

# MELiSSA

Memorandum of Understanding  
ECT/FG/MMM/97.012

## TECHNICAL NOTE 74.1

**Anaerobic Waste Compartment modelling and simulation toolbox  
-AWC\_MS -**

**Bioreactor modelling  
Toolbox description  
Toolbox user manual**

Version 1  
Issue 0

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## Document change log

<b>Version</b>	<b>Issue</b>	<b>Date</b>	<b>Observations</b>
0	0	January 2003	Draft version
1	0	February 2003	Final version Release of Awc_MS v1.0 toolbox

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## **I Introduction**

The Anaerobic Waste Compartment Modelling and Simulation toolbox (AWC\_MS) presented in this technical note is not designed to be "the model of the anaerobic waste compartment of the MELiSSA loop". It is designed as a tool for

- 1 - the study and the development of biological dynamic models for the first compartment, in order to find the most reliable model and to fix the biological parameters;
- 2 - the study of the process itself by enabling to test easily the operating variables and the design of the first compartment.

As a consequence, the toolbox was designed in order to be flexible enough to allow a large range of scenarii. The AWC-MS toolbox is developed under MatLab™ R12.

The previous studies of the MELiSSA compartment I, both in the MELiSSA project and in the EWC project are used as the starting point for the design of the process and the reactions modelled by the toolbox. These points will be briefly reviewed in the first part of this work, which will also details the models (biological and physical models) implemented in the toolbox.

In the second part of this work will be presented the architecture of the toolbox itself and its components will be detailed. A manual for the use of the toolbox, explaining all of its interfaces, the required data and the different possibilities of simulation is presented in the last part of this document.

## II The anaerobic Waste Compartment : design and modelling

In this section are reviewed the previous studies of the anaerobic compartment which were used as the core for the building and the development of the AWC-MS toolbox. The models implemented in the AWC-MS toolbox, as presented in section III, are detailed here. These models concern :

- The model of the process itself, its hydrodynamic and its differential equations
- The biological models
- The physical equilibria models

### II.1 Design principle (TN 71.1)

First of all, it is necessary to fix what is the anaerobic waste compartment. The most recent description is developed in TN 71.1 (Hermans et al. 2002) and is reported in figure 2.

This concept of the first compartment can be split into 4 parts (Figure 2.2):

- 1 Pre-treatments and reactor feed preparation
- 2 The core of the process: the reactor and the filtration unit (FU)
- 3 Post-treatment of the anaerobic products
- 4 The links with the others MELISSA compartments

The anaerobic waste compartment is then a set of several units operation, and for simplicity, **we will restrict the development of the toolbox to the part (2) of the compartment (Reactor + Filtration Unit).**

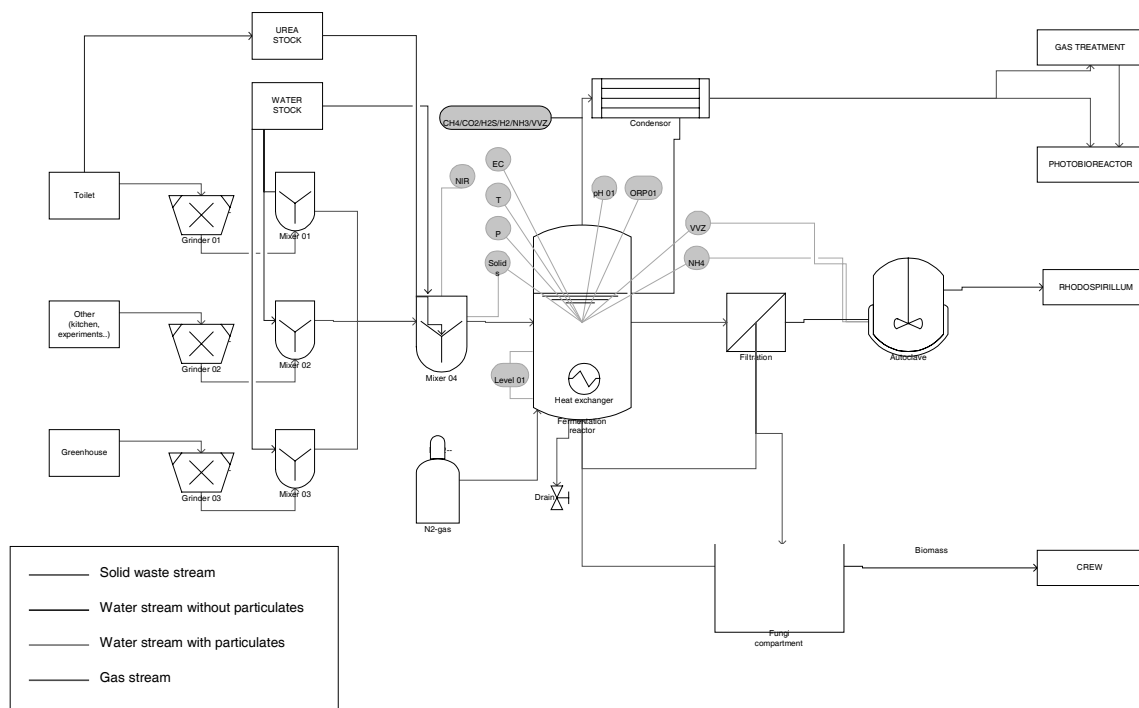


Figure 2.1 Concept of the MELISSA anaerobic waste compartment (from TN 71.1)

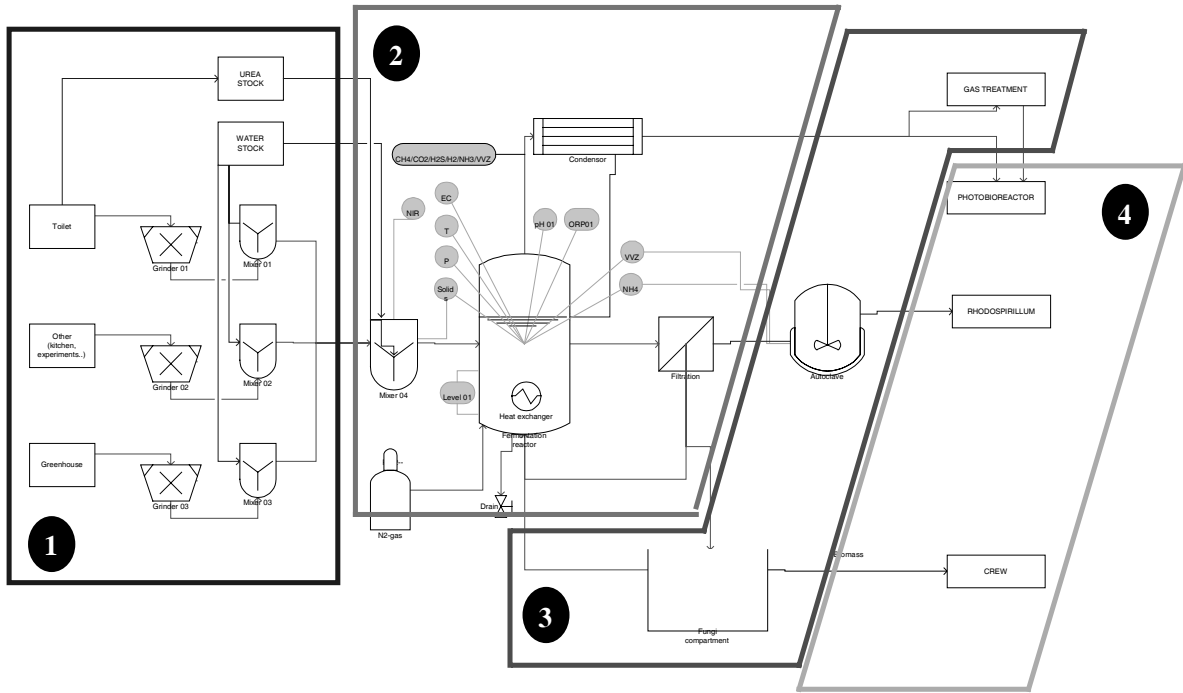


Figure 2.2: The 4 parts of the anaerobic waste compartment

## II.2 Modelling of the anaerobic reactor

### II.2.1 Modelling principles

For the development of the modelling and simulation toolbox of the anaerobic compartment, the classical mechanical engineering approach is used (Figure 2.3). This means that the process is divided into biological and fluid-flow dynamics.

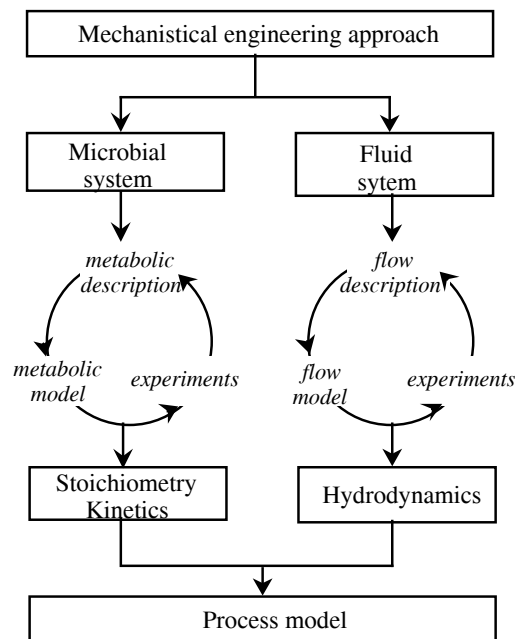


Figure 2.3: Mechanical engineering approach (from Noorman, 1991).

It can be noticed that the same approach was used for the compartment III (nitrifying), but at the difference of this third compartment, the difficulty will be in the microbial system modelling, as a consortium of unknown species is more complex to described than known bacteria.

The model by itself is a set of differential equations, established from the hydrodynamic equation for the processes (report to section II.2.2 and II.2.3). In this equations are integrated the different rates for the biological reactions (section II.2.4) and the physical equilibria reactions (section II.2.5).

## II.2.2 Bioactor modelling (hydrodynamic modelling)

### ***Simple chemostat approach***

The most simple hydrodynamic model for a bioreactor is the constant volume continuous or batch chemostat. Constant volume means that in the reactor it is assumed that both liquid and gas volume **are constant**. It is also assumed that **the pressure is constant**. As it is known that their is a gas production, this implies that **the output gas flow rate is variable**.

<b>Liquid phase</b>	$V_L \cdot \frac{dC_{Si} _L}{dt} = F \cdot C_{Si}^{in} _L - F \cdot C_{Si} _L + V_L \cdot \phi_{Si} _{GL} + V_L \cdot \phi_{Si} _{Reac}$
<b>Gas phase</b>	$V_G \cdot \frac{dC_{Si} _G}{dt} = G_{in} \cdot C_{Si}^{in} _G - G_{out} \cdot C_{Si} _G - V_G \cdot \phi_{Si} _{GL}$ <p>The Gas output is calculated in order to maintain volume and pressure constant in the reactor (see below)</p>
<b>Notations</b>	<p><math>V_L</math> and <math>V_G</math> : respectively liquid and gas reactor volumes (l)</p> <p><math>F</math> : the input/output liquid flow rate (l.h<sup>-1</sup>)</p> <p><math>G_{in}</math> : the input gas flow rate (l.h<sup>-1</sup>)</p> <p><math>G_{out}</math> the output gas flow rate (l.h<sup>-1</sup>)</p> <p><math>C_{Si}^{in} _L</math> and <math>C_{Si}^{in} _G</math> : respectively the liquid and gas input concentration of Si (g/l)</p> <p><math>C_{Si} _L</math> and <math>C_{Si} _G</math> : respectively the liquid and gas reactor/output concentration of Si (g/l)</p> <p><math>\phi_{Si} _{GL}</math> : gas liquid transfert rate (g.l<sup>-1</sup>.h<sup>-1</sup>)</p> <p><math>\phi_{Si} _{Reac}</math> : Liquid reactions rate for Si (g.l<sup>-1</sup>.h<sup>-1</sup>) ; <math>\phi_{Si} _{Reac} = \sum r_{Si}</math> , <math>\phi_{Si} _{Reac}</math> is the sum of all the reaction rates <math>r_{Si}</math> (biological and acid-base) of compound Si</p>

Table 2.1 : Simple chemostat principle. C are concentrations; V are volumes;  $\phi_{Si}|_{GL}$  is the phase exchange term and  $\phi_{Si}|_{Reac}$  is the reactionnal rate (biological, chemical or/and physical) term

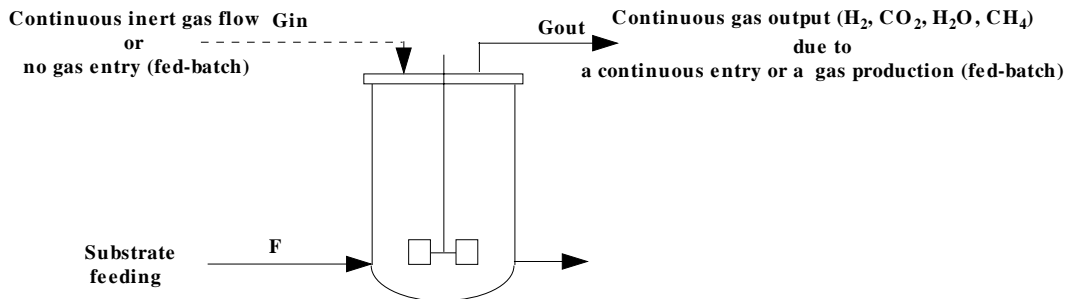


Figure 2.4 : scheme of a classic chemostat. Only variable inputs and outputs

The output gas flow rate is calculated using the following procedure:

- 1) Volumic gas flow rate is converted into molar flow rates. ***It is important to notice that in the formula expressed here, the volumic gas flow is assumed given in Normal units (i.e. 0°C, 1atm).***

$$G_{in} \text{ molar} = \frac{G_{in}}{R_G * T_0} \quad R_G=8.3144 \text{ and } T_0=273.15 \text{ K}$$

- 2) The moles exchanged between the gas and the liquid is calculated:

$$dn_{exch\_tot} = \sum \frac{\phi_{Si}|_{GL}}{M_{Si}} * V_L \quad (\text{in mol.h}^{-1}; M_{Si} \text{ is the molar mass of Si})$$

- 3) the molar gas output flow rate is then :

$$G_{out} \text{ molar} = G_{in} \text{ molar} + dn_{exch\_tot}$$

and then

$$G_{out} = G_{out} \text{ molar} * 8.3144 * 273.15 \quad (G_{out} \text{ in Normal units})$$

### **chemostat modelling with variable volumes and pressure**

The model is under investigation

#### **II.2.3 Filtration Unit (FU) modelling**

Considering preliminary tests presented by EPAS (TN 56.1, 2001), based on VITO tests, the WFF4385 membrane was selected. This is a porous (30nm pore size), hydrophilic tubular membrane which is operated in tangential microfiltration mode.

Membrane processes present basically a very simple flowsheet. There are no moving part (except for pumps and compressors), no complex control schemes and little ancillary equipment compared to any to other unitary processes. Nevertheless, due to the various kind of possible processes and membranes compositions the modelling of filtration operations (from reverse osmosis to filtration) is a huge and highly studied topic.

#### **Flux and driving forces**



For pressure driven liquid phase separation, the flux of a component A through a membrane can generally be described by the equation (Humphrey et Keller, 1997) :

$$N_A = \frac{P_A}{L} (\Pi - \pi_A)$$

$N_A$  : Flux of A through the membrane (mass/time-area)

$P_A$  : permeability of A (mass-length/time-force)

$L$  : thickness of the separating layer of the membrane (length)

$\Pi$  : pressure difference across the membrane (driving force)

$\pi_A$  : osmotic pressure of A

The osmotic pressure effect can be neglected for species with molecular weight greater than few thousand daltons.

### Separating capability

For liquid phase separation, it is common to use the term "rejection" when describing a membrane's ability to retain a solute and permeate a solvent. Rejection is defined as:

$$R = \left[ 1 - \frac{C_{Ap}}{C_{Af}} \right]$$

$R$  : rejection (ranging between 0 and 1 ; can also be expressed as a percentage)

$C_{Ap}$  : solute concentration in permeate

$C_{Af}$  : solute concentration in feed

### Operation of the filtration unit: dynamics and fouling.

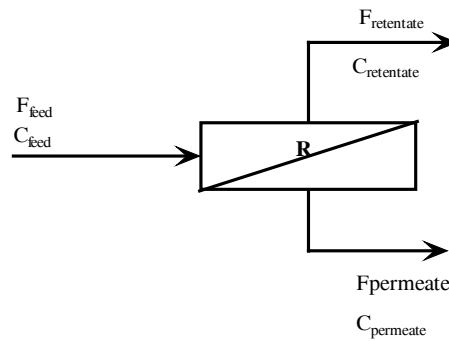
As illustrated in preliminary tests (report to TN 53.1), the filtration unit possesses its own dynamic behaviour. First, it is observed transient behaviour in the permeate flux (as well in the pressure, the two parameters being linked) before reaching a steady-state.

Secondly, it was also observed that there is not a constant proportionality between compounds concentrations in retentate and in permeate, what can suggest a not-constant separating capability.

Another problem often encountered is the fouling of the membrane which leads also to changes in the permeability and in the flux of permeate.

### Modelling of FU operation in AWC-MS

The modelling of FU operation is then not a simple task, especially if a dynamic model is required. Usually, for preliminary studies, a simple separation model is used which represents the separating capability of the membrane in steady-state. This is the modelling approach used at this time. This implies that transient behaviours and fouling are neglected.



The current modelling of the FU is then based on

- the separating capability  $R$ , which must be given for all the compounds involved in the process. The concentration in the permeate is then calculated for each compound from the solute concentration in the feed :

$$C_{Ap} = [1 - R]C_{Af}$$

- The permeate flux itself is not calculated. Preliminary tests must be made in order to validate theoretical flux calculation and experimental one. Then the permeate flux must be given as one of the variable of the process

The Operation of the Filtration Unit is then dynamically modelled as an equilibria between two flows (the feed and the permeate). It is written:

$$\frac{dC_{Si}|_{permeate}}{dt} = 10^6 \cdot ([1 - R]C_{Si}|_{feed} - C_{Si}|_{permeate})$$

The concentration in the retentate flow is then :

$$C_{Si}|_{Retentate} = \frac{(C_{Si}|_{feed} \cdot F_{feed} - C_{Si}|_{permeate} \cdot F_{permeate})}{F_{feed} - F_{permeate}}$$

$F_{feed} - F_{permeate}$ , being the flow rate of the retentate

#### II.2.4 Biological reactions

Biological reactions for anaerobic degradation processes were already discussed and detailed in TN 39. and TN 45.3. It was shown that often the reactions and the parameters presented in the literature are specific to the process for which they are used. Our objective here is not to give a complete functional biological model for the anaerobic compartment I reactor, but to propose the basic tools which must enable to built this model. Then even if the equations and relations describing the models are given, the parameters of the models must be identified and adapted to the process.

The tools currently proposed are a set of 4 different kind of reactions, which would be combined together in order to built a complete biological model. These reactions are:

- enzymatic reaction associated to a Michaelis-Menten kinetic model with competitive and non-competitive inhibition
- growth reaction associated to a Monod model with the haldane inhibition expression and the endogenous maintenance expression (Pirt model)

- decay reaction
- decomposition reaction for a compound into other ones

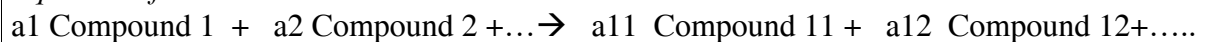
#### II.2.4.1 Principle of biological reaction description

The biological activity can be represented by **one or more** reaction.

Each reaction can be a stoichiometric mass balanced equation or a non –balanced equation. The first one is preferable as this allows having a mass balanced process.

At each reaction is associated a specific rate (as the growth rate for growth reaction) based on a kinetic model, which enable via the yields of the reaction to calculate the consumption/production rates of each compound involved.

*Equation of the reaction :*



$a_1, a_2, \dots$  are the coefficients of the reaction

$Y_{1/12} = \frac{a_1}{a_{12}}$  is the yield for compound 1, with compound 12 as reference

*Kinetic equations associated to the reaction:*

$r_{12}$  being the rate of production of the compound 12 by this reaction ( $r_{12}$  being derived from a kinetic model such as Monod, michaelis model.....), then  $r_1$  for the reaction is calculated by :

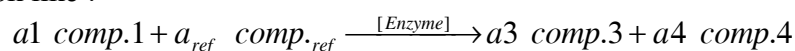
$$r_1 = Y_{1/12} r_{12}$$

Table 2.2 : Example of the principle for a modelling of a reaction

#### II.2.4.2 Details of the anaerobic reactions involved

##### 1 - Enzymatic reaction

The reaction look like :



- $a_1, a_{ref}, \dots, a_4$  are the molar coefficients of the reaction
- E is the enzyme which catalyse the reaction; its concentration is [Enzyme]
- Ref denotes for the reference compound of the reaction (usually a substrate)

The kinetic model associated to enzymatic reaction is :

If  $V_{Ref}$  is the reaction rate associated to the reference compound,  $V_{Ref}$  is expressed as the rate of compound Ref. by unit of time and by unit of enzyme, i.e. units are [Compound Ref]  $\text{time}^{-1}$  [Enzyme] $^{-1}$

For each compound  $S_i$ , the reaction rate  $r_{S_i}$  can be calculated as :

$$r_{S_i} = Y_{S_i/Ref} \frac{1}{K_{i_{NC}}} \left( \frac{[S_i]}{K_{S_i} K_{i_C} + [S_i]} \right) V_{Ref} [S_{ref}] [Enzyme] \text{ in } [S_i] \text{ time}^{-1}$$

- $K_{Si}$  is the half saturation constant for Si (Michaelis –Menten model)
  - $Ki_C$  is the competitive inhibitory factor, defined as :  $Ki_C = 1 + \sum \frac{[Si]}{Ki\_Si\_C}$ , where
- $Ki\_Si\_C$  is the competitive constant of compound Si
- $Ki_{NC}$  is the non-competitive inhibitory factor, defined as :  $Ki_{NC} = 1 + \sum \frac{[Si]}{Ki\_Si\_NC}$ ,
- where  $Ki\_Si\_NC$  is the competitive constant of compound Si
- $[Enzyme]$  is concentration of Enzyme catalysing the reaction. This concentration is assumed to be proportional to the quantity of the biomass producing the enzyme, then it can be written  $[Enzyme] = \alpha[Biomass \text{ producing the enzyme}]$

## 2 - Biological reactions and micro-organisms growth

The biological kinetic model described in TN 45.3 is used as the basis for the model proposed for all the biological reactions in the AWC-MS toolbox.

### The growth

The growth reaction must look like :



- $a1, a_{Biomass}, \dots, a4$  are the molar coefficients of the reaction
- Biomass is the biomass produced by the reaction

For the biomass, the growth rate  $r_x$ , which is the reference rate of the reaction is :

$$r_x \Big|_{GROWTH} = \mu \max [Biomass] \cdot \prod \frac{[Si]}{K_{Si} + [Si] + \frac{[Si]^2}{Ki_{Si}}}$$

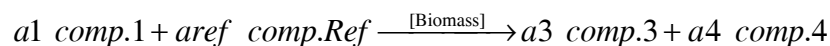
- $K_{Si}$  is the saturation constant for Si (Si must be a substrate)
- $Ki_{Si}$  is the inhibitory constant (Si is not necessary a compound involved in the reaction)

For other compound than the biomass, the reaction rate  $r_{Si}$  is :

$$r_{Si} \Big|_{GROWTH} = Y_{Si/Biomass} r_x \Big|_{GROWTH}$$

### The maintenance

An endogenous maintenance reaction can be associated to the growth reaction. This maintenance represents a consumption of substrate not associated to a biomass production. Then this reaction look like :



with an associated reaction rate :

- $a1, a_{ref}, \dots, a4$  are the molar coefficients of the reaction
- Ref denotes for the reference compound of the reaction

The consumption rate of the reference substrate used for the maintenance is expressed by:

$$r_{Ref} \Big|_{MAINTENANCE} = m \cdot [Biomass] \cdot \prod \frac{[Si]}{K_{Si} + [Si]}$$

An for the other substrates involved in the maintenance reaction :

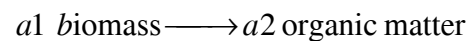
$$r_{Si} \Big|_{MAINTENANCE} = Y_{Si / Ref} \cdot r_{Ref} \Big|_{MAINTENANCE}$$

### **Overall biological reactions rates**

Finally, the reaction rates of a biological reaction is the sum of the growth rate and of the maintenance rate :  $r_{Si} \Big|_{REACTION} = r_{Si} \Big|_{GROWTH} + r_{Si} \Big|_{MAINTENANCE}$

### **3 - Biomass decay**

The biomass decay is considered in the toolbox as a separate reaction, which has the form:



The decay rate ( $k_D$ ) is assume to be constant, and then the reaction rates are:

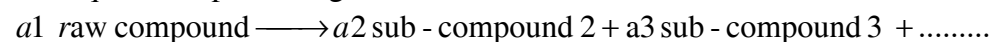
$$r_{Biomass} = -k_D [Biomass]$$

$$r_{Organic\ matter} = Y_{OM / Biomass} \cdot r_{Biomass}$$

### **4 - Decomposition reaction**

In fact, this is not exactly a reaction. This is only a way to represent the splitting of a compound in several others compounds. As an example, we can prefer feeding with compound named "Manure" instead of directly its sub-composition named "degradable manure" and "non degradable manure" which will be the compounds involved in further reactions. This kind of reaction was included in the toolbox as it offers a higher flexibility when a process is described, allowing to make simulations with various composition for a raw substrate.

The equation representing this reaction should look like:



There is no reaction rate for such reactions as this is only a way to represent sub-composition of a compound. Nevertheless as this description is integrated into a dynamic system with variable feed conditions a pseudo reaction rate was built in order to maintain the homogeneity of the representation of the reactional system. The specific rate of  $10^6 \text{ h}^{-1}$  was chosen in order to have a very quick reaction rate compared to all the other reactions:

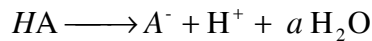
$$r_{Si} = 10^6 \frac{S_{Raw\ compound}}{K_S + S_{Raw\ compound}} \cdot Y_{Si / Raw\ compound}$$

## **II.2.5 Equilibria reactions**

Two kinds of equilibria are considered: the acid/base equilibrium and the gas liquid equilibrium. As the biological reaction, these equilibria are taken as dynamic phenomenon (implying then the definition of a rate).

### II.2.5.1 Acid-base equilibria

Acid-base equilibria is a reaction of the form:



It can be noticed that such reaction implies that the ionic forms of a compound were defined in the list of the compounds involved in the process.

The equilibrium constant  $K_A$  of the reaction, gives the theoretical repartition of the compound HA between its two forms HA and  $A^-$ .

$$K_A = \frac{[A^-]_{eq} [H^+]}{[HA]_{eq}} \quad \text{and} \quad [HA]_{tot} = [HA]_{eq} + [A^-]_{eq}$$

From these two relations is then possible to calculate at each time, the equilibria values  $[HA]_{eq}(t)$  and  $[A^-]_{eq}(t)$ . It is assumed that the acid/base reaction reaches quickly this equilibrium from initial  $[HA](t)$  and  $[A^-](t)$  concentration which are varying because of biological reactions and input/output flows. The difference between equilibrium value and current value can be taken as the gradient force of the acid-base reaction, and the reaction rate can be written:

$$r_{Si} = 10^6 \left( [Si]_{equ}(t) - [Si](t) \right)$$

Notes:

- 1) this reaction rate is added to the other biological rate for each compound (see table 2.1)
- 2) details for acid-base equilibrium can be found in TNs 23.1, 27.1 and 39.1
- 3) as for the decomposition reaction, the specific rate of  $10^6 \text{ h}^{-1}$  is arbitrary chosen sufficiently high to have a reaction very rapid compared to other reaction or transfer rates

### II.2.5.2 Gas-liquid equilibria

The gas-liquid equilibrium is equilibrium of a compound between two phases. There no reaction but only a transfer between the two phases. The transfer rate is written:

$$\phi_{Si}|_{GL} = k_L a \left( [Si]_{\text{Gas or Liq}}^* - [Si](t)|_{\text{Gas or Liq}} \right)$$

$[Si]^*$  is the saturation constant (it can be in gas or in liquid)

Notes:

- 1) details for gas-liquid equilibrium can be found in TNs 23.1, 27.1 and 39.1

### **III The AWC MS toolbox**

This section will describe the gridlines of the AWS\_MS MatLab toolbox. The toolbox is composed of about 60 scripts, most of them being related to data capture and graphical interfaces (GUI). The building of the GUI will not be detailed in this work and the use of the GUI for the data capture will be presented in the next chapter (user manual).

This chapter will focus on the architecture of the toolbox, the functions of the scripts and their interdependencies.

#### **III.1 Functions and objectives of the Toolbox**

The toolbox will allow to perform simulations of the process as described in the previous chapter. The system is composed of a 2 phases (gas-liquid) bioreactor with or without inputs/outputs flow associated to an external filtration unit.

The system of differential equations (ODE) resulting from this process (sections II.2.2 and II.2.3) is integrated in the toolbox, as well as the equations required to represent the biological reactions, the gas-liquid equilibria and the acid-base equilibria. The ODE system is composed of [3xnumber of compound + 1] (i.e. for 5 compounds involved a system of 16 ODE is solved). But it is important to keep in mind that the toolbox is NOT a model of the compartment I, but a tool for testing and developing various models for the process, in the limits of the core models that are implemented in the toolbox.

The toolbox was built in order to be able to :

- Define and change the set of compounds involved in the process
- Choose, define and fix the parameters of the set of biological reactions involved in the process. The reactions must be chosen in the set of the 4 models currently implemented in the toolbox (see II.2.4.2)
- Design the reactor and to fix all the operating variables (temperature, input flows rate and input composition....) only through a GUI
- Save parameters of a deigned process
- Perform simulations of the system with the choice of the ODE solver and the possibility to continue a simulation with new operating variables (typically by changing inputs flows or composition)
- Visualise and to save the results. This also implies that the toolbox can reload the saved data.

It exists some restrictions in the toolbox:

- The maximum number of compounds is currently fixed to 24
- There is a maximum of 40 growth reactions, 10 enzymatic reactions and 10 decomposition/decay reactions
- The toolbox is limited to the models and the process detailed in section II (but the architecture allow to implement quite easily new models)
- The toolbox is not optimised in terms of computing time. As the ODE system is generated for all compounds in all phases of the process, some differential equations that are useless are computed (typically the ODE for a compound that not exist in the gas phase is also solved).

**AWC\_MS toolbox Version 1.0**  
Structure of the toolbox composed of 58 scripts and functions

**Main Windows interface of AWC\_MS**

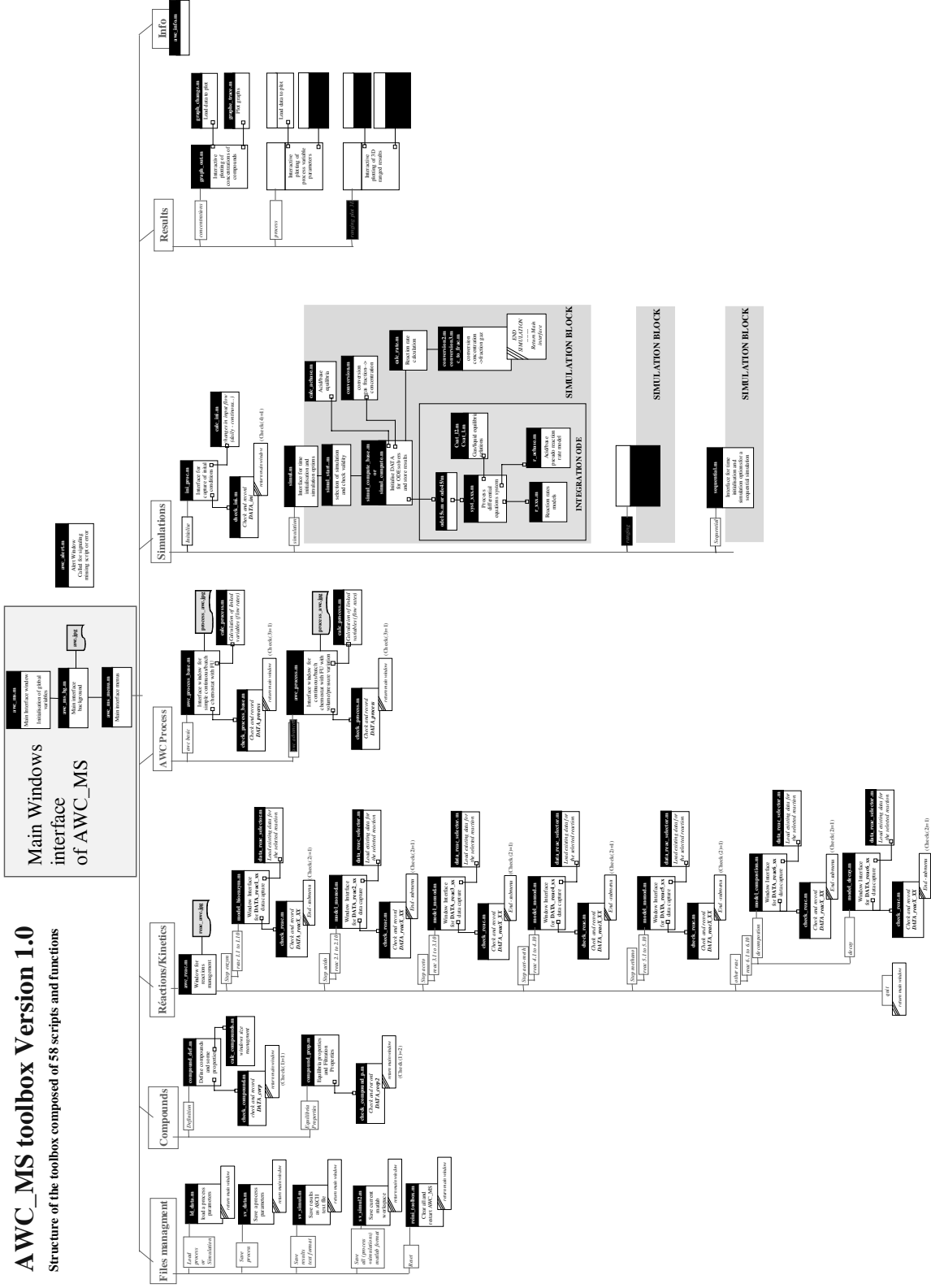


Figure 3.1: Global view of the architecture of the AWC\_MS toolbox (detailed views of menu trees are given in appendices)



### III.2 Structure and building of the toolbox

The toolbox is composed of a set of MatLab scripts and functions (57 in the current V1.0 release). There are 4 kind of scripts and functions:

- Scripts for the toolbox itself (graphic interface and user interaction)
- Scripts and function for data capture. Those are graphic interfaces for managing and designing the process (compounds, reactions and reactor parameters)
- Scripts and functions for simulation and computation of the process. They include the rate calculations and ODE computing.
- Scripts for the visualisation of results.

#### III.2.1 Global architecture and scripts dependencies

When launched in the MatLab environment (see section IV, Users Manual), A graphical interface (Figure 3.2) allows through menus to access the different interfaces for data capture, parameters management, process simulation and results visualisation.

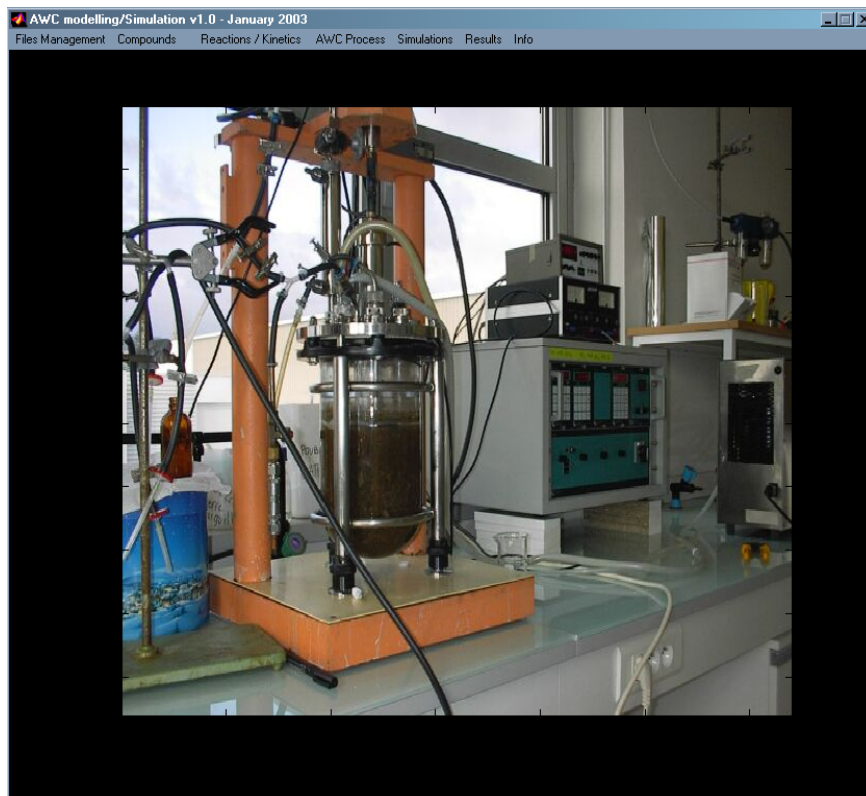


Figure 3.2: Main windows interface of AWC\_MS

Each menu and sub-menu is associated to a set of scripts. A raw view of the dependency of scripts and functions with the different menus and sub-menus of the main AWC\_MS windows is presented in figure 3.1 (each of the 7 main menus of the toolbox are detailed in appendices).

As illustrated in figure 3.3 for the choice of a reactionnal model and the capture of its parameters, each function of the toolbox is built on a common template, what gives a good flexibility for the management of the toolbox and the addition of new functionality without completely changing the toolbox.

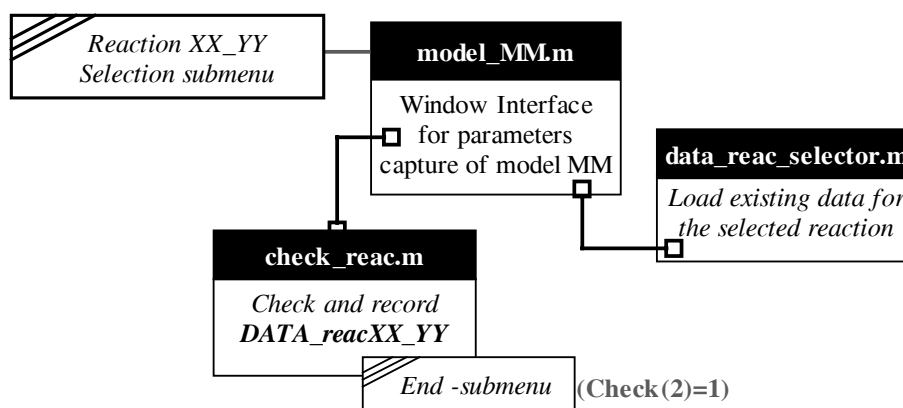


Figure 3.3: Template for building the scripts related to the **description** of a reaction (capture of reaction parameters). Model\_MM can be any kind of model of a reaction

### III.2.2 List of scripts and their functions

The 57 scripts of the toolbox are listed below. All scripts (S) or function (F) are called by another one, excepting awc\_ms.m, which is the script for starting the toolbox. There is also 3 pictures which are used to illustrate the toolbox : reac\_awc.jpg, for the reaction window ; process\_awc.jpg for the process window and awc.jpg for the main AWC\_MS window

Script/function name	Function in AWC_MS	Called by....
awc_alert.m	S Display alert/warning windows	When required
awc_info.m	S Display information for AWC_MS	awc_ms_menu.m
awc_ms.m	S Main script Definition of global variables Initialisation of the toolbox and of the main window	First script
awc_ms_bg.m	S Define background of main window	awc_ms.m
awc_ms_menu.m	S Define menus and sub-menus of the main window and call the related scripts	awc_ms.m
awc_process_base.m	S Display an independent window for the design of a process (reactor and FU parameters)	awc_ms_menu.m
awc_reac.m	S Display an independent window for the selection of reactions involved in the process by using menus and sub-menus	awc_ms_menu.m
calc_acbase.m	F Calculation of equilibrium concentrations for acid/base compounds	Simule_compute_xx.m syst_awc_xx.m
calc_compound.m	S Resize and reload the GUI for the compounds data capture (compound number, names and basic properties)	Compound_def.m
calc_ini.m	S Conversion g/l $\leftrightarrow$ g/day of liquid input flow concentrations	Ini_proc.m
calc_process.m	S Calculation of dependent variables for the process GUI (calculation of drain flow from other liquid flows given)	awc_process_base.m
calc_rates.m	F Compute reactions rates from concentrations (after simulation)	Simul_compute_xx.m
Check_compound.m	S Check validity of data given for the compounds (basic properties) Store data in <b>DATA_corps</b> and <b>Nom_corps</b> and close the compound GUI	Compound_def.m
Check_compound_p.m	S Check validity of data given for the compounds equilibrium properties Store data in <b>DATA_corps2</b> and close the compound equilibrium properties GUI	Compound_p.m

Check_ini.m	S	Check validity of data given for the initial compounds concentrations for the simulation Store data in <b>DATA_in</b> an <b>DATA_input</b> and close initial concentrations conditions for simulation GUI	ini_proc.m
Check_process_base.m	S	Check validity of data given for the process parameters. Store data in <b>DATA_process</b> and close process GUI	awc_process_base.m
Check_reac.m	S	Check validity of data given for the reactions parameters Store data in <b>DATA_reac_xxx</b> and close the reaction data capture GUI.	All scripts for model reaction data capture : model_xxxx.m
Compound_def.m	S	Display an independent GUI window for the capture of compounds (number, names, basic properties)	awc_ms_menu.m
Compound_prop.m	S	Display an independent GUI window for the capture of compounds equilibrium properties (pH, gas/liquid)	awc_ms_menu.m
Conversion.m	F	Convert gas fraction into gas concentrations	
Conversion2.m	F	Convert gas concentration into gas fraction	
csat_1.m	F	Calculation of the saturation concentration of a gas compound in a liquid phase	
csat_12.m	F	Calculation of the saturation concentration of a gas compound in a liquid phase	
csat_g.m	F	Calculation of the saturation concentration of a liquid compound in a gas phase	
data_reac_selector.m	F	Give the vector containing the parameters of a given reaction	
Graph_3d.m	S	GUI window for 3D graphical representations of range simulations	awc_ms_menu.m
Graph_3d_change.m	F	Load the results to display in 3D graphs	Graph_3d.m
Graph_3d_trace.m	F	Trace in the 3D graphs window the graph to display	Graph_3d.m
Graph_change.m	F	Load the results to display in graphs	Graph_out.m
Graph_out.m	S	GUI window for graphical representations of simulations (compounds concentration in reactor and outputs flow)	awc_ms_menu.m
Graph_p_change.m	F	Load the results to display in process variables graph	Graph_process.m
Graph_p_trace.m	F	Trace in the in process variables graph window the graph to display	Graph_process.m
Graph_process.m	S	GUI window for graphical representations of the process variable operating parameters	awc_ms_menu.m
Graph_trace.m	F	Trace in the concentration graphs window the graphs to display	Graph_out.m
ini_proc.m	S	Display an independent GUI window for the capture of compounds initial concentrations (gas and liquid feed)	awc_ms_menu.m
ld_data.m	S	Load a matlab format file (*.mat) – restore saved matlab environment variable	awc_ms_menu.m
Model_bioenzym.m	S	Display an independent GUI window for the capture of parameters related to an enzymatic reaction	awc_reac.m
Model_composition.m	S	Display an independent GUI window for the capture of parameters related to a decomposition reaction	awc_reac.m
Model_decay.m	S	Display an independent GUI window for the capture of parameters related to a decay reaction	awc_reac.m
Model_monod.m	S	Display an independent GUI window for the capture of parameters related to an growth reaction (monod/haldane/pirt model)	awc_reac.m
r_acid_base.m	F	Compute the reaction rate for an acid/base reaction	Syst_xxxx.m Calc_rate.m
r_bioenzym.m	F	Compute the reaction rate for an enzymatic reaction	Syst_xxxx.m Calc_rate.m
r_decay.m	F	Compute the reaction rate for a decay reaction	Syst_xxxx.m Calc_rate.m
r_decomposition.m	F	Compute the reaction rate for a decomposition pseudo reaction	Syst_xxxx.m Calc_rate.m

r_monod.m	F	Compute the reaction rate for a biological growth reaction	Syst_xxxx.m Calc_rate.m
Ranging.m	S	Display an independent GUI window for the initialisation and the launch of a range simulation	awc_ms_menu.m
Ranging_start.m	S	Check and Initialise conditions for range simulation	Ranging.m
reini_graph.m	S	Reinitialise results GUI	Graph_out.m
reini_toolbox.m	S	Reinitialise completely the AWC_MS toolbox (all variables are reset)	awc_ms_menu.m
Sequential.m	S	Display an independent GUI window for the initialisation and the launch of a fixed sequential (fed-batch) simulation	awc_ms_menu.m
Sequential_start.m	S	Check and initialise conditions for a fed-batch simulation	Sequential.m
Simul.m	S	Display an independent GUI window for the initialisation and the launch of a simulation	Awc_ms_menu.m
Simul_compute_base.m	S	Load initial conditions (concentrations and process parameters) for a basic reactor+FU process and launch simulations (calling ODE15 or ODE45)	All XXX_start.m scripts
Simul_start.m	S	Check and initialise conditions for a simulation	Simul.m
sv_data.m	S	Save compounds/reaction/process parameters in a MatLab format	Awc_ms_menu.m
sv_simul.m	S	Save simulation results in ASCII/text format	awc_ms_menu.m
sv_simul2.m	S	Save the complete MatLab Environment (including parameters+results)	awc_ms_menu.m
syst_awc_base.m	F	Compute the ODE system to solve for the process which is simulated	ODE solvers Simul_compute_base.m

Table 3.1: list of the scripts of AWC\_MS V1.0. S is for a script and F is for a function.

### III.2.3 List of the main variables of the toolbox

In the following table 3.2 are listed and explicated the main variables used in the toolbox for the storage of the different parameters of the models. Most of the variables are defined as global variable (i.e. they are common to all functions of the toolbox). The global variables are initialised in the first script of the toolbox (awc\_ms.m).

It can be noticed that most of the variables are created by the check\_XXX.m scripts.

Other variables that are used are usually temporary variable for the management of the interfaces and the computations. They are deleted and cleared when the interfaces are closed.

Some standart are applied when using a variable :

- Gui\_xxx\_xxx are variable related GUI objects
- R\_xxxx are variables related to reaction rates
- DATA\_xxx are variables for the storage of parameters (models, process, compounds....)
- C\_xx are variables related to compounds concentration and  $dC_{xx}$  variables are related to  $\frac{dC_{xx}}{dt}$  expressions

In principle, the names of variables are explicated in the header of the script which use or create it.

Variable name	Description	Detailed description is given in...
C	Concentration of compounds (simulation result)	Simul_compute_base.m
C_acbase	PH concentration matrix	Check_compound_p.m
Check(1:6)	Indicate the status of checking of the toolbox (0=no entry ; 1=validated) Check(1)→ =1: compounds def ; =2 : compound equilibrium properties check(2) → reactions check(3) → reactor check(4) → initial conditions check(5) → results of simulation check(6) → existence of a previous simulation	All check scripts
DATA	Temporary vector containing initial conditions used for a simulation	Simul_compute_base.m
DATA_corp	Contain the compounds basic properties	Check_compound.m
DATA_corp2=0;	Contain the compounds Equilibria properties	Check_compound_p.m
DATA_ini	Contain initial concentrations (t0 and inputs)	Check_ini.m
DATA_input	Index of the liquid input feed type (1→in g/l ; 2→ in g/day ; 3→ sequential feeding in g)	Check_ini.m
DATA_process	Contain operating parameters for the reactor and the FU	Check_process_base.m
DATA_reac_1_1 to DATA_reac_1_10	Contain the Kinetic parameters of reaction 1 to 10 in step 1	Check_reac.m
DATA_reac_2_1 to DATA_reac_2_10	Contain the Kinetic parameters of reaction 1 to 10 in step 2	Check_reac.m
DATA_reac_3_1 to DATA_reac_3_10	Contain the Kinetic parameters of reaction 1 to 10 in step 3	Check_reac.m
DATA_reac_4_1 to DATA_reac_4_10	Contain the Kinetic parameters of reaction 1 to 10 in step 4	Check_reac.m
DATA_reac_5_1 to DATA_reac_5_10	Contain the Kinetic parameters of reaction 1 to 10 in step 5	Check_reac.m
DATA_reac_6_1 to DATA_reac_6_10	Contain the Kinetic parameters of reaction 1 to 10 in step 6	Check_reac.m
M_acbase	PH equilibria matrix	Check_compound_p.m
model_process	Type of AWC process modelled	Check_process_base.m
N_corp	Number of compounds	compound_def.m Check_compound.m
N_reac(1:6)	Number of reaction for each reactional steps	Check_reac.m
reac_model(1:6,1:10)	Index of kinetic model of reaction 1-10 and step 1-6 i.e. : reac_model(3,2)=2 means that the reaction number 2 of step 3 is a reaction of type 2. The type of reactions are : 1 : enzymatic model 2 : monod model 3 : decay model 4 : decomposition model	Check_reac.m
t	Time vector (after simulation)	Simul_compute_base.m
Tps	Simulation duration	Simul_start.m Simul_compute_base.m
Tps_preced	Time at which start the simulation	Simul_start.m Simul_compute_base.m

Table 3.2: List of main variables used in AWC\_MS V1.0.

## IV AWC MS toolbox user manual

Manual for release V1.0 of AWC\_MS MatLab toolbox.

The AWC\_MS toolbox is composed of 3 parts :

- The data management part, which is a set of Graphic User Interfaces used to enter the model parameters and variables (number of compounds, compounds properties, biological reaction, process operating conditions...)
- The model part itself which is solved during simulation
- The result part which allows to visualise results in a graphical form.

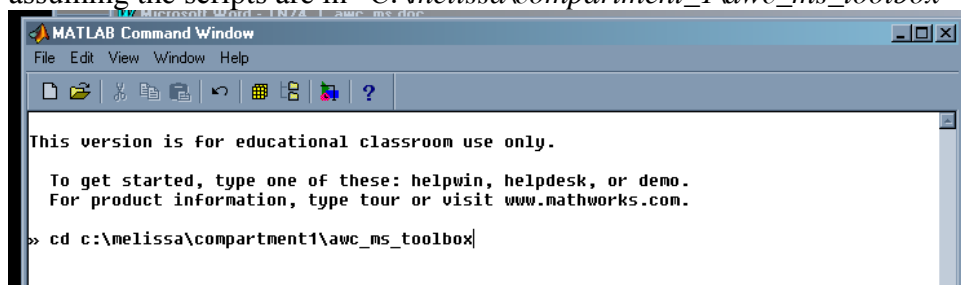
### IV.1 Starting the AWC\_MS MatLab toolbox

The script launching the toolbox is awc\_ms.m. A 1024x764 screen display is required (1280x1024 is recommended).

To start the toolbox :

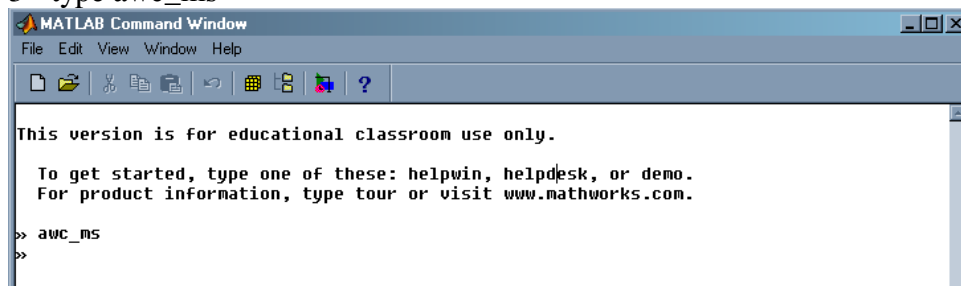
1- run MatLab

2- in MatLab environment go in the directory containing the AWC\_MS scripts (here assuming the scripts are in "C:\melissa\compartment\_1\awc\_ms\_toolbox" directory)



```
MATLAB Command Window
File Edit View Window Help
This version is for educational classroom use only.
To get started, type one of these: helpwin, helpdesk, or demo.
For product information, type tour or visit www.mathworks.com.
>> cd c:\melissa\compartment1\awc_ms_toolbox|
```

3 - type awc\_ms



```
MATLAB Command Window
File Edit View Window Help
This version is for educational classroom use only.
To get started, type one of these: helpwin, helpdesk, or demo.
For product information, type tour or visit www.mathworks.com.
>> awc_ms
>>
```

The main Graphic User Interface (GUI) of AWC\_MS toolbox must appear (figure 4.1).

**IMPORTANT NOTE :**  
**WITH THE GUI WINDOWS, DO NOT USE THE CROSS (X) OF THE MENU BAR TO CLOSE THE WINDOWS, BUT THE VALIDATE OR CANCEL BUTTONS**

## IV.2 Description of the AWC modelling and Simulation Graphic User Interface

This interface (figure 4.1) posses 7 menus for managing and operating the toolbox. The different menus will be presented in the order in which they must be used when entering and checking the data for a simulation

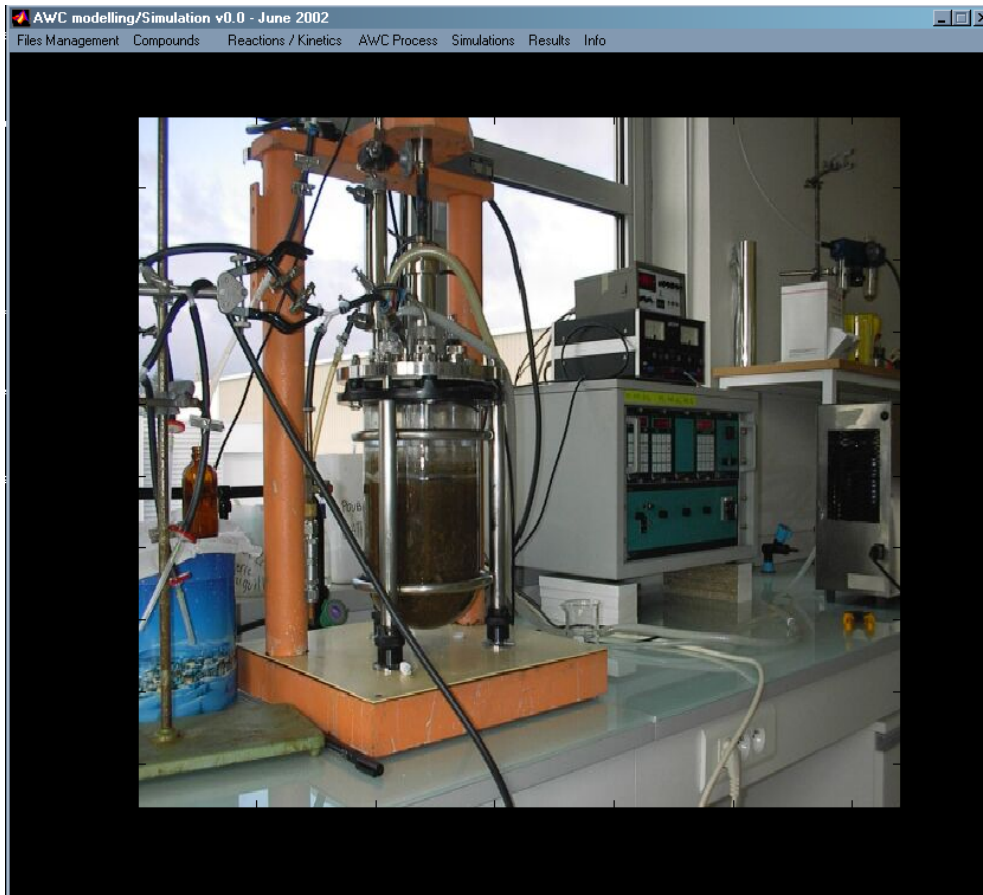


Figure 4.1: Main graphic User Interface of the AWC\_MS toolbox (v1.0 release)

### IV.2.1 File management menu

This menu is for saving/loading process parameters and simulation results. It is composed of 5 sub-menus:

**Load process/simulation :** Load MatLab variables saved to a MatLab file (\*.mat) format. The variables are directly load in the workspace of the MatLab environment. The variables that are saved and that can be then used by the toolbox are the main DATA\_xxx variables detailed in section III.2.3.

**Save Process :** Only process parameters data are saved in a MatLab format (\*.mat) file. The parameters concern the compounds and their properties, the biological reaction, the process operating conditions and the initial conditions for simulation. It is recommended to save Process parameters before starting a simulation (this avoid having to capture again the data if simulation crashes).

**Save Results (ASCII) :** this save simulation results in a text format (ASCII ; \*.dat) which can further be imported in excel for example.

**Save Simulation:** this save the whole workspace of MatLab environment (all variables) i.e. process parameters and simulation results. This can be used to save intermediate results for multiple step (fed-batch) simulations.

**Reset:** reset the MatLab workspace and the toolbox variables. It must be used before loading or creating a new process.

#### IV.2.2 Compounds menu

This menu manage the list of compounds involved in the models and their properties (mass, equilibrium constants...).The compound menu is composed of 2 sub-menus. The first sub-menu control all other management GUI and then any changes in this menu require to re-validate and re-check all the other management interfaces.

**Compounds definitions:** it the first step for the description of the process. Here are set the number of compounds involved and their main properties (figure 4.2).

The number of compounds is chosen (between 1 and 24).

Each compound is defined by its name, and its basic properties are :

- the CHONSP composition - **unused** in calculation of preliminary release -
- the molar mass (g/mol) - **required** and positive
- the volumetric mass - **unused** in calculation of preliminary release –
- FU separating capability (between 0 and 1)

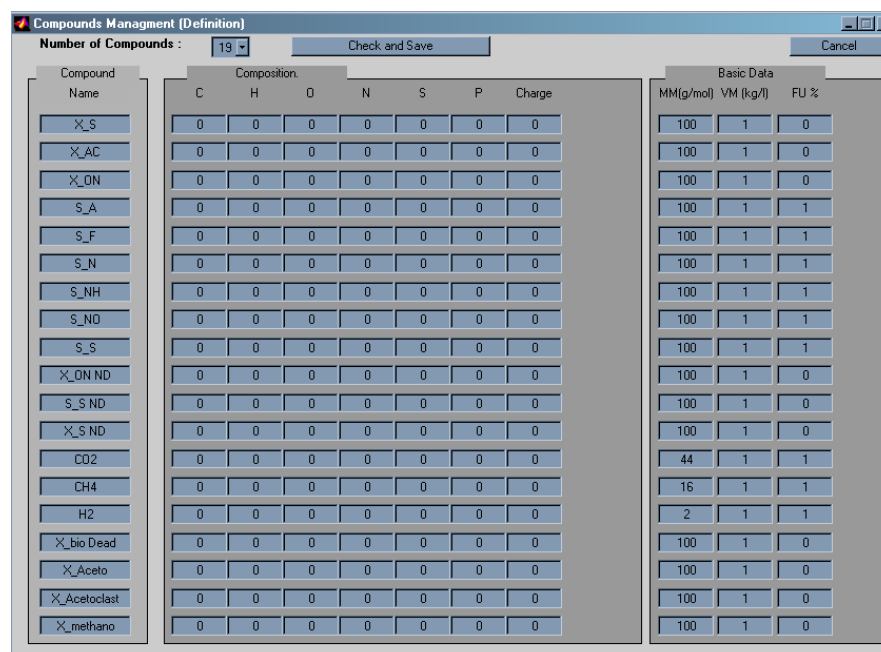


Figure 4.2: Compound definition GUI (v1.0 release)

**Compounds equilibria properties:** this interface (Figure 4.3) must be validated, even if no equilibrium phenomena are considered. The equilibria considered are gas/liquid equilibrium and acid/base equilibrium.

- The gas/liquid equilibrium for a compound requires to set-up the gas/liquid partition coefficient  $k_i$  ( $k_i = \frac{y_i}{x_i}$ ) given at a defined temperature (but note that



temperature is only indicative as no correction is applied). The type of equilibrium must be given, i.e. if the equilibrium is a gas, which is dissolved, or a liquid, which is vaporised.

- The acid/base equilibrium requires to set-up the acid/base reaction (acid→base + H<sup>+</sup> + H<sub>2</sub>O), and the equilibrium constant for a fixed temperature (temperature is only indicative and no correction is applied). For acid/base equilibrium, the compound h2o or H<sub>2</sub>O **must be in the list** of the compound involved in the process

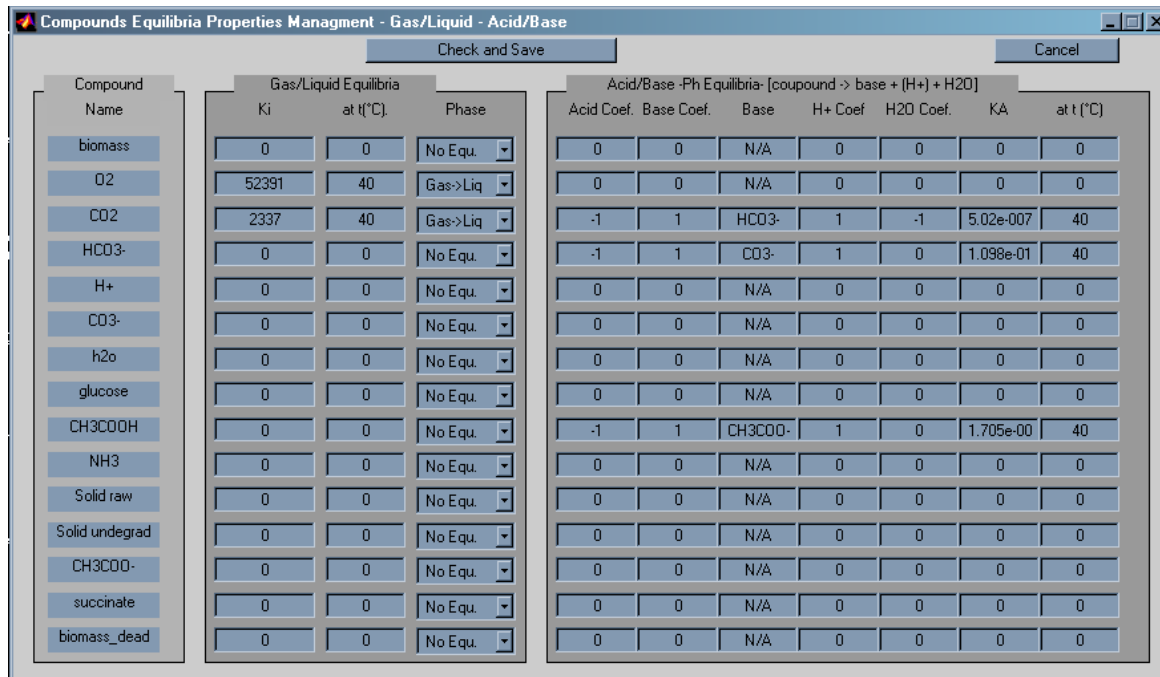


Figure 4.2: Compounds equilibria properties GUI (v1.0 release)

### IV.2.3 Reactions/Kinetic menu

The interface opened illustrates the principles of the anaerobic digestion. The biological anaerobic digestion is separated into 6 steps, which compose the menu of the Biological reactions interface (Figure 4.3).

For each step a set of 10 reactions can be defined. Even if it is not necessary to have a reaction for each of the steps, in each step the reaction N-1 must be defined before the reaction N.

In the GUI for the models, it must be kept in mind that the "check and save" button must be used to save the data captured. **The "quit" button should be used to close cleanly the windows without saving, instead of the "x" button.**

For each reaction the consistency of the mass balance equation is checked. If the reaction is not mass-balanced a warning is displayed. It must be kept in mind that if a reaction is not balanced, the process itself (i.e. the results obtained by simulation) is also not mass balanced.

The significance of the parameters in the different models is detailed in section II.2.4.

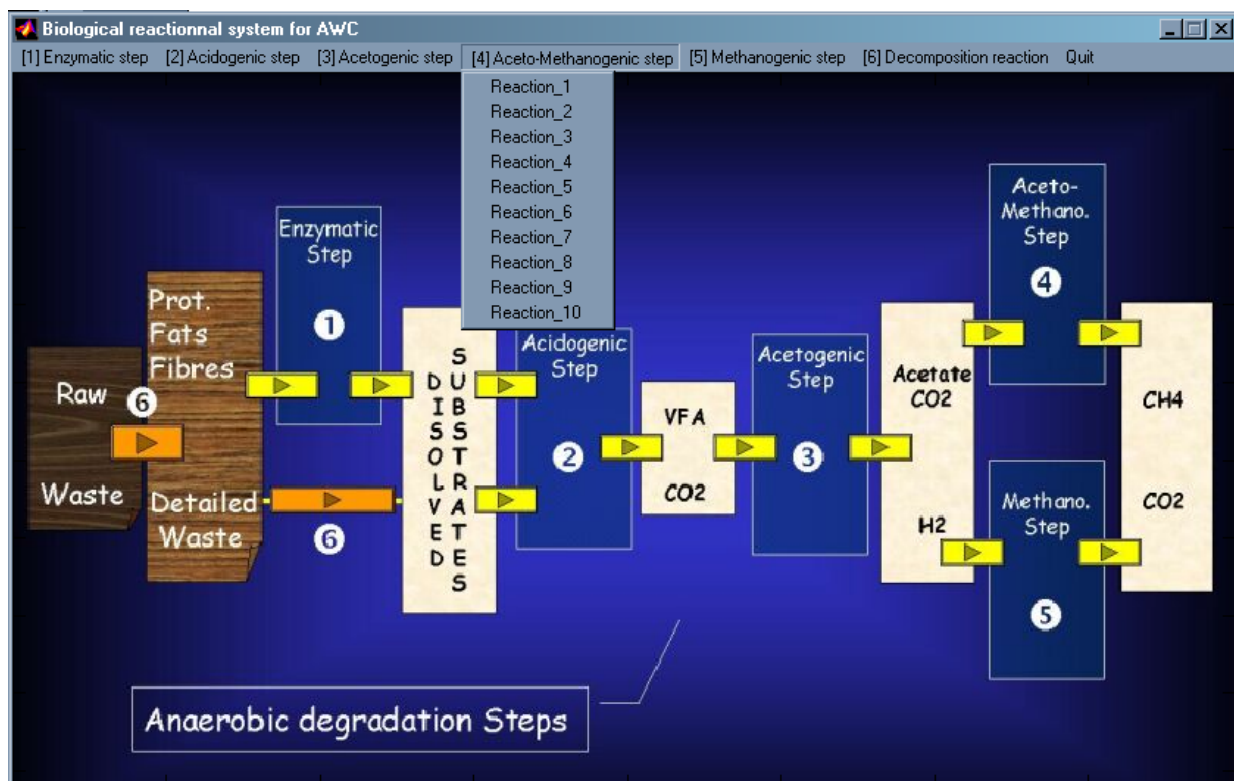


Figure 4.4: Biological reaction GUI (v1.0 release)

#### IMPORTANT NOTES:

When a reaction is created and validated, it can only be modified (changing stoichiometric equation and kinetics parameters) but it can not be remove. This drawback may be corrected in further releases

**(1) Bio-Enzymatic Step :** This menu opens for each reaction an interface which enables to set-up the parameters of an enzymatic reaction (i.e. no growth is associated to the reaction). The parameters of the Bio-Enzymatic model are:

- the coefficient of the stoichiometric reaction (given in moles),
- the ratio between the enzyme and the biomass which produce this enzyme. This ratio is given in the cell corresponding to the biomass.
- the enzymatic kinetic parameters ( $V_{max}$ ,  $K_s$ , competitive inhibition and non-competitive inhibition). These values are given in cells corresponding to the substrate.

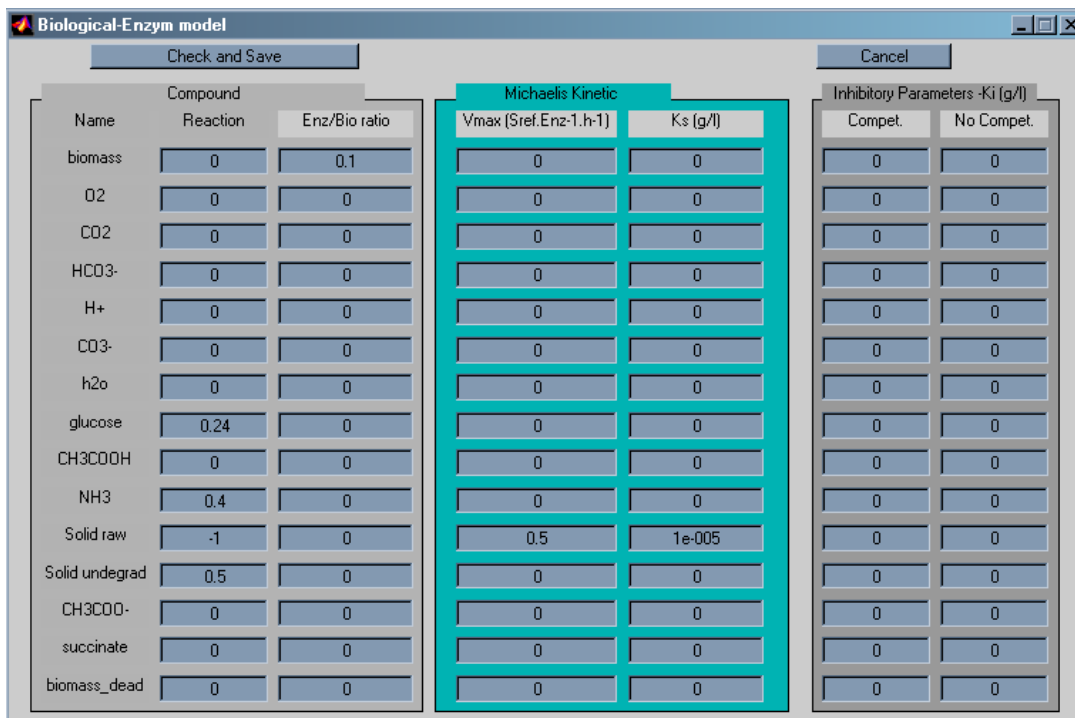


Figure 4.5: Bio-Enzymatic model GUI (v1.0 release)

(2) (3) (4) (5) **Biological reactions Step:** the same kind of model, and then of interface, is used for all the biological reactions. The model is a Monod-Haldane-Pirt model. The parameters of the model are:

- the coefficient of the stoichiometric reaction (given in moles)
- the Monod model kinetic parameters ( $\mu_{max}$ ,  $K_s$ )
- the Haldane model parameters (inhibition constants)
- the Pirt model parameters (endogenous maintenance terms).

The screenshot shows a software window titled "Monod/Haldane/Pirt model" with a "Check and Save" button and a "Cancel" button. The window contains a table with columns for "Compound", "Reaction", "Monod model", "Inhibition", and "Endogenous Maintenance". The "Monod model" column is further divided into  $\mu_{MAX}$  (h<sup>-1</sup>) and  $K_s$  (g/l). The "Inhibition" column is  $K_i$  (g/l). The "Endogenous Maintenance" column is divided into  $m_s$  (S<sub>r</sub>/h/bio) and Stoic.

Compound	Reaction	Monod model		Inhibition	Endogenous Maintenance	
		$\mu_{MAX}$ (h <sup>-1</sup> )	$K_s$ (g/l)	$K_i$ (g/l)	$m_s$ (S <sub>r</sub> /h/bio)	Stoic
biomass	0.5	0.5	0	0	0	0
O2	0	0	0	0	0	0
CO2	1.5	0	0	0	0	0
HCO3-	0	0	0	0	0	0
H+	0	0	0	0	0	0
CO3-	0	0	0	0	0	0
h2o	0	0	0	0	0	0
glucose	-1	0	0.001	0	0	0
CH3COOH	2	0	0	0.1	0.001	0
NH3	-0.1	0	0.001	0	0	0
Solid raw	0	0	0	0	0	0
Solid undegrad	0	0	0	0	0	0
CH3COO-	0	0	0	0	0	0
succinate	0	0	0	0	0	0
biomass_dead	0	0	0	0	0	0

Figure 4.6: Monod/Haldane/Pirt GUI (v1.0 release)

**(6) Decomposition and decay reactions:** These steps deal with biomass decay (Biomass → dead biomass at a given decay rate) and decomposition of matter (i.e. Biomass = proteins+carbohydrate+lipids). The decomposition of matter is not a reaction, it can only be used to detail a complex compound.

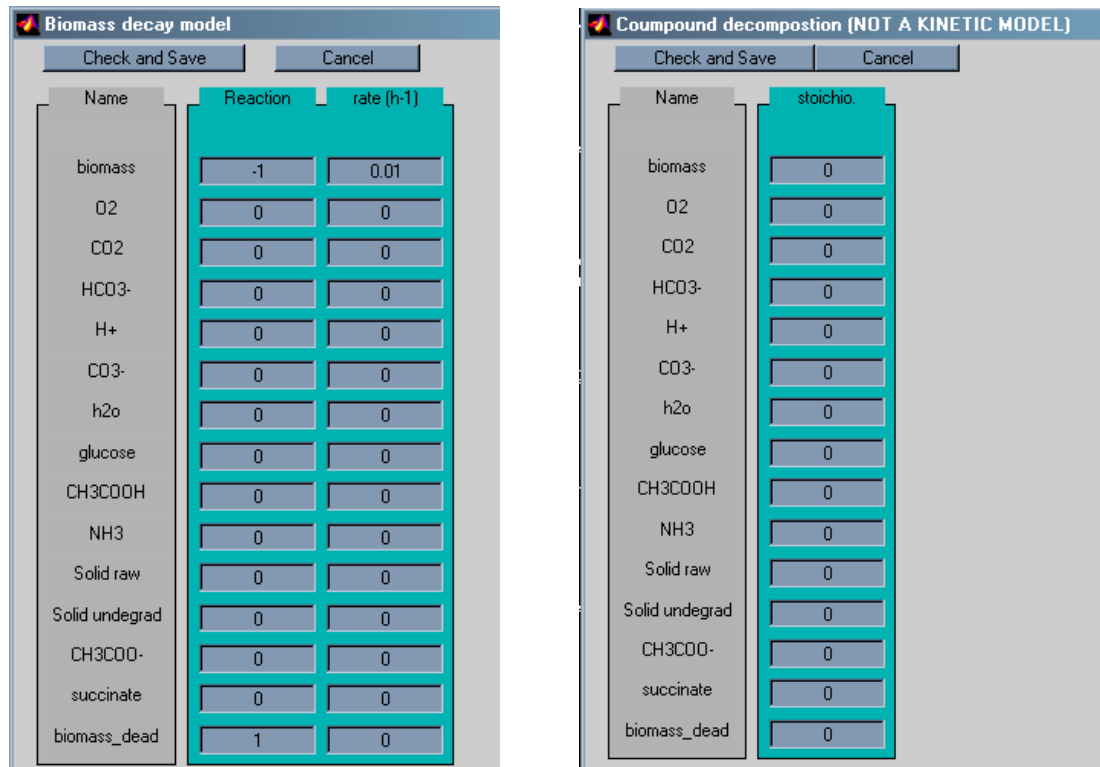


Figure 4.6: Biomass decay model and Decomposition GUI (v1.0 release)

#### IV.2.4 AWC process menu

With this menu are managed the operating condition of the process itself.

#### **The basic AWC process.(Figure 4.7)**

The process is composed of a biological reactor, which can be operated in continuous, batch and fed-batch. 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).

All operating conditions are fixed and cannot evolved during the simulation of the process (i.e. no volume variations in the reactor, no pressure variation, no pH variation). The liquid output flow rate is equal to the input flow rate. The gas output is calculated depending on the input flow rate (**which is given at normalised conditions 0°C and P=1atm.**) and on the gas production in the reactor.

The process variable evolving in time is then the total volume of gas at the output of the reactor

The picture of the GUI window used to capture the operating parameters of the system is a schematic representation of the process.

The parameters involved in the basic AWC process model are :

- The total volume of the reactor (used to calculate the gas volume)
- The liquid volume of the reactor
- The pH (for acid/base equilibria calculation)
- *The Redox (unused in calculations – only indicative value)*
- A  $k_L a$  value (used for all compounds in gas/liquid equilibria calculations)
- The input liquid flow rate
- The gas input flow rate (in N.L/h)
- 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 output (and reactor) reference pressure (important for gas calculation in  $PV=nRT$  relations)
- The input liquid flow rate on the FU (unused)
- The output liquid flow rate on the FU (permeate flow rate). Note that in order to maintain constant liquid volume, the drain flow rate is calculated as  $\text{drain} = \text{Liquid input on reactor} - \text{permeate}$

#### **IMPORTANT NOTE:**

**The operation of the Filtration Unit is consistent only for continuous processes (continuous liquid output is required)**

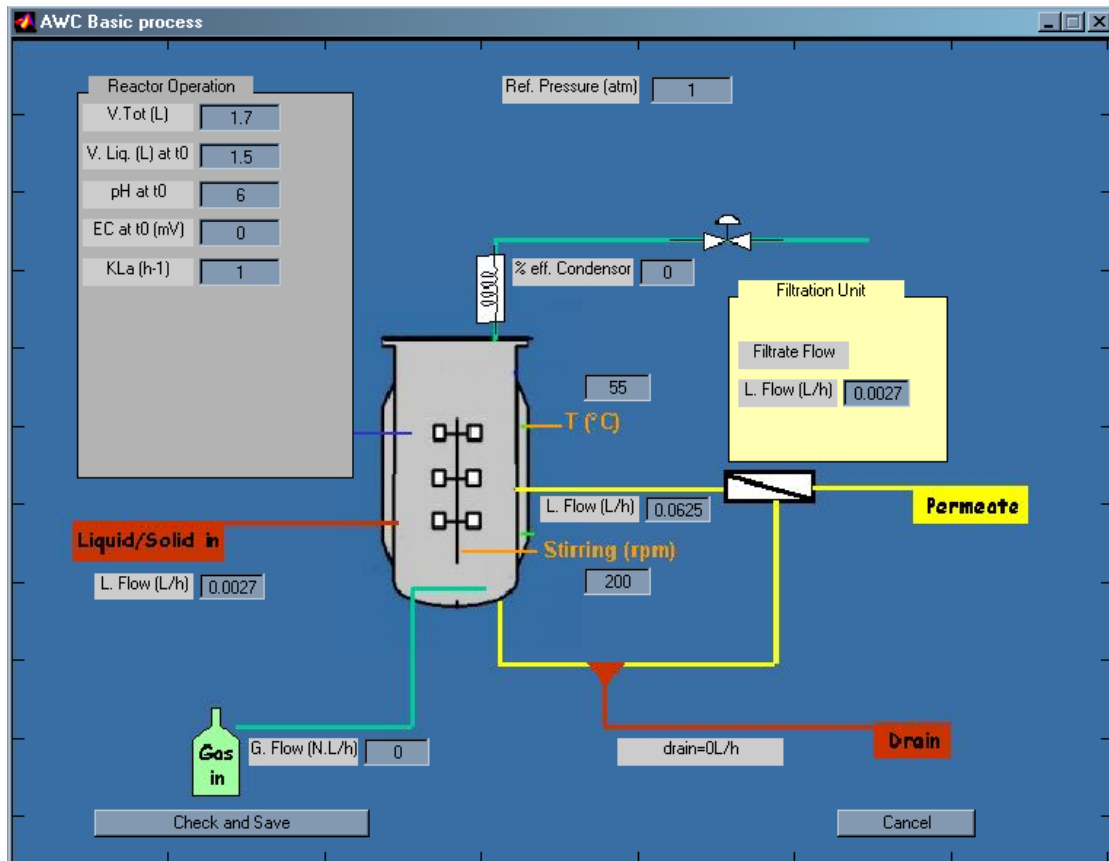


Figure 4.7: AWC process GUI (v1.0 release)

#### IV.2.5 Simulation menu

In simulation tree menu are sub-menus for :

**Initialising the process (figure 4.8):** the initialisation concerns the inputs (gas and liquid) and the reactor content (gas and liquid). It must be kept in mind that if the flow rates are null, the compositions of the feeds are useless.

In the reactor :

- The concentrations are given in g/l for liquid phase while for gas phase a gas fraction is used. These concentrations are taken as the initial reactor conditions at time 0 for a simulation starting at time 0.
- In case of a simulation that is the continuation of a previous one (simulation starting at time t), the initial reactor concentrations used are the last concentrations computed by the previous simulation. **If in the column 3 (see figure 4.8) "reactor at t\_start, liq g/l", there are non-zero values, these values are taken as a mass (in g) of the compound that is added to the reactor at t\_start, and initial concentrations at t are recomputed taking into account these additions of matter.**

For the liquid input before entering the data, the units must be chosen:

- **concentrations in g/l or daily input in g/day.** For daily input, concentrations of input flow are calculated in the toolbox according to the liquid flow rate. It

can be noticed that changing units  $g/l \leftrightarrow g/day$  is associated to a program, which convert all values captured in the new unit. These two choices are for normal simulations and range simulations.

- quantity of matter feeding the reactor (in g), at fixed time intervals (this time interval is fixed after). This option must be used only when a fed-batch simulation (or sequential simulation) is chosen.

Compound Name	Inputs Flow		Reactors at t_start	
	Liq g/day	Gas fraction	Liq g/l	gas fraction
X_S	Liq g/l	0	12	0
X_AC	Liq g/day	0	1.8	0
X_ON	Liq Seq. g	0	3.3	0
S_A	0.46	0	4.5	0
S_F	0.034	0	0.36	0
S_N	0	0	0	0
S_NH	0	0	0.87	0
S_NO	0.0077	0	0.678	0
S_S	0.132	0	3.8	0
X_ON ND	0.71	0	0	0
S_S ND	0	0	0	0
X_S ND	0	0	0	0
CO2	0	0	0	0
CH4	0	0	0	0
H2	0	0	0	0
X_bio Dead	0	0	0	0
X_Aceto	0	0	0	0
X_Acetoclast	0	0	0	0
X_methano	0	0	0	0

Figure 4.8: AWC GUI for initialisation of inputs and reactor compositions (v.1.0 release)

**Starting a simulation (figure 4.9)** : This is the standard way for a simulation. The simulation duration must be given in hours, and the computing options, which are

- The choice of the ODE solver (default recommended ODE15s)
- The calculation of the reaction rates after the simulation for each compound. This option allow to display the reaction rates in the results
- If a previous simulation was performed it is asked if the new simulation is a continuation of the previous one or a completely new one. This option is useful when we want to change one or more operating condition (i.e. starting with a flow rate of 4l/h during 150h and then a flow rate of 2l/h during 50h)



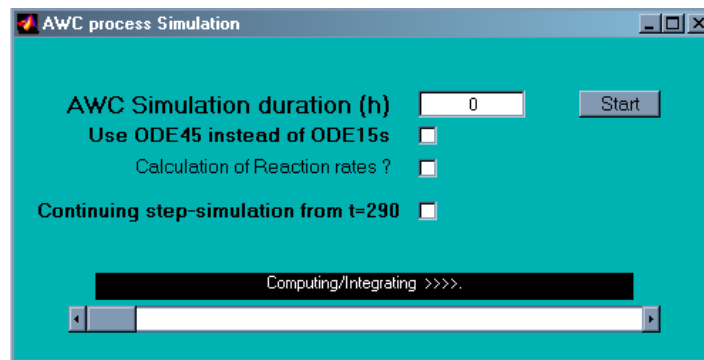


Figure 4.9: AWC simulation start GUI (v.1.0 release)

The start button runs the simulation program. During the simulation, a slider shows the evolution of the computation. In the black bar is also indicated the current time of the process simulation (in hours), and an estimation of the remaining time before the end of the simulation (in minutes).

#### IMPORTANT NOTES:

- 1) During the simulation, the MatLab windows are frozen and it is not possible to STOP before the end of the simulation. In order to stop, the MatLab processus (or application) must be killed (crt+alt+sup under windows)
- 2) If the simulation is the continuation of a previous one, the compounds number and parameter must not be changed, as well as the option "calculation rate". In this case, it must be kept in mind that the values given in the "reactor liquid content at t0" in the initialisation GUI (see above) are treated as matter added (in g) to the reactor.
- 3) With ODE15s, the start of the simulation can take from several seconds to several minutes, depending on the number of compounds and the initial values for the process.

#### Starting a simulation over a range for a process variable (figure 4.10)

Using this menu allows to perform automatically 11 simulations varying one of the operating parameter "reactor volume" or "liquid flow rate" in a specified range (the step for changing the operating parameters is range/10).

This range simulation operates as the standard simulation, except that it is not possible to continue a previous simulation. This kind of simulation is useful to study the influence of the operating parameters on the dynamic of the process. (TN 71.1)

The results obtained can be displayed only with the "range results" sub-menu (see below).

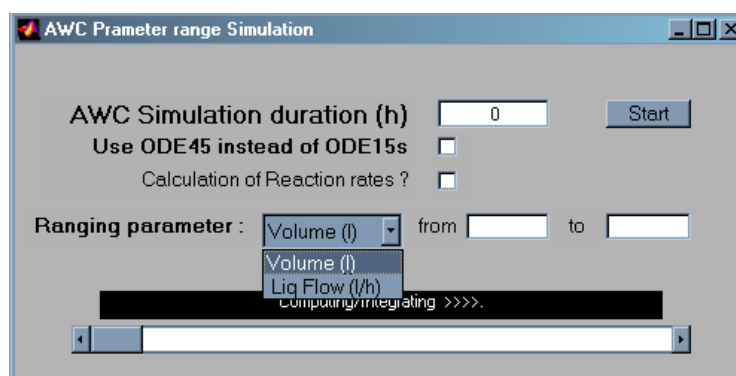


Figure 4.10: AWC range simulation start GUI (v.1.0 release)

### Starting a simulation with sequential inputs (fed-batch) (figure 4.11)

#### IMPORTANT NOTES:

- 1) This procedure was not fully tested. Its validity remains to be checked.
- 2) As this is a non continuous fed-batch system, the FU can not be used and liquid flow rates must be set to 0
- 3) In the initialisation menu, the liquid feed must be given as sequential quantity of matter added to the reactor.

This simulation sub-menu allows to simulate a reactor operated in fed-batch. This kind of reactor can also be simulated with the standard simulation sub-menu, but in this case it requires to manually change the feed of the reactor. With this fed-batch procedure it is not necessary to stop and restart the simulation for each feed of the reactor. On the other hand, the fed-batch is "formatted", this means that the feed, sampling and dilution of the reactor are at the same time interval during all the simulation. It must be noticed that if sampling and dilution volumes are different, this led to change the liquid volume of the reactor during the simulation.

The following informations must be given :

- The sequential fed-batch time (in hour) is the time after which a new fed-batch operation is realised. In figure 4.11, the value 1 hour means that for the 1000 hours of simulation, every 1 hour matter addition, sampling and dilution operations are realised.
- The sampling volume is the volume sampled from the reactor. This volume has the same composition as the liquid phase of the reactor at the time of the sampling. The sampling is treated before any addition of matter in the reactor.
- The dilution volume is the volume of water added. If for example in the reactor are added 10 ml of a solution of a compound at 5g/l, this means that
  - 1)  $5 \cdot 10 \cdot 10^{-3} = 5 \cdot 10^{-2}$  g of the compound is added (information given in the initialisation GUI),
  - 2) the dilution volume used is  $10^{-2}$  l. (information given in this GUI)

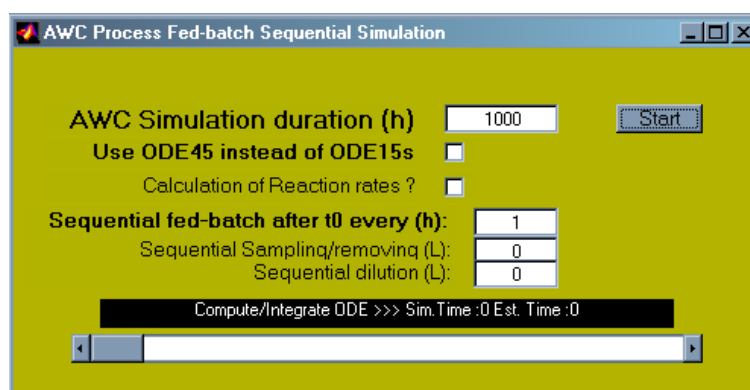


Figure 4.11: AWC Fed-batch simulation GUI (v.1.0 release)

#### IV.2.6 Results menu

The results menu is for the plotting of the simulation results. The windows for the results plotting would be self-understandable.

**The compound sub-menu** (figure 4.12) presents the output concentrations (liquid phases) and the output gas fractions. Liquid and gas composition can be displayed for the reactor content and the output flows. The compound and its location are chosen using select menus at the bottom of the window. Up to 5 compounds can be displayed at the same time.

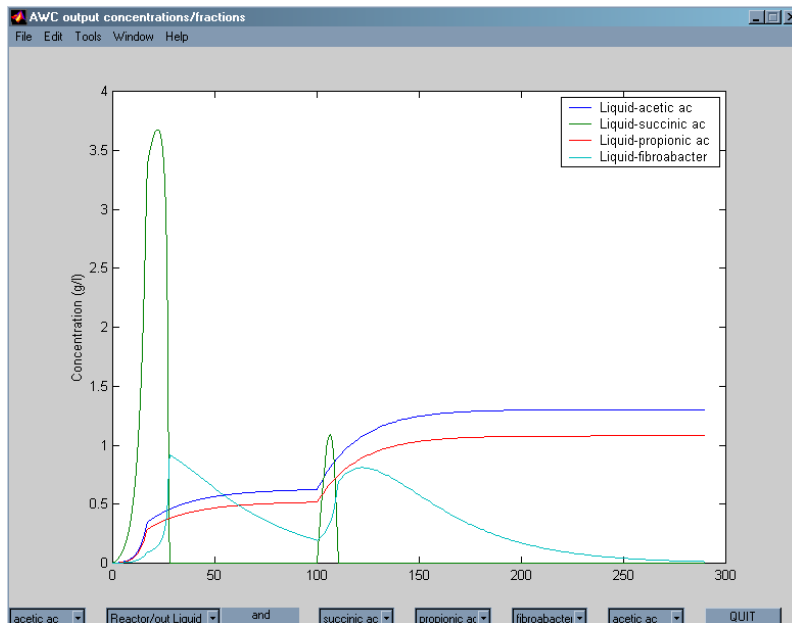


Figure 4.12: AWC plotted results (v.1.0 release)

**The process sub-menu** presents the variation of the process operating variables. In the current release v1.0, only the gas volume production is presented. If there is no gas flow rate, this gas volume is the cumulative gas output flow during the simulation. If there is a gas flow rate, the output gas flow rate is variable taking into account this gas production in order to maintain gas volume and pressure constants in the reactor

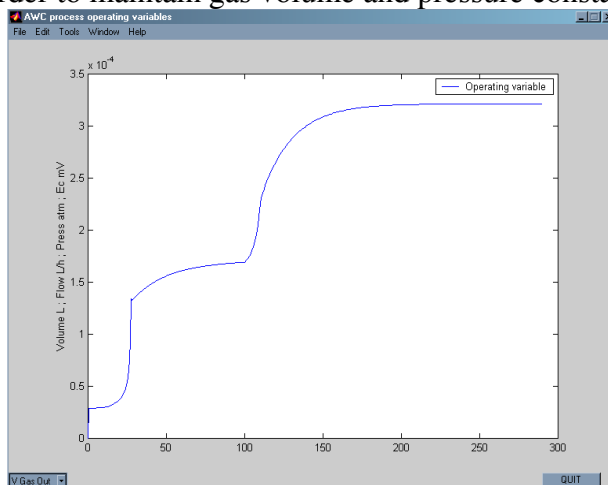


Figure 4.13: AWC plotted results (v.1.0 release)

**The range simulation result sub-menu (figure 4.13).** This representation of the results is only for the simulations performed when ranging one of the operating variable. This is a 3-Dimensional representation of the concentrations of compounds in reactor and in flow rate, for one compound as a function of time and of the value of the operating variable.

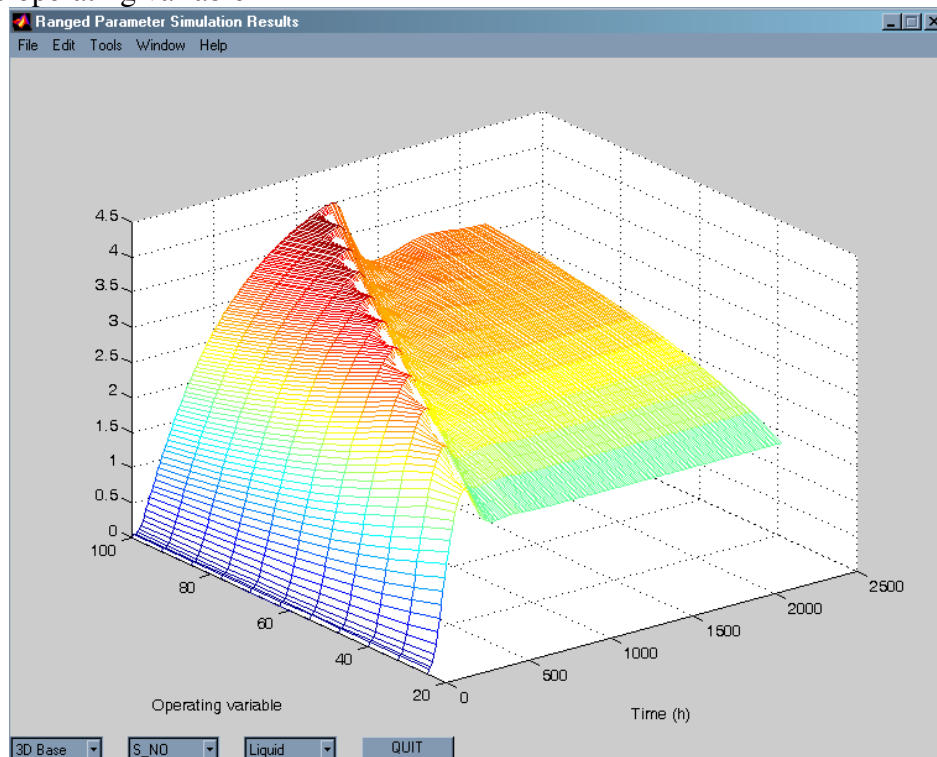


Figure 4.13: example of a 3-D plotting result for a range simulation (v.1.0 release)

#### IV.2.7 Info menu

It indicates where can be found informations about the toolbox

## **Conclusion**

In this technical note is presented the first release of the toolbox for the modelling and the simulation of the first compartment. In principle the toolbox is flexible enough to develop several kind of model, from simples to complicated ones. It would be possible too use it with most of the models already developed for anaerobic degradation processes.

The architecture of the toolbox itself would permit to add new models if it is required.

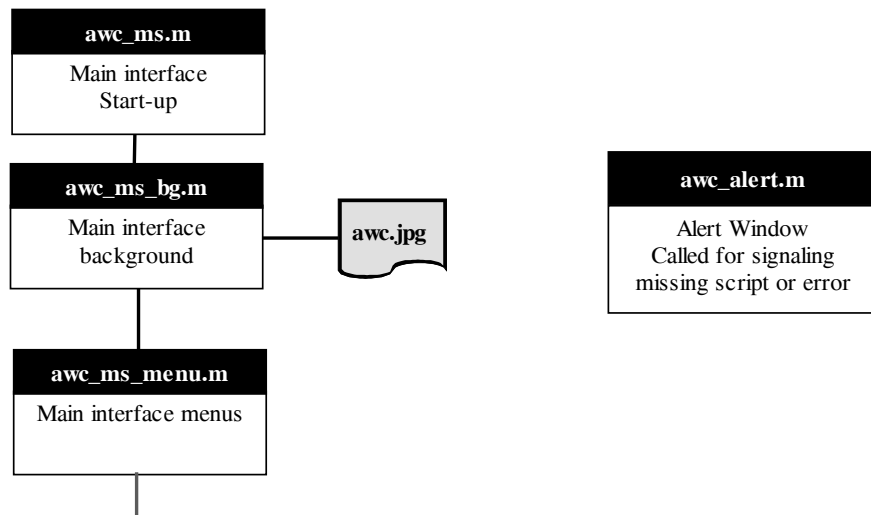
The current version offers only one kind of process a chemostat+FU without change in the volumes and the gas pressure. It would be developed another model enabling pressure and volume variation in the reactor.

Another point concerns the modelling of the Filtration Unit, which is currently assumed to work in steady-state, with constant and fixed performances. A more dynamic modelling of the FU could be possible, but it would require deeper knowledge of the functioning of the membrane, and probably would also require specific studies and experiments to validate such a model.

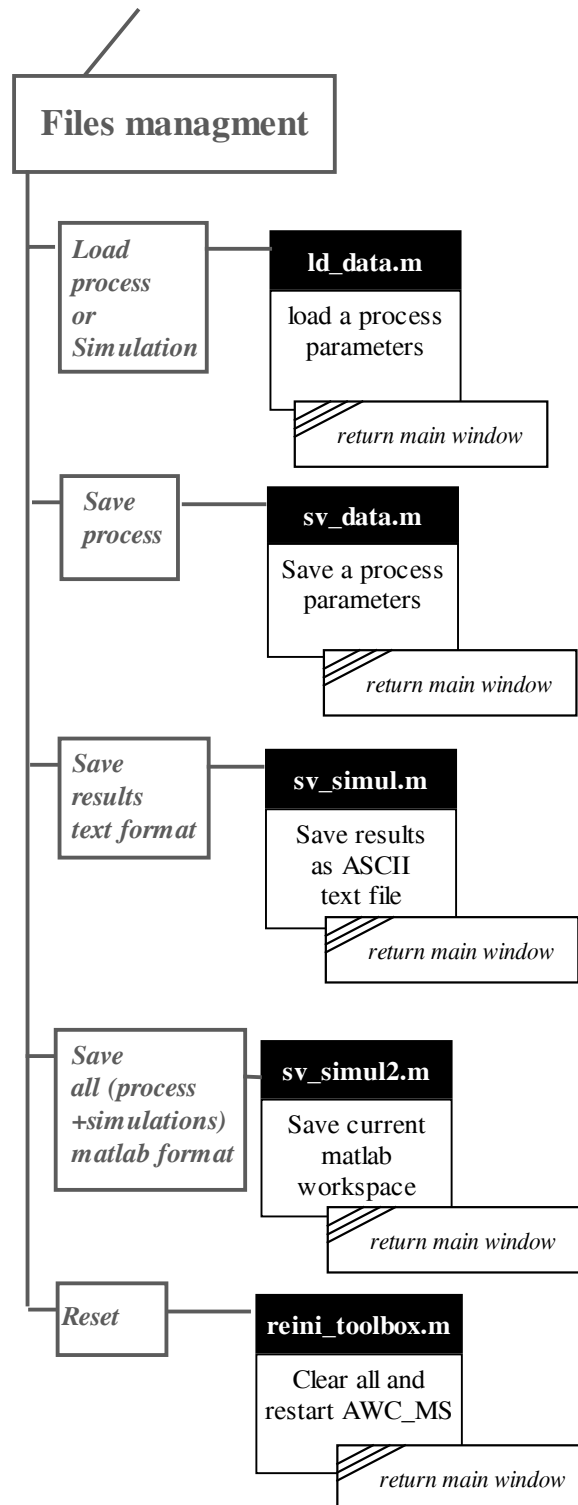
## References

Humphrey J.L. and Keller G. E.(1997). MembraneProcesses. In Separation Process Technology. MacGraw-Hill Editor. New-York.

## APPENDICES

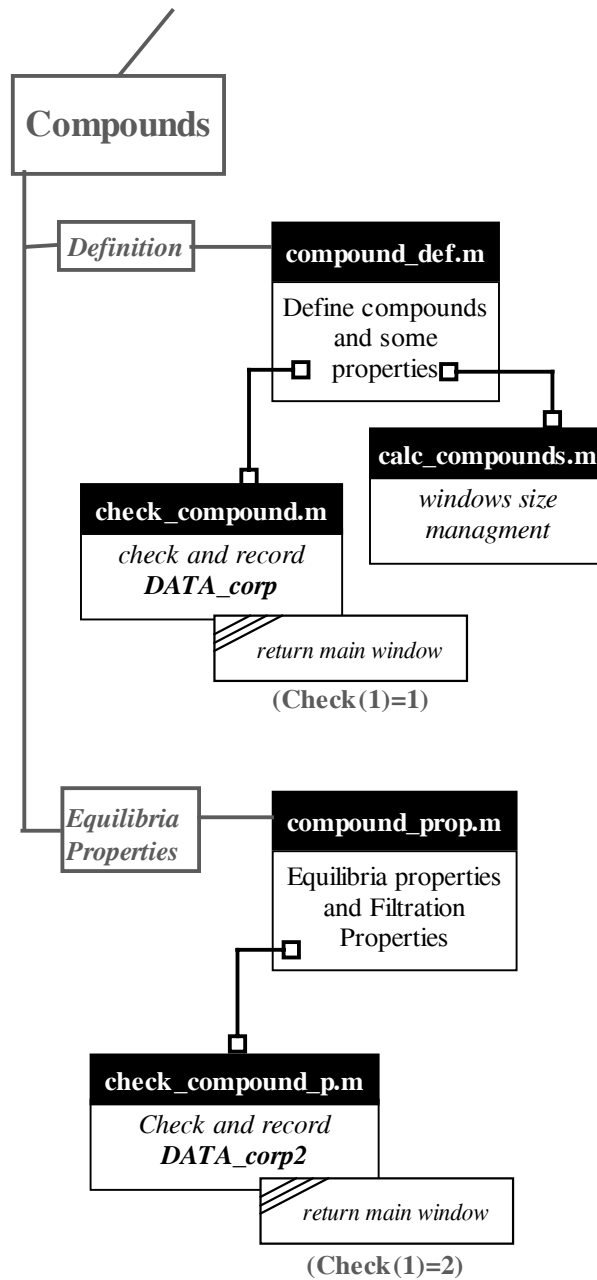


Detailed view of the architecture of the AWC\_MS toolbox : Start-up scripts

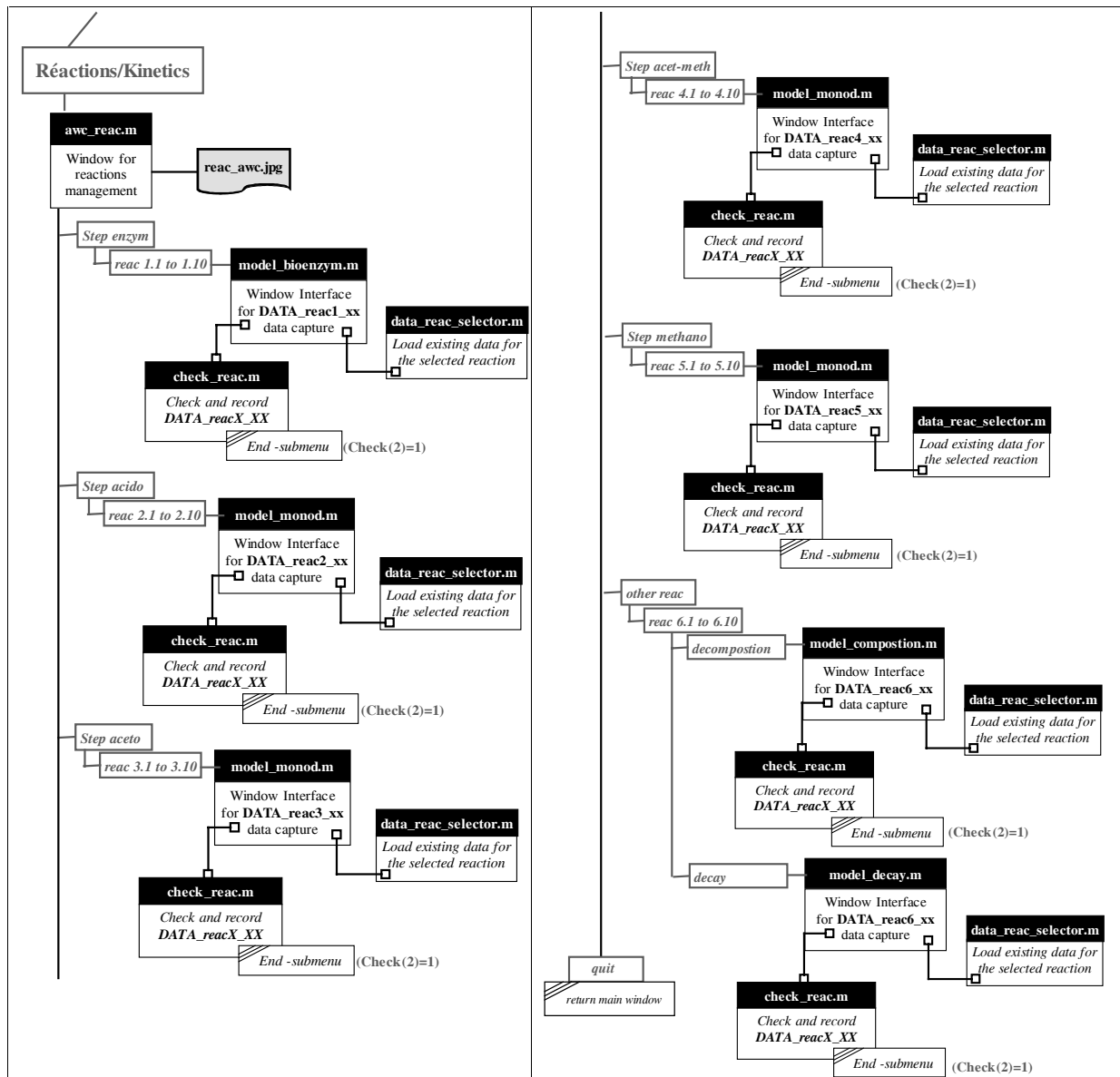


Detailed view of the architecture of the AWC\_MS toolbox :  
Scripts of the file management tree menu

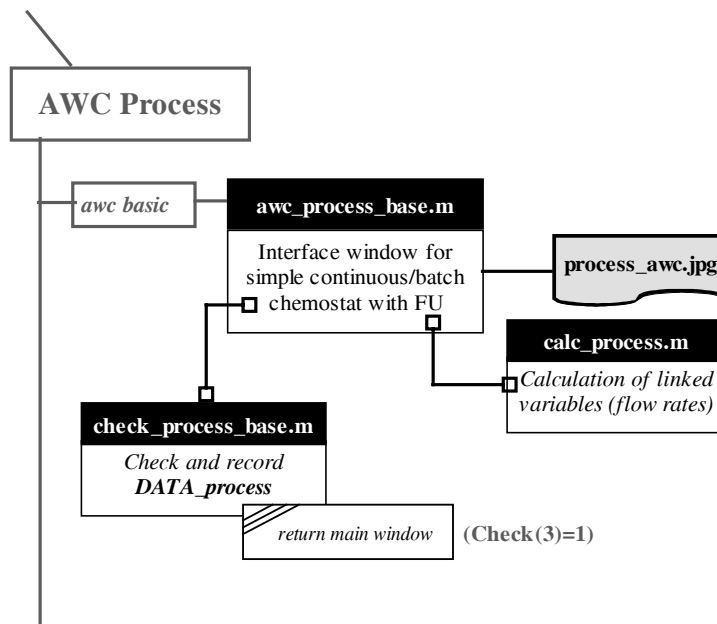




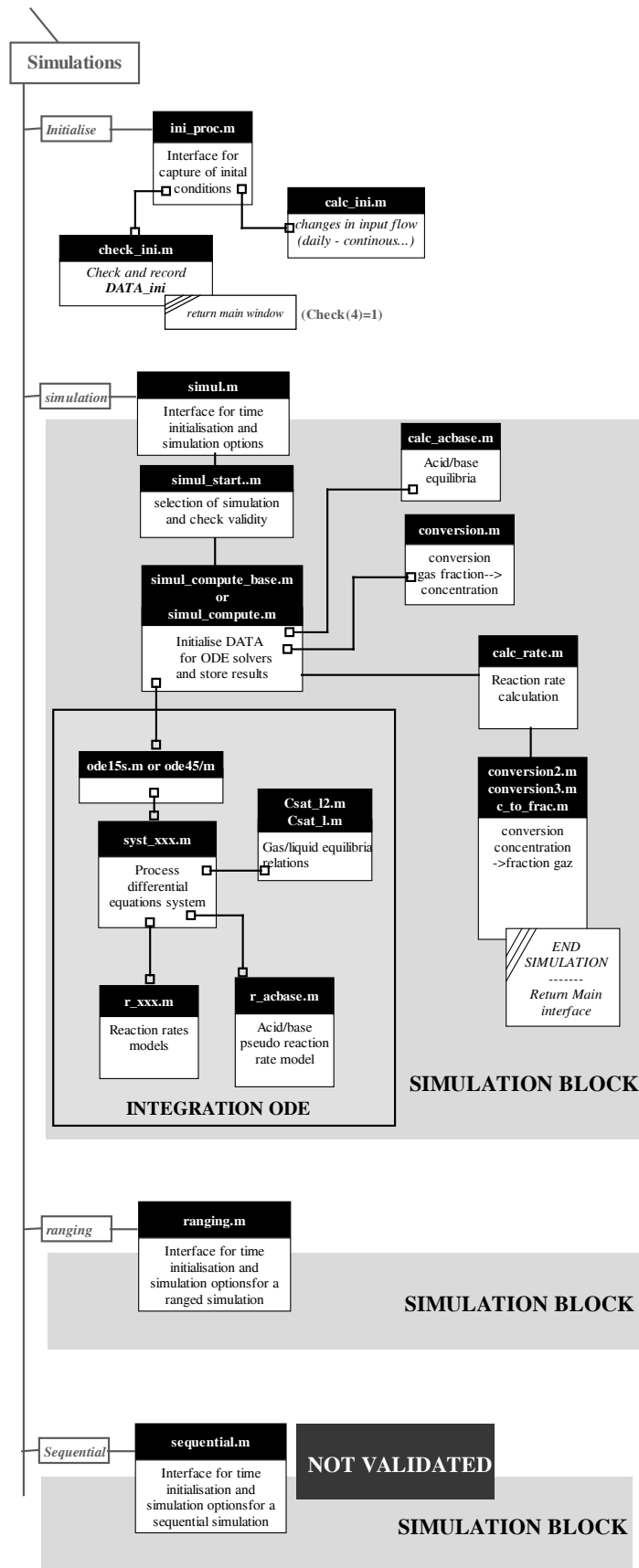
Detailed view of the architecture of the AWC\_MS toolbox :  
Scripts of the compounds management tree menu



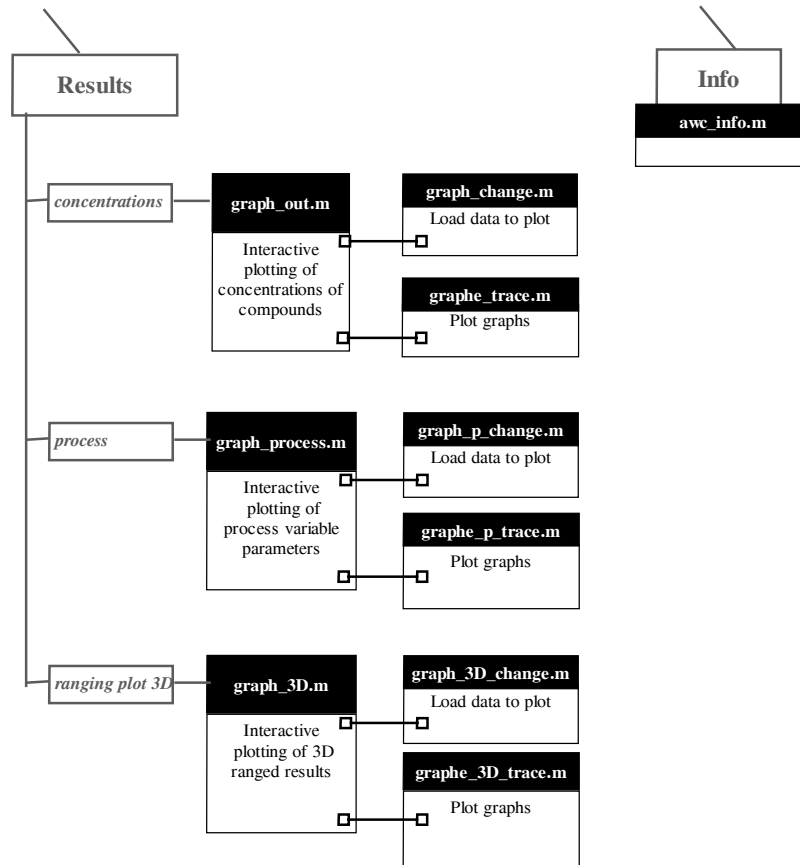
Detailed view of the architecture of the AWC\_MS toolbox :  
 Scripts of the reactions management tree menu



Detailed view of the architecture of the AWC\_MS toolbox :  
Scripts of the process management tree menu



Detailed view of the architecture of the AWC\_MS toolbox :  
Scripts of the simulation tree menu



Detailed view of the architecture of the AWC\_MS toolbox :  
Scripts of the results tree menu

### Using AWC\_MS with an example

In order to illustrate the use of the toolbox a simple example is detailed. This example was made with a previous v0.1 version of AWC\_MS, but the principle is the same.

4 compounds involved :

CO<sub>2</sub> : PM = 44 g/mol

Carbohydrate = 100 g/mol (in fact molar mass unknown)

Biomass = 23 g/mol

VFA = 60 g/mol (in fact molar mass unknown)

The gas/liquid equilibria for CO<sub>2</sub> is considered :

K<sub>i</sub> = 2337 for T=40°C

1 biological reaction is considered :

Carbohydrate → 1.2 biomass + 1.2 CO<sub>2</sub> + 0.5 VFA

*(note that reaction is not mass balanced)*

With μ<sub>max</sub> = 0.3 h<sup>-1</sup>

The operating parameters of the reactor are :

Total Volume : 2 liters

Liquid Volume 1.2 liters

No gas or liquid inputs (i.e. batch culture)

T=40°C

P=1atm

PH=5

K<sub>L</sub>a=40 h<sup>-1</sup>

No FU

### Managing model parameters

All GUI for data management include a "check and save button" which must be used to store the data parameter and to validate the checking sequence of data capture. Simulation and some GUI are only available if previous data were validated.

The normal sequence is :

- 1 - Compounds definition
- 2 - Compounds properties
- 3 - Biological reactions
- 4 - Process parameters
- 5 - Initialisation

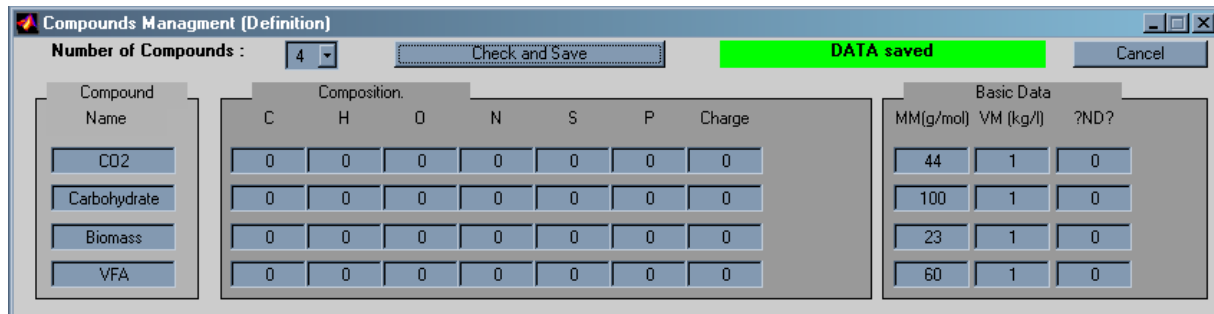
After any kind of Step of the process parameter management you can use the " **Save Process** " menu to save the data entered. You must remember that the "check and Save" button of GUI save data into MatLab workspace and that these data are lost when the workspace is cleared or when MatLab is closed. Only the data saved into a \*.mat file can be recovered in further session of MatLab.

**Compounds definitions:**

Use the first menu "Compounds definitions" to define the compounds involved and to set their properties.

- 1 ) Select the number of compounds and enter their names
- 2 ) CHONSP are not defined, but they are only indicative values in the current AWC\_MS version.
- 3 ) Molar masses are important as they are related to the calculus of yields in biological reaction and in conversion between gas fraction and gas concentrations.
- 4 ) Density is not used in current calculation (probably involved in liquid solid separation)  
 Last column is unused but must be set to zero.

- 5 ) Validate and save the results. A green message "DATA SAVED" must appear during few seconds before the window close.



Compounds definition GUI example

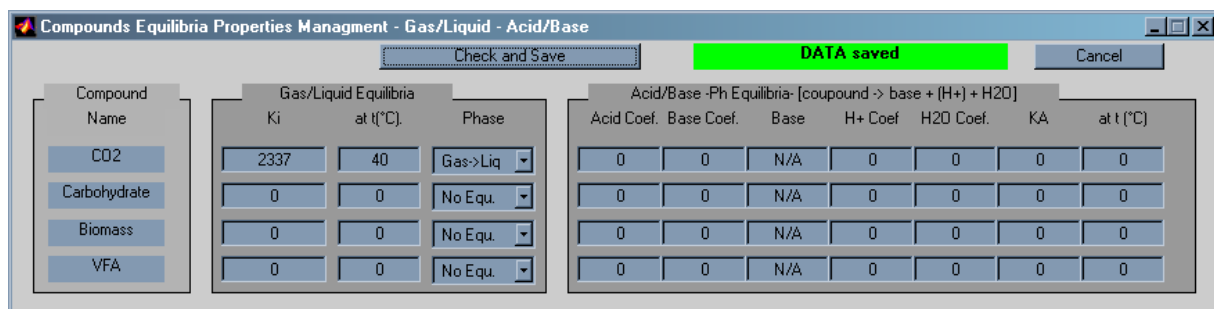
Use the " Save Process " to save the data entered. You can check that by closing matlab and re-launch matlab and the toolbox you can load and recover your data by using the "Load data" menu

**Compounds equilibria properties**

Use the menu "Compounds Equilibria" to define the compounds equilibria properties. **Even if there is no equilibria**, the menu must be involved and the "check and save" button must be hit.

By default all parameters are set to "No equilibria values"

In this example, CO<sub>2</sub> partition coefficient must be given and the equilibria direction must be set to "gas>liq" (i.e. CO<sub>2</sub> is normally a gas compound)



Compounds equilibria properties GUI example

Then Validate and save the results. A green message "DATA SAVED" must appear during few seconds before the window close.

### **Biological reaction**

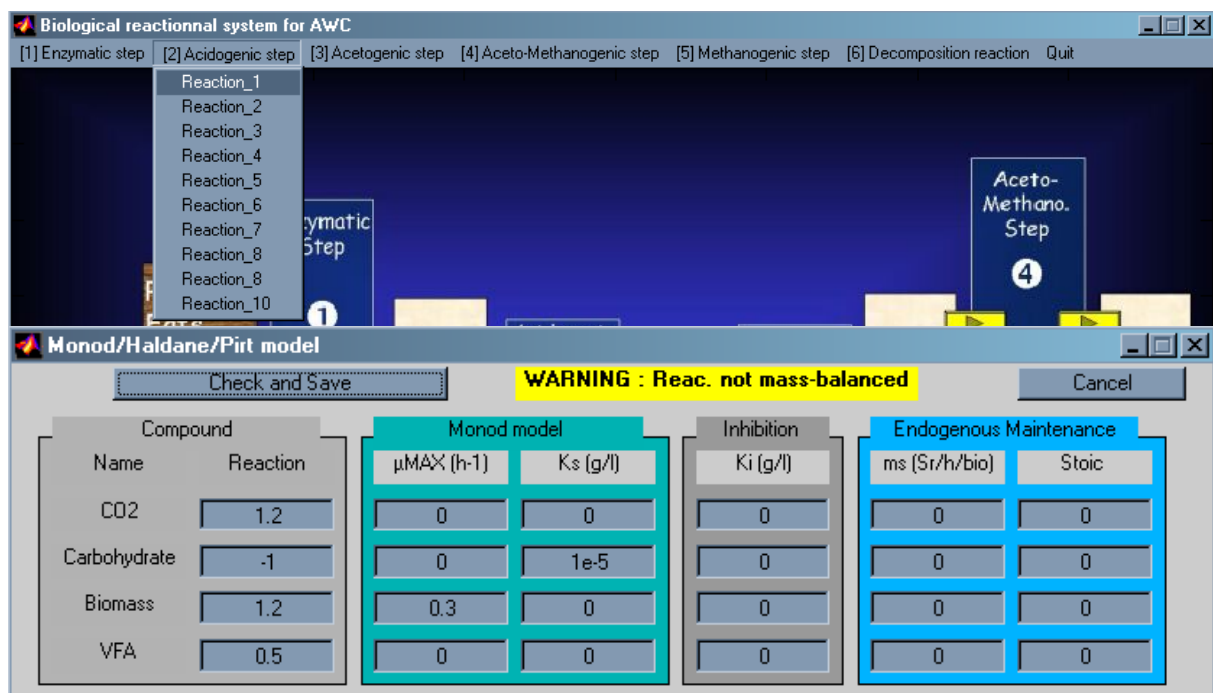
In this simple example only one biological reaction is involved, which correspond to a Step 2 (acidogenic) reaction. In the Biological reaction window, chose menu "[2] acidogenic Step > reaction 1".

You must enter:

- 1) the stoichiometric coefficients of the reaction (molar coefficients). **Substrates have negative coefficient and products positive coefficients.**
- 2) the kinetic parameters for Monod growth model :
  - maximum growth rate (in  $\text{h}^{-1}$ ), **given on the line corresponding to the biomass.**
  - Saturation constant (in  $\text{g/l}$ ). **It is recommended to give a saturation constant to all the substrate involved (use 10-6 if no values are known) to avoid inversion of reaction after substrate exhaustion.**
- 3) the kinetic parameters for inhibition (Haldane term) and endogenous maintenance (Pirt term) are facultative

Then Validate and save the results. A yellow message "Warning: reaction not mass balanced" must appear during few seconds before the window close. This is only a warning and the data are saved. If the reaction is well balanced only the message "DATA SAVED" appears.

To cleanly close the biological reaction window use the QUIT menu.

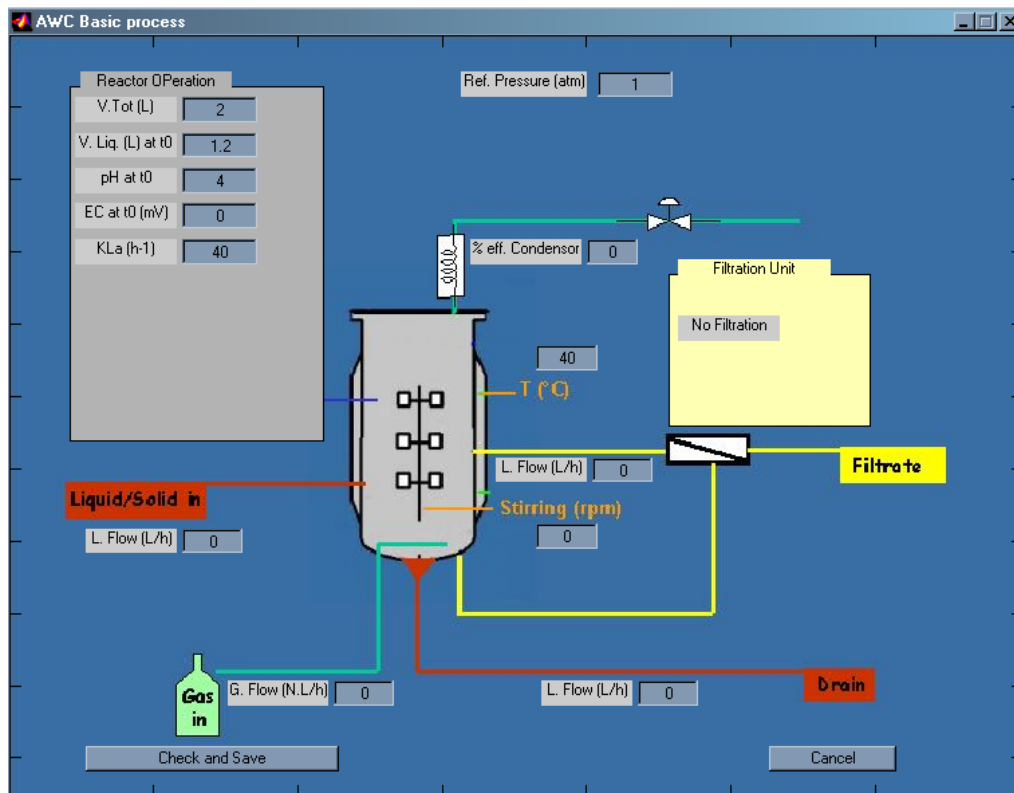


Biological reaction GUI example



### Process operating conditions

After selecting in Process menu the **basic AWC process** enter the process operating conditions and validate with the "Check and Save Button".



AWC process GUI example

### Initial (t=0) conditions

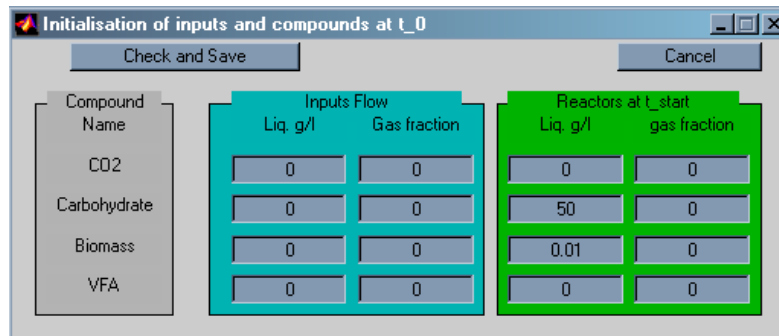
In this example, inputs flows (blue frame) are useless (batch process) and the reactor content at t=0 (green frame) is set to:

- 0.01 g/l of biomass
- 50 g/l of substrate (carbohydrate)

By setting the gas fraction to 0 for CO<sub>2</sub> means that the gas phase is composed of compounds not involved in reactions (inert gas).

Note that if no biomass is given at t=0, there is no biological reaction.

Validate and save the results. A green message "DATA SAVED" must appear during few seconds before the window close. At these step it is recommended to save the process parameters (" **Save Process** " menu), as the next step is the simulation (computation of the system).



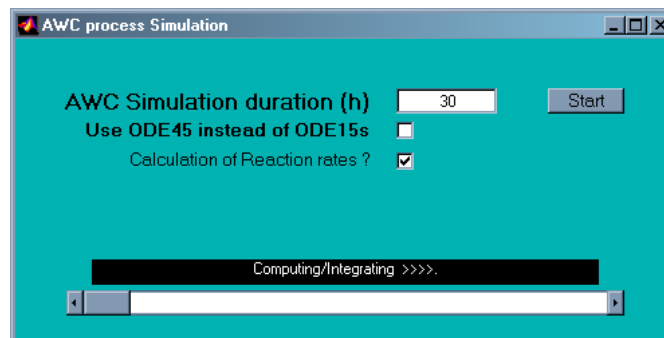
t=0 initial conditions GUI example

## Simulation and results

### First simulation

As it is the first simulation of the process ( $t_{start}=0$ ), it is only ask for the simulation :

- The simulation duration (in h)
- The choice of the ODE solver. By default ODE15s is used, but in some cases ODE45 should be used. ODE45 is slow but can succeed when ODE15s failed.
- The calculation of the reaction rate enables to have the biological reaction rate of the compounds in the liquid phase in the results



t=0 start simulationGUI example

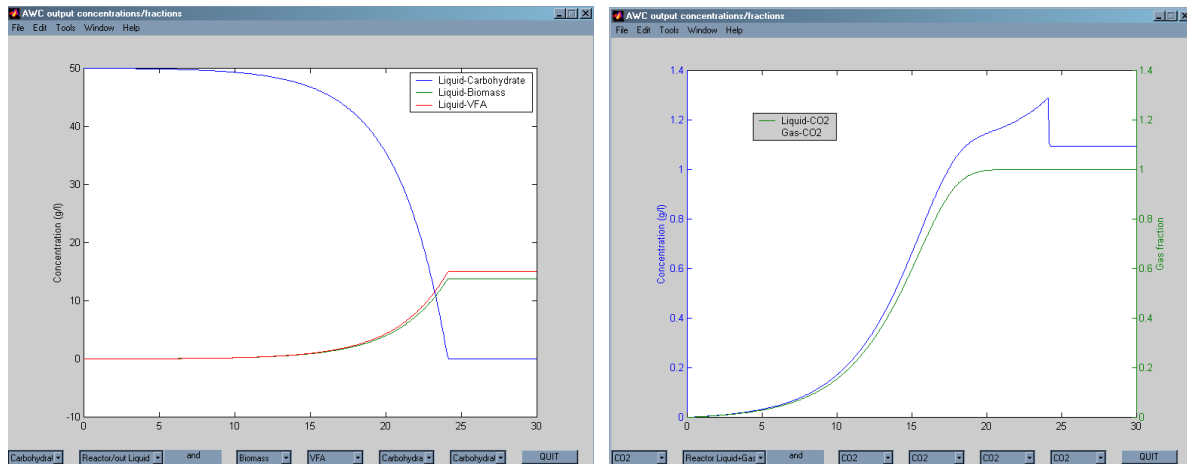
During the simulation the slider indicates the progression of the simulation. The time of the simulation is also displayed. Note that for ODE15s, it can takes some minutes for the solver to initialise its parameters (depending on the number of reactions and of compounds).

The simulation cannot be stopped.

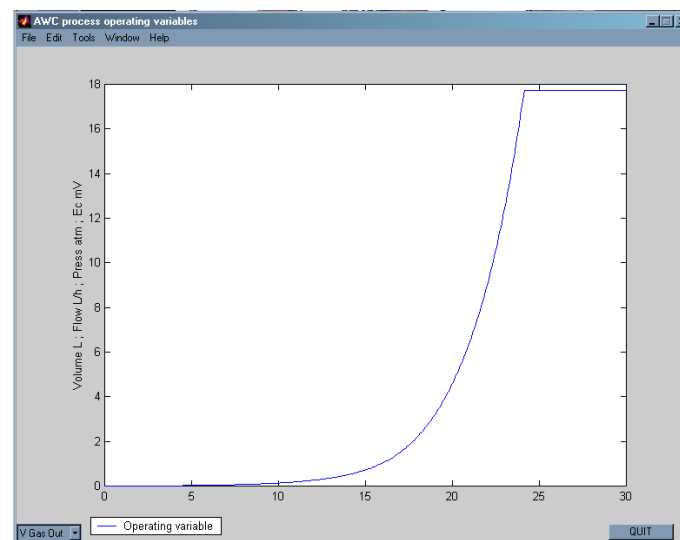
The GUI for simulation disappears only at the end of the simulation.

Once the simulation is ended, the result menu is accessible. Two kinds of results are presented:

- The compounds liquid concentration, gas fractions and biological rates (if option selected for simulation). Up to 5 compounds can be displayed at the same time
- The cumulative gas production at the reactor output, composed volume produced by normal gas flow rate and gas production due to reactions. Keep in mind that the volume is given for the operating conditions fixed for the reactor.



Concentration results at reactor output



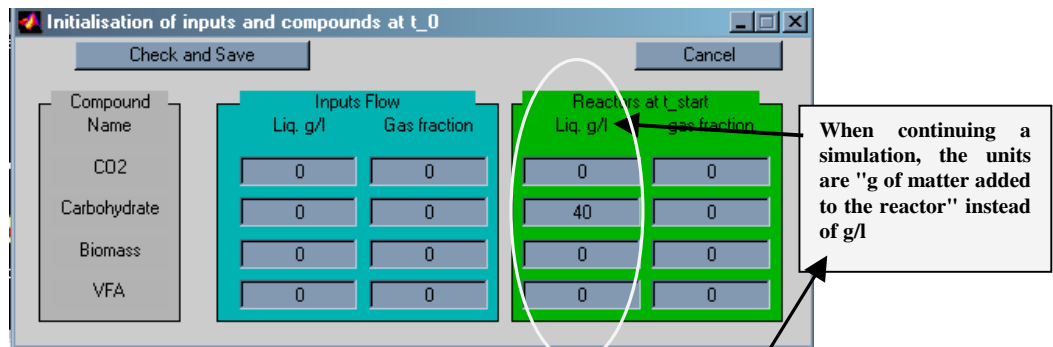
Cumulative gas volume production at the reactor output

At the step it is recommended to save the simulation with the " **Save Simulation** " menu. The whole process and the simulation results can then be reloaded later if needed.

### **Step by Step (Fed-batch like) simulations**

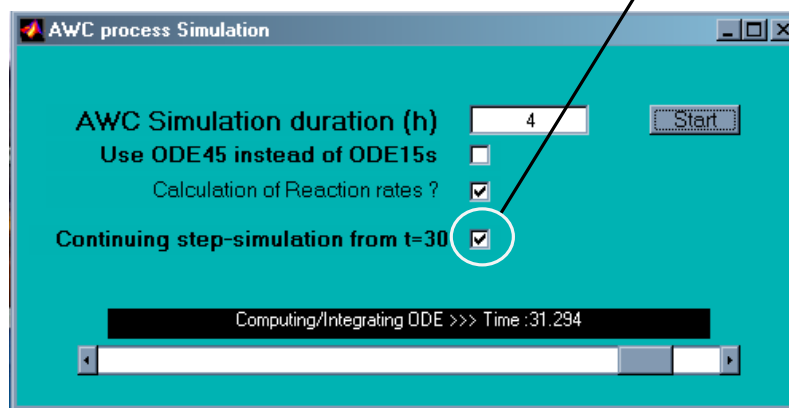
After this first simulation, it is possible to continue the simulation. It is required then to re-check:

- The process operating condition, it is possible to change the operating condition (flow rates,  $K_{La}$ ,....)
- The initial conditions of simulation. The input flow compositions can be changed. The  $t_{start}$  reactor conditions must be reset to zero if you only want to use the last concentrations (gas or fractions) calculated during the previous simulation. If there is addition to reactor, the **mass (and not the concentration)** of compound added in liquid phase is given. In the example, 40g of carbohydrate are added in the 1.2 liters of the reactor.



Example of the new initialisation for continuing the simulation

If there was a previous simulation for the current process, an option appears in the simulation GUI: "Continuing step-simulation from t=xxx". By selecting this option, the computation starts from the end of the previous simulation.



Continuing the simulation from a previous one

The new simulation results are cumulated with the previous ones. In the graphical representation, the results are given from the t=0 time.

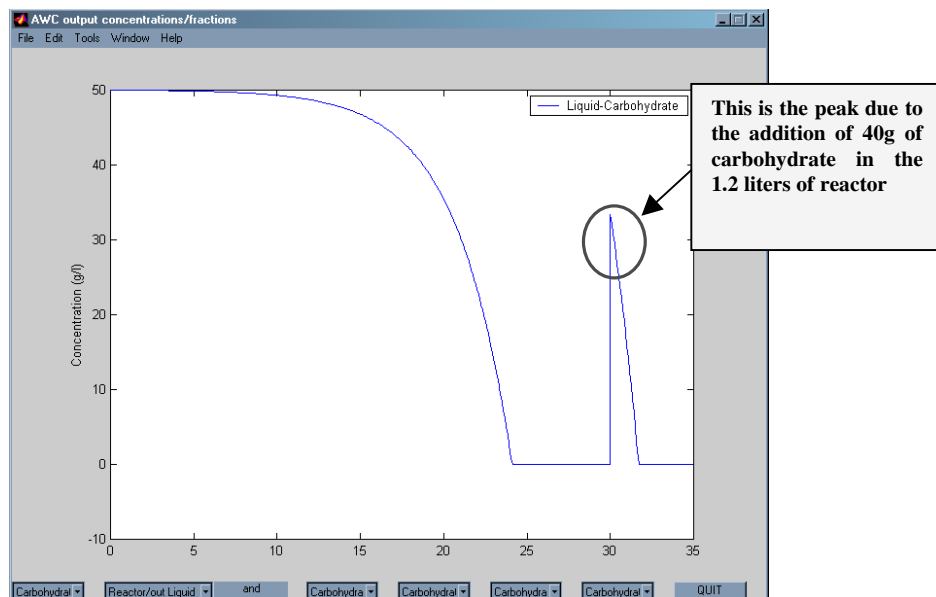


Figure 4.21 : Results of a two step simulation