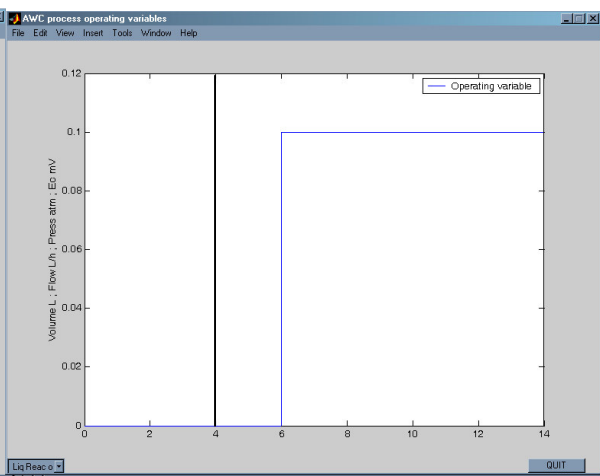
f) Input liquid flow rate   g) output liquid flow rate

II.6.4.6 Test 6 : Over-pressure control and volume control for continuous gas flow and liquid flow rates

This test is quite similar to the test 4, excepted that there is an input of liquid. Then during the first hour of the simulation the increase of pressure results both from the gas volume reduction and from the input gas flow rate. The model takes well into account the two phenomena, as the first opening of the valve occurs before 1 hour (figure c). Pressure variations are more rapid than in test 4 because of a reduced gas volume.
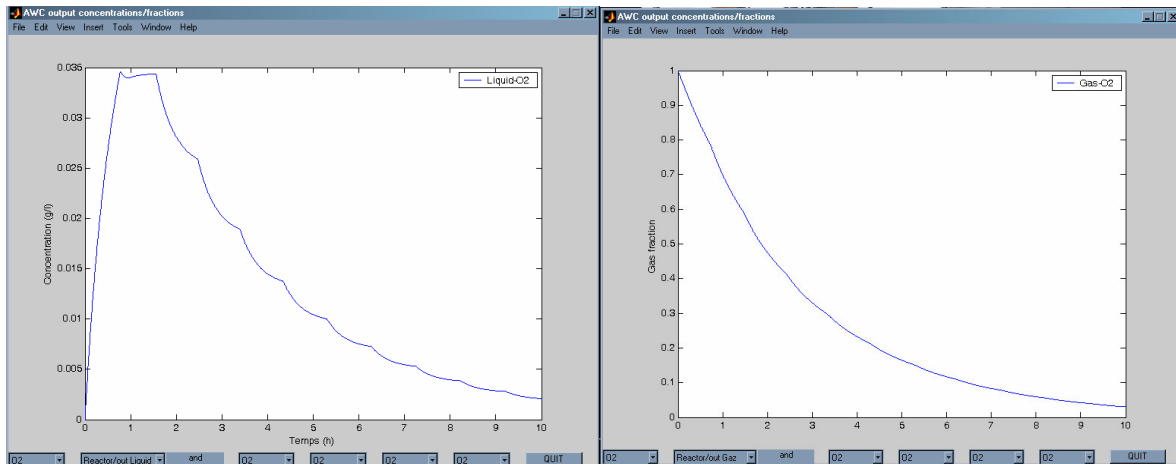
a) O_2 liquid concentration
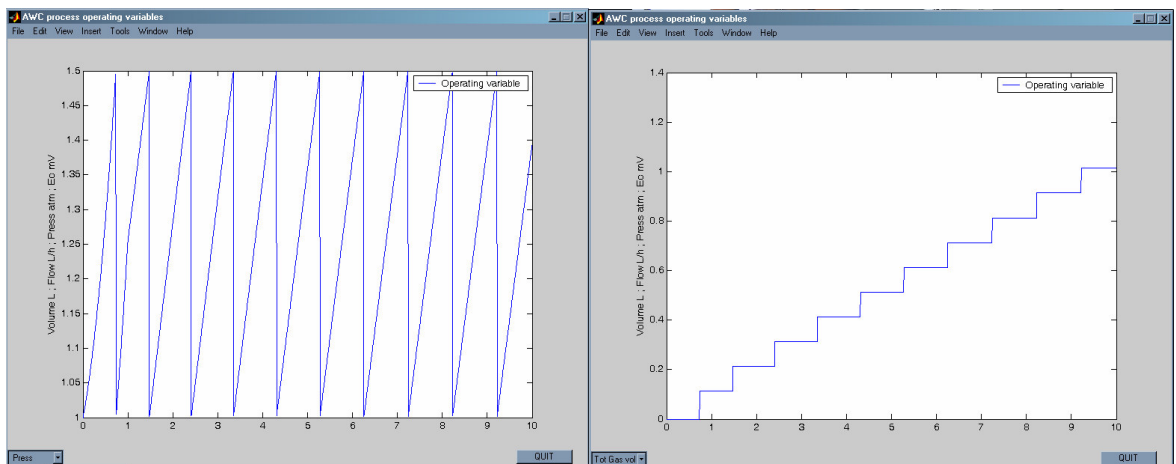
b) O_2 gas fraction

c) Gas pressure in reactor

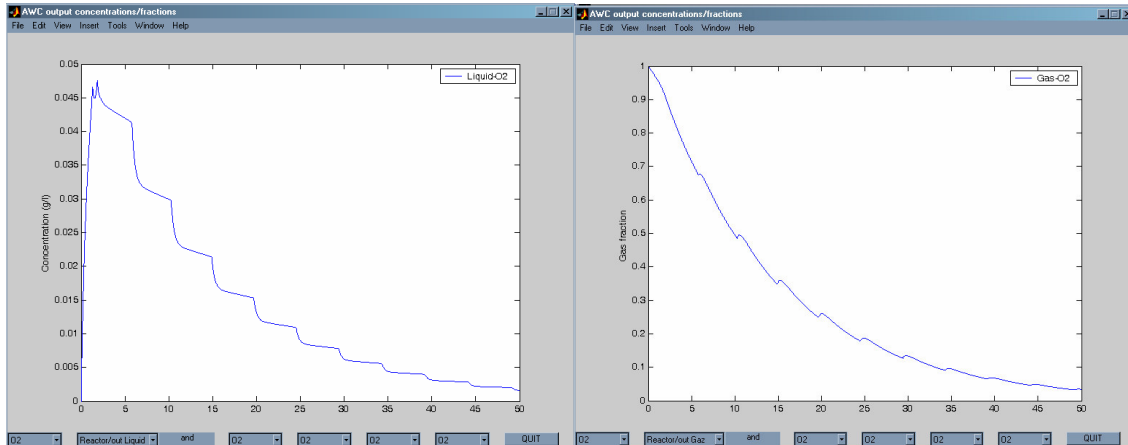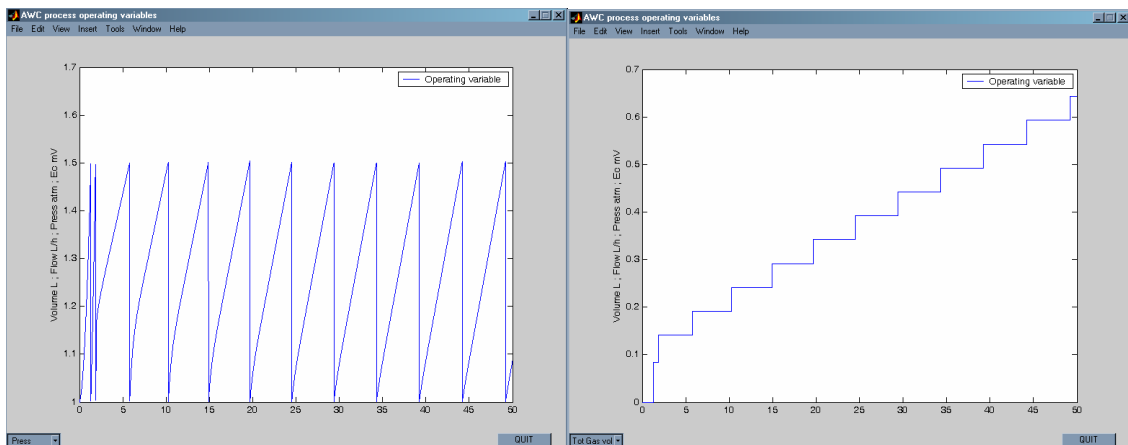d) Cumulative volume of gas produced
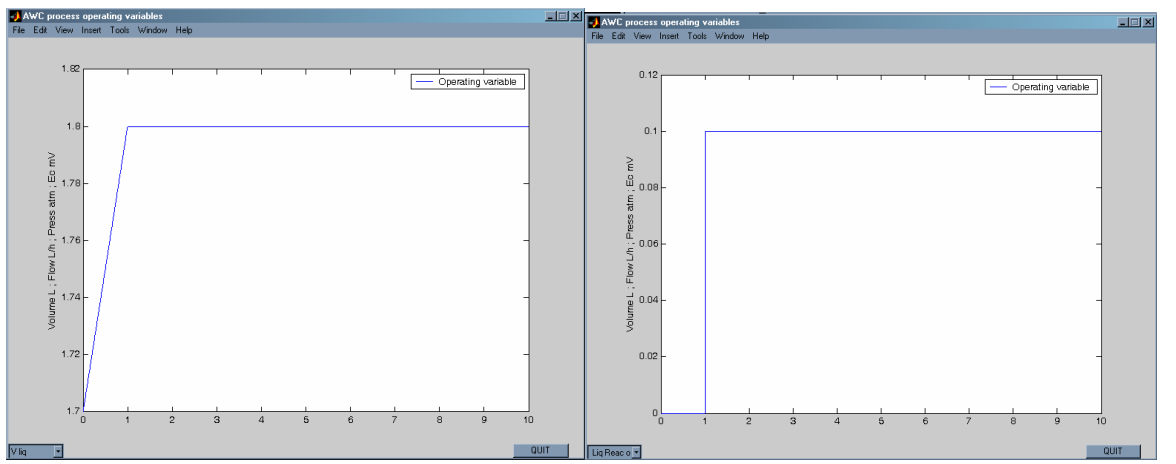
e) Liquid volume

f) output liquid flow rate

II.6.4.7 Test 7 : Uncontrolled increase of liquid volume and over-pressure control

This test is similar to the test 5, but at the contrary of test 5 for the second step of the simulation (from t0+4h) we don't control the liquid volume of the reactor. With this test we try to manage a reactor with a constant input liquid flow rate, without output and no maximum for the liquid volume (no control). By this way an output liquid flow rate is generated only if the liquid volume reach 99.99% of reactor volume. There is no gas input but the pressure is controlled by the over-pressure valve.

During the first 7 hours the model is well computed. But when the gas volume reaches a too low value the pressure variations becomes too rapid for the ODE solvers and the simulation starts to slow down. Even if the simulation not failed, the quick pressure variations did not allow to have a good accuracy (figure c)

We can identify one limitation for the use of the model: it is difficult to manage very rapid (less than 1 minute) open/close sequences of the valve. But it can be outlined that these situations are not realistic operating conditions for the biological processes.

a) O_2 liquid concentration

b) O_2 gas fraction
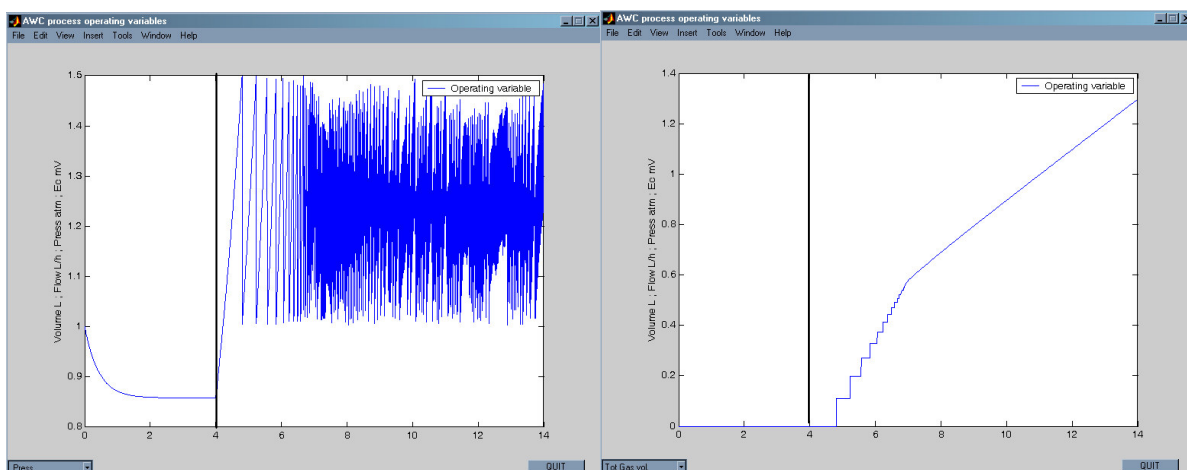
c) Gas pressure in reactor

d) Cumulative volume of gas produced

e) Liquid volume of the reactor
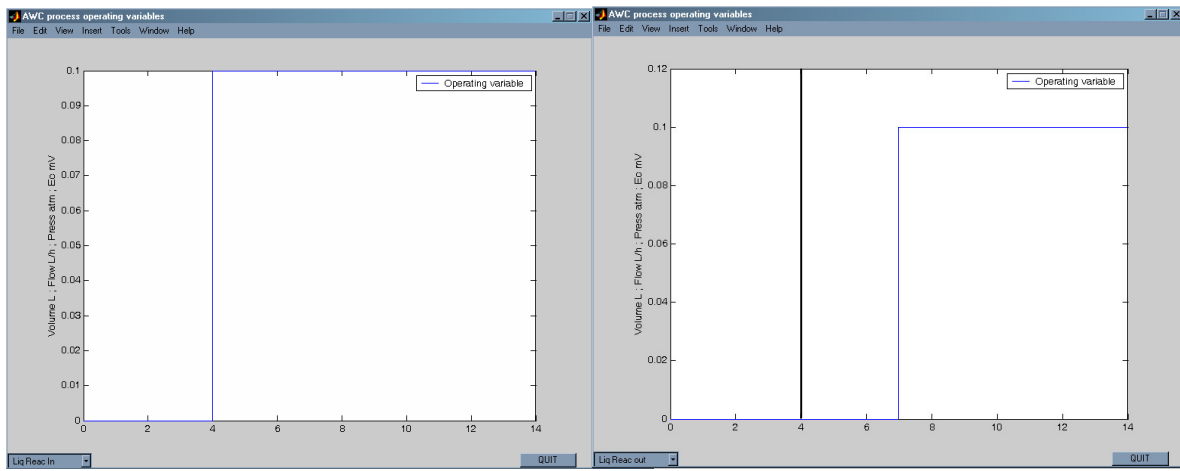
f) Input liquid flow rate   g) output liquid flow rate

II.6.4.8 Test 8 : Effect of low gas flow rate and gas/liquid equilibrium on pressure
This test is similar to the test 6 with a lower gas input flow rate (0.01NL/h). Using a lower gas flow rate allows to perform simulation during 50 hours and to observe interaction between gas/liquid equilibrium and depressurisation sequences (figures a, b and c). In figure c, it can be noticed the increase of pressure due to the equilibrium between liquid and gas after a rapid change of pressure. This effect is reduced with the decrease of the quantity of dissolved gas in the liquid (figure a).


a) O_2 liquid concentration   b) O_2 gas fraction

c) Gas pressure in reactor   d) Cumulative volume of gas produced
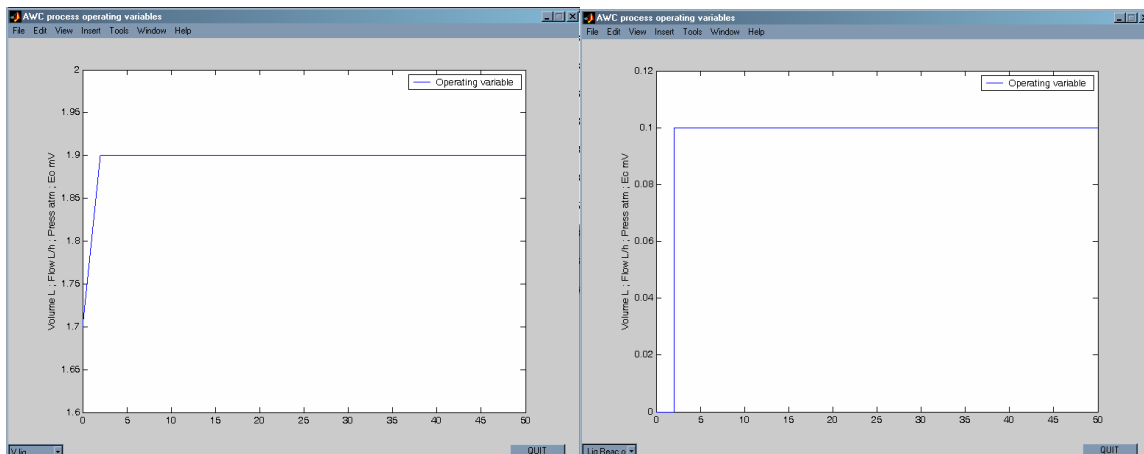
e) Liquid volume   f) output liquid flow rate

II.6.4.9 Test 9 : Liquid volume steady-state operating conditions

In order to test the steady-state for the liquid volume, with the dynamic control of the volume we take the operating conditions used in test 8. The liquid output flow rate of the reactor is set to the same value as the input flow rate. Moreover the drain flow rate is also set to reactor liquid output flow rate and the permeate is set to 0 in order to avoid recycling to the reactor.

As can be seen in figure e), neither the dynamic control of the reactor volume or the pressure control affect the steady-state of the liquid volume.
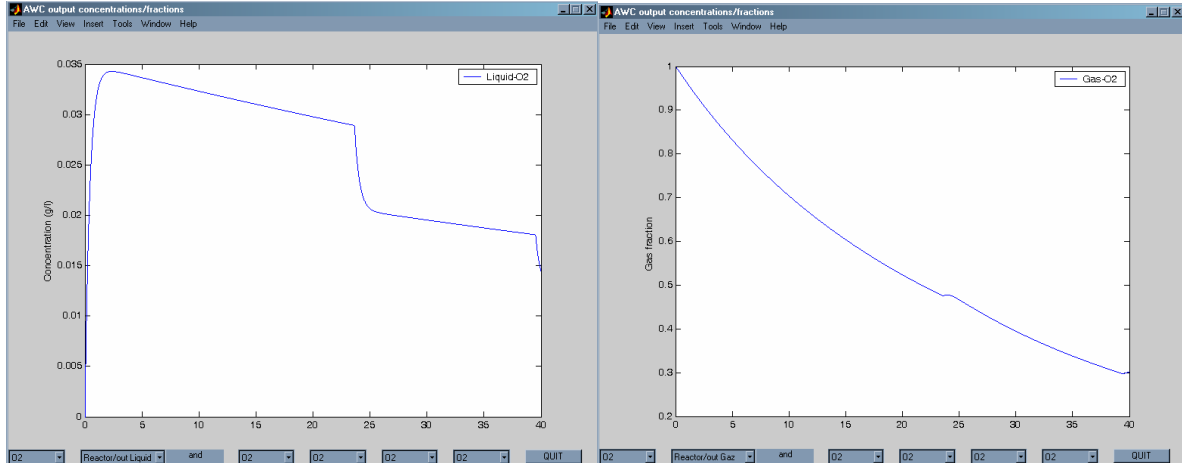
a) O$_2$ liquid concentration   b) O$_2$ gas fraction
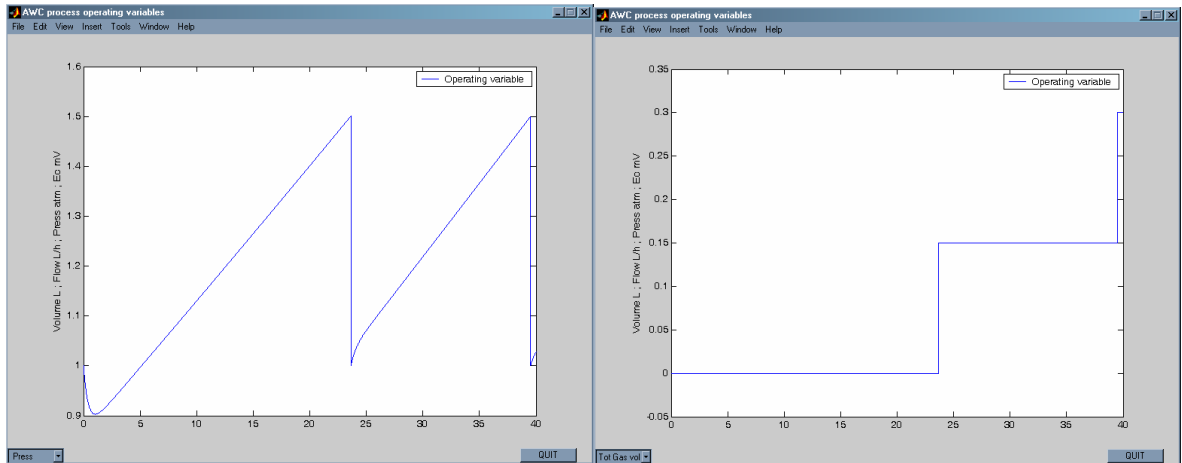
c) Gas pressure in reactor   d) Cumulative volume of gas produced
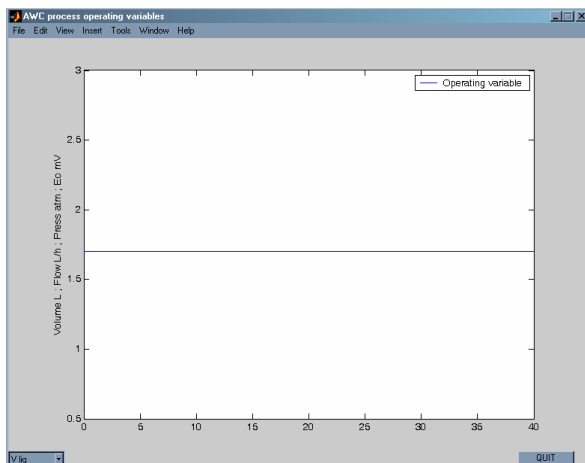
e) Liquid volume

II.6.4.10 Test 10 : Pressure control by a variable output gas flow rate

This is quite the same method that is used in the previous model for the bioreactor (report to TN 74.1).

In the new model developped, it must be noticed that the pressure is calculated and not fixed (table 2). Then even if the objective is to maintain a constant pressure, the manipulated variable being the output gas flow rate, the pressure is not necessary maintained constant. This is illustrated by the figure c. In this test the problem of pressure decrease at the start-up is linked to the gas/liquid equilibria for O2 (figure a). The model tries to compensate the decrease by dcreasing the gas output flow rate (figure f), but this decrease is insufficient.

It can be asked if the time constant in the manipulation of the gas outout flow rate is sufficient, but as we can see in figure f, even if there is a test to constraint the gas output flow to remain positive, the time constant used is so high that this test is by-passed for a short time (figure f). It is not possible to increase the time constant for the manipulation of the gas output flow rate without numerical risk for the model.
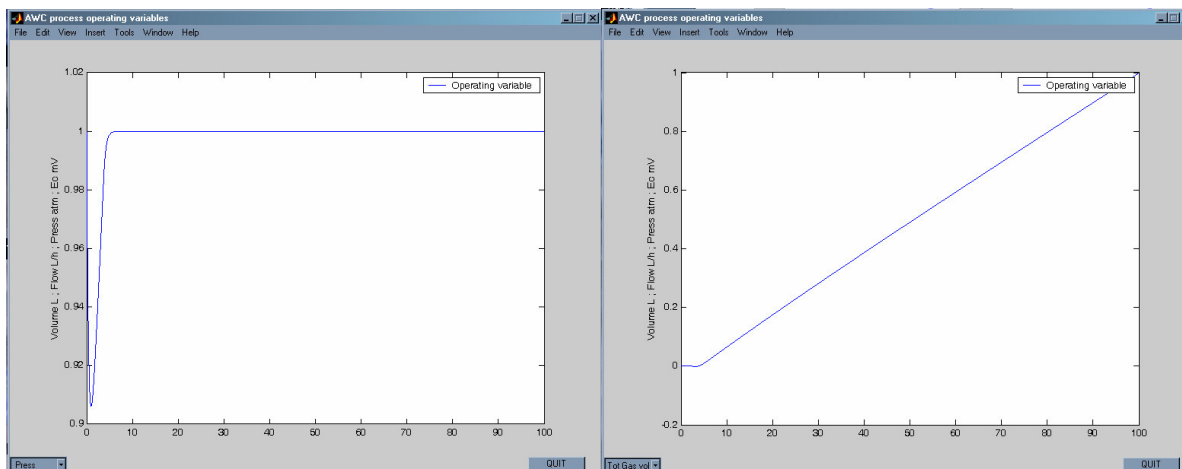
On the other hand, it can be observed that the model is well adapted as the gas output flow rate starts again only when the pressure reaches the reference value of 1 atm.

If the gas output flow rate is higher than the input one, it is because of the O_2 gas release from the liquid phase (figures a and f).
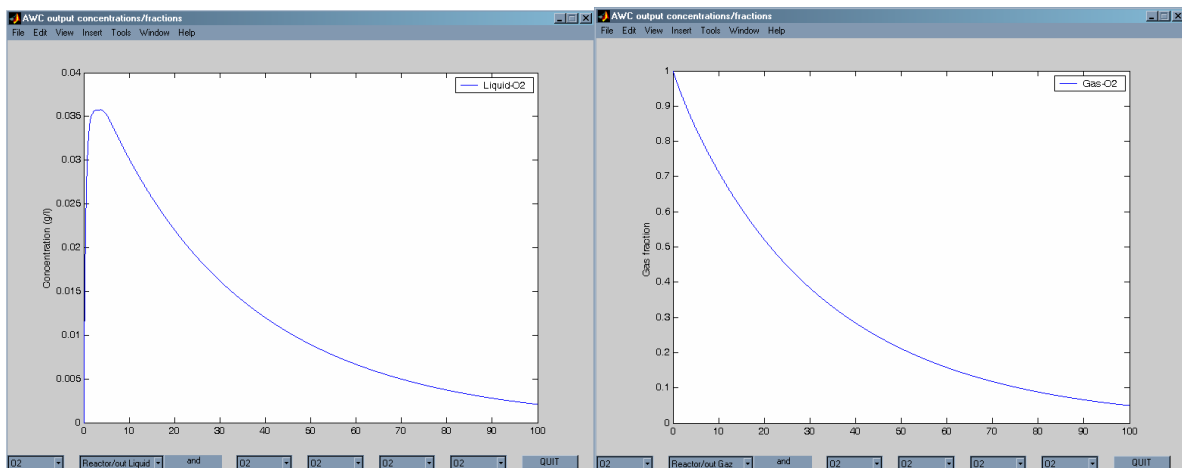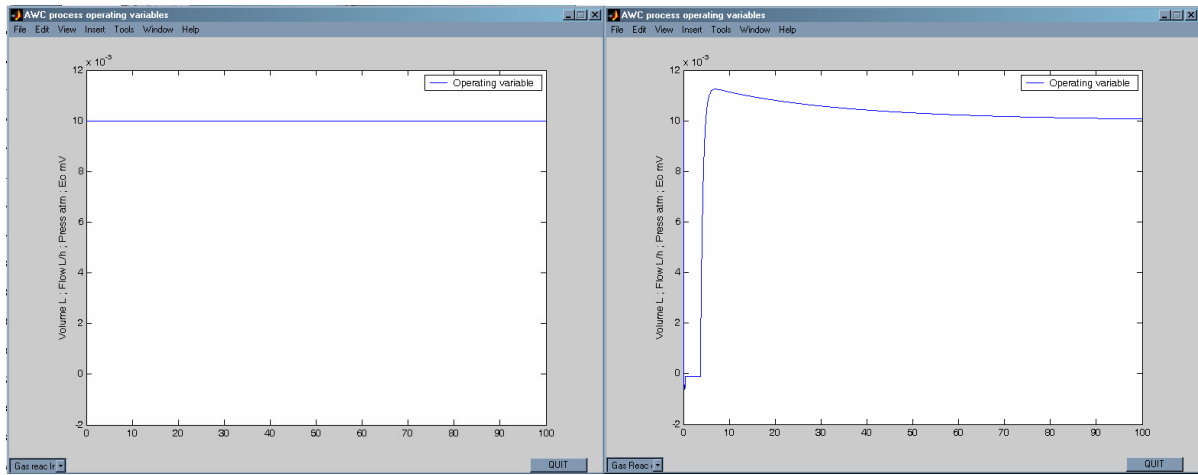

a) O_2 liquid concentration

b) O_2 gas fraction

c) Gas pressure in reactor

d) Cumulative volume of gas produced

e) Gas input flow rate   f) Gas output flow rate

II.6.4.11 Tests : conclusions

The tests performed were focused on the ability of the model to :

- manage the gas phase
- check the overpressure valve
- check the control of the reactor liquid volume

As dynamic equations for the reactions and the filtration unit were unchanged since version 1 of AWC, they were not tested.

The tests 1, 2 and 3 were used to check the functioning of the model for gas/liquid transfer phenomenon associated to pressure increase or rapid depressurisation (when over-pressure valve opens). In test 1 and 3 the moles transferred by time units is important (important unbalance between gas and liquid phase) what lead to rapid pressure increase (1.5 atm is reached in about 6 minutes). When valve is open the two phenomena: moles transferred from the liquid and moles lost by valve occur at the same time. The leakage by opening the valve is more rapid than the moles released by the liquid phase but it can be observed that the pressure does not exactly fit within the fixed limits (1 atm − 1.5 atm). This is probably due to difficulties for the model to compute at the same time a rapid pressure increase (transfer of moles from liquid to the gas) and a rapid pressure decrease (valve opened). But as the gradient for the transfer of moles ($\phi_{Si}\big|_{GL}$) remains low compared to the leakage by the valve the solver can manage the problem. It will be more problematic when the pressure increase will be more rapid, as illustrated by the following figure (test 1 with a k_La of 200 h^{-1} instead of 2h^{-1}).
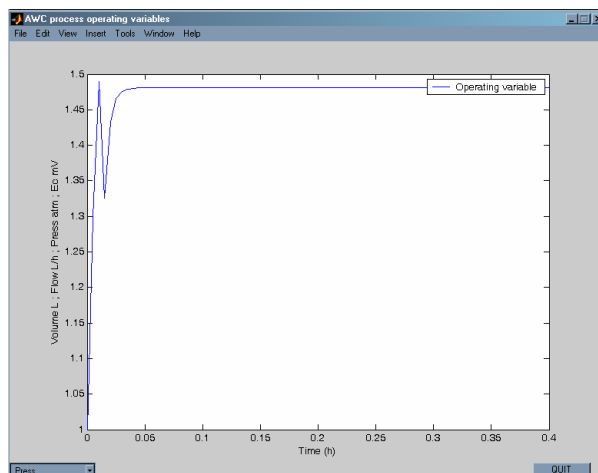
Pressure variations for a simulation comparable to the test 1, but with a k_La of 200 h^{-1} instead of 2h^{-1}.

The pressure increase from 1atm to 1.5 atm occurs in 1 minute, and when valve is opened, the decrease is to slow compared to the transfer of moles from the liquid phase.

Another point identified with these test is that the gas fraction (tests 1 and 3) is not exactly 1, as this fraction is calculated at each time function of pressure and moles of gas. The calculation is sensitive to the numeric precision (fixed at 10^{-10}). In principle this is sufficient.

In tests 4, 5, 6, 8, 9 and 10 the functioning of the model (over-pressure valve and liquid volume variation) with inputs flows is checked. The frequency of the pressure variation being lower (about 1 hour) than in the previous tests, it can be seen that the model gives accurate results. The influence of pressure on the dissolved O2 saturation concentration can also be observed.

The test 7 is interesting as it illustrates both the robustness of the model and its limits. When the gas volume is very small compared to the gas flow rate and/or the gas/liquid transfer rate, the frequency of pressure change is very high, and it is difficult to reach the ranges of the pressure limits that were fixed. The simulation takes a long time because of the lot of sharp oscillations, but the results obtained remain reliable.

III **Improvements and updating of AWC toolbox**
Some minor changes were made in the version 1.1 of the AWC_MS toolbox.

III.1 Gas liquid equilibrium model
An error in the calculation of the saturation constant (C*) from the gas composition was corrected. The calculation of C* was also modified in order to take into account the effect of pressure on C*.
It is important to keep in mind that the modifications require now to give a partition coefficient k_{Si} calculated for a reference pressure of 1 atm.

III.2 Matlab ODE solvers
In the interface for starting the simulations it is now possible to choose the Matlab® ODE solver in the list of the 7 solvers available. By default the solver ode15s is selected. This is the recommended solver, as most of the problems to compute are stiff problems.
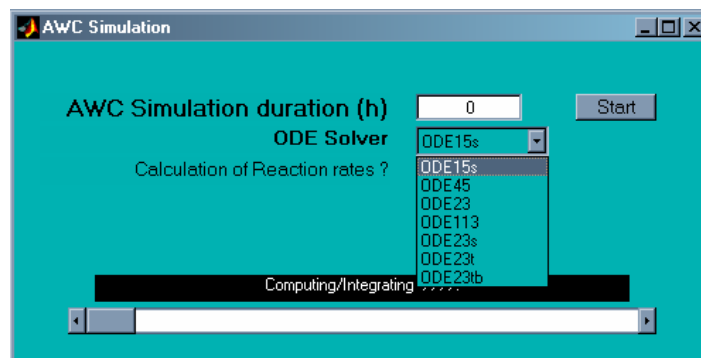
III.3 Unfrozen windows during computations
The problem of frozen windows during simulations was solved.
The advantage is that windows can be minimised during computation, and then it is easier to continue using the computer while simulations are being performed. It is also possible to abort a simulation by clicking the "Quit" button of the simulation progress interface. It is important to notice that all unsaved work is lost is this case.
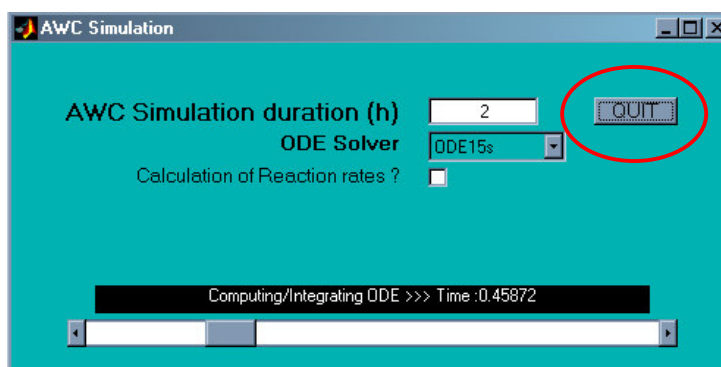
The drawback is that all menus and buttons are also unfrozen. Using the menu and other actives interfaces during a simulation can lead to unexecpeted results.

IV <u>Conclusion</u>

In this technical note, the second release of the toolbox for the modelling and the simulation of the first compartment AWC_MS v1.1 is presented

This version offers a new kind of process: a bioreactor that can be operated in gas and liquid fed-batch conditions with variable volumes and pressure.
From the tests performed the model seems reliable enough for the biological anaerobic processes that would be simulated. The main limitation observed concerns the rate for the sequence of open/close for the over-pressure valve, as the dynamic model developed cannot be used for rapid sequences.