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Université Blaise Pascal
Laboratoire de Génie Chimique et Biochimique
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MELiSSA LOOP MASS BALANCE MODELLING WITH MATLAB® / SIMULINK

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1 INTRODUCTION

Since the end of year 2000 the modelling and simulation of the complete MELiSSA loop was stopped, mainly because of the limitations of the software used to solve the system (ProSim 96.01 ®). The last studies performed were done in order to have a preliminary estimation of the flows and of the liquid volumes of the biological reactors (L; Poughon, 2000). During this last years the advance of the project requires to have a tool for the steady-state and for the dynamic modelling of the loop which can be used by the MELiSSA partners in order to compute the behaviour of the loop under various operating conditions and to evaluate the efficiencies and the size of the loop. This tool must also be able to be associated to the control models developed for the loop.

On the basis of the past models of the complete loop (TN 32.3), a new model was developed under MatLab/Simulink ®. This software was chosen because it is used (at this time) for the study of the dynamic models of the biological compartments at LGCB-UBP, and also as the tool for the study of control models by SHERPA.

In a first step a model for the simulation of the loop in steady-state (i.e. mass and elements balanced based models) was built. This is the work presented in this report. This work must be taken as a starting point as some models (especially for compartment I) are not fully validated and as the flowsheet and the operating constraints for the loop are not completely fixed.

The technical note is divided into 3 parts.

The first part presents the mass balance model of the 6 MELiSSA compartments and of the other subsystem elements built for the loop as well as the building of the loop itself under Matlab/Simulink. This is more devoted for the understanding and the development of the models than for their use. This part is required for anyone who wants to modify the model, but requires some basic knowledge on Matlab and on Simulink. To be useful, this part must be read in parallel with the MELiSSA loop model version 1 program.

The second part explains how to use and install the model, how to perform simulations and how to analyse the results.

The third part is a summary of the tests performed in order to check the loop model and to identify several problems.

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2 MELISSA LOOP MODELING WITH SIMULINK

2.1 Principles of the approach used

2.1.1 MATLAB SIMULINK®

Simulink® is a matlab® graphical and interactive software package for modelling, simulating and analysing dynamic systems. It support linear and non-linear systems, modelled in continuous time, sampled time (discrete modelling) or a hybrid of the two. System can also be multirate. Simulink is then a tool which is interesting for the complex dynamic system of MELiSSA. As it is not the objective to fully describe and explain here how to use Matlab and Simulink it is recommended to every who wants to develop and modify models to read the software documentation (http://www.mathworks.fr/support/books/).
For modelling, Simulink 5 provides a graphical user interface (GUI) for building models and systems as block diagrams, using click and drag mouse operation. It is then simple to build and manipulate a system with blocks. Models can be built using several layers of hierarchy which simplfy the manipulation, the building and the understanding of the system (Figure 2.1).

Simulink includes a comprehensive block library of sink, sources, linear and non-linear components and connectors. Obviously there is no block for modelling the compartments of MELiSSA, even if it could be possible (but difficult) to develop models with combinations of linear and non linear Simulink blocks. But it is possible to customize and create our own blocks by creating “S-functions”. As this is by this way that all models for the MELiSSA loop were developed, the S-functions were presented here after.

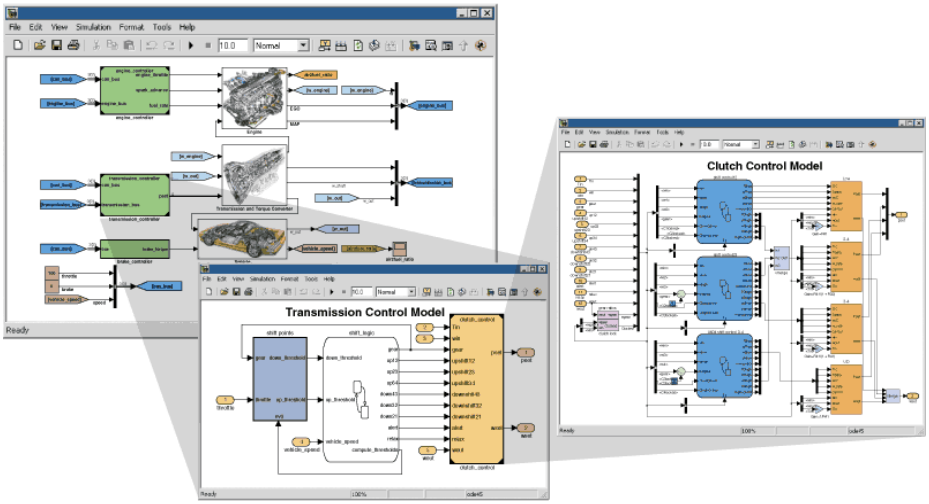

Figure 2.1: Simulink Graphical end user interface. Models are built from block. There is several layers to go deeply in the details in the building of the model. [From Matworks ™ website]

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2.1.2 SIMULINK AND S-FUNCTIONS

An S-function is a computer language description of a Simulink block. S-functions can be written in MATLAB®, C, C++, Ada, or Fortran. C, C++, Ada, and Fortran languages. S-functions use a special calling syntax that enables you to interact with Simulink equation solvers. This interaction is very similar to the interaction that takes place between the solvers and built-in Simulink blocks. The form of an S-function is very general and can accommodate continuous, discrete, and hybrid systems. By following a set of simple rules, we can implement any kind of algorithms in an S-function. If for details it is recommended to report to the Matlab documentation, some principles of S-function are explained here after as these function will be the core of the MELiSSA Loop model.

After writing a S-function its name is placed in an S-Function block (available in the User-Defined Functions block library), which user interface can be customised (Figure 2.2).
The "S-function dialog block's" S-function parameters field allows specifying parameter values to be passed to the corresponding S-function. The parameters are separated by a comma, in the order required by the S-function (it is necessary to know the source code). The parameter values can be constants, names of variables defined in the model's workspace, or MATLAB expressions (Figure 2.2).

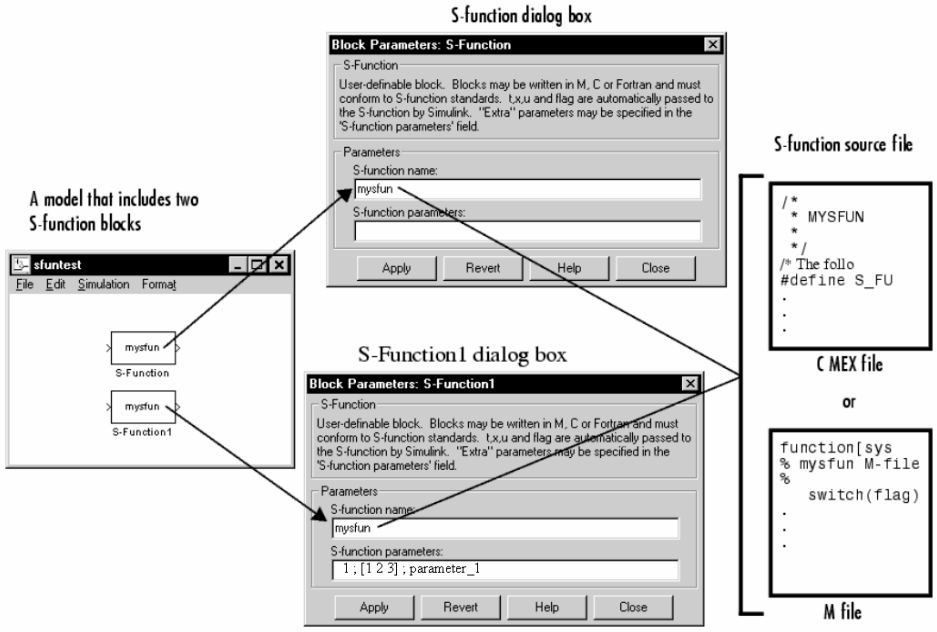

Figure 2.2: Relationship between an S-Function Block, its Dialog Box, and the Source File that defines the Block's bhavior. In this example, the model contains two instances of an S-Function block. Both blocks reference the same source file (mysfun, which can be either a C MEX-file or an M-file). If both a C MEX-file and an M-file have the same name, the C MEX-file takes precedence and is the file that the S-function uses. [From Simulink S-function manual]

To create S-functions, we need to know how S-functions work. Understanding how S-functions work, in turn, requires understanding how Simulink simulates a model, and this, in turn

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requires an understanding of the mathematics of blocks. The table 2.1 explains the mathematical relationship between a block's inputs, states, and outputs.

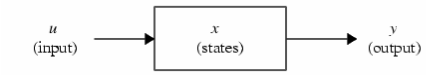
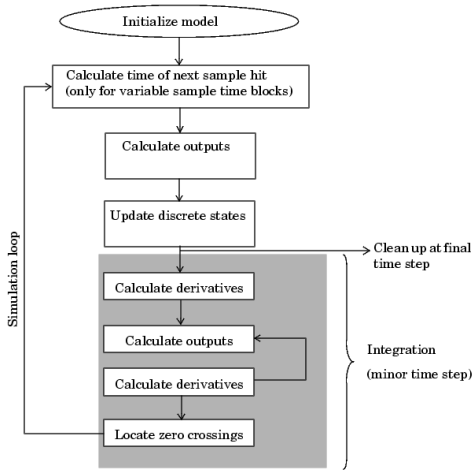
Mathematics of Simulink Blocks	**Simulation Stages**
A Simulink block consists of a set of inputs, a set of states, and a set of outputs, where the outputs are a function of the sample time, the inputs, and the block's states.  The following equations express the mathematical relationships between the inputs, outputs, and the states. $y = f_0(t, x, u)$ (Output) $\dot{x}_c = f_d(t, x, u)$ (Derivative) $x_{d_{k+1}} = f_u(t, x, u)$ (Update) where $x = x_c + x_d$	Execution of a Simulink model proceeds in stages. First comes the initialization phase. In this phase, Simulink incorporates library blocks into the model, propagates widths, data types, and sample times, evaluates block parameters, determines block execution order, and allocates memory. Then Simulink enters a simulation loop, where each pass through the loop is referred to as a simulation step. During each simulation step, Simulink executes each of the model's blocks in the order determined during initialization. For each block, Simulink invokes functions that compute the block's states, derivatives, and outputs for the current sample time. This continues until the simulation is complete. 

Table 2.1 How Simulink S-function works [From Matworks ™ website]

As previously said S-function can be coded using different languages. Each ones has its advantages and its drawbacks. We choose to develop our S-function in Matlab as its is a more simple language and more easily to integrate in Simulink simulations. The main drawback of Matlab coded S-function is that this function allows only one input (and output) argument (or signal, or flux). This function is coded into a classical M file.
An M-file S-function consists of a MATLAB function of the following form:

[sys,x0,str,ts]=f(t,x,u,flag,p1,p2,...)

where **f** is the S-function's name, **t** is the current time, **x** is the state vector of the corresponding S-function block, **u** is the block's inputs, **flag** indicates a task to be performed, and **p1**, **p2**, ... are the block's parameters. During simulation of a model, Simulink repeatedly invokes function f, using flag to indicate the task to be performed for a particular invocation (Table 2.1). Each time the S-function performs the task, it returns the result in a structure having the format shown in the syntax example.

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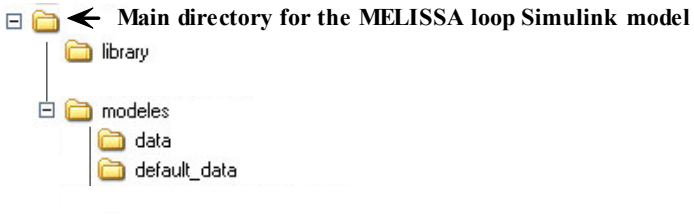
2.1.3 MELISSA LOOP MODELLING (PRINCIPLES)

The modelling of the loop with Simulink is simple in its principle but more complex in its development. The principle is to build **S-blocks** for each compartment of the loop and for special process operations (filtration, divider…), then to **link** the blocks with gas, liquid and solid matter fluxes and finally to **close** the loop with several loop operating constraints. In order to avoid the mixing of the files created for the modelling and during the simulation of the loop, the following directories hierarchy is used :



The S-blocks

Each block is build as a S-function block (as described above), thus a S-function (i.e. a M file) is created for each process. At this time we want only to perform mass-balance (i.e. steady-state) simulations of the loop; Thus in S-functions, only the "output" state must be defined (Figure 2.1). The models developed are then models which for a defined input calculate an output. For biological processes (MELiSSA compartments) the models are then the mass balance equations (stoichiometric equations) characterising each compartment. For each model, the building of the corresponding S-function (report to section 2.2) will follow always the same scheme (Figure 2.3):

1 – Initialising and recovery of process/reaction parameters

2 – Recovery of input compound and analysis of the composition if necessary (complex compound) using composition files

3 – Building of stoichiometric reactions

4 – Execution of the reactions using stoichiometric coefficients. This step takes into account the substrates limitations to avoid negative quantity of compounds and is always carried out by the function **"reaction.m**" by all S-functions. The reaction applies to each stoichiometric equation using a key compound for which is also given an efficiency yield (between 0 and 1). The objective of the reaction is to eliminate, if possible (depending of complete exhaustion of other limiting substrate), the key compound with the efficiency given. For example for efficiency of 0.5, the reaction tries to eliminate 50% of the key compound with the stoichiometric equation, and calculates the new mixture composition after the reaction.

5 – Calculation of outputs and creation of compositions files of complex products if necessary (i.e. residual organic matter, biomasses….). In bioreactor, the gas/liquid thermodynamic equilibria is also calculated by the function" **flash.m**". The flash function calculates for a mixture of compound the distribution of the compounds into 2 phases depending on their partition coefficient in the phases. Details on the principles of partition coefficients can be found in TN 17.1 and 23.1.

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The models and their respective S-functions will be detailed in the next sections. All files are located in "/library/" directory. **The S-blocks created for MELiSSA were also stored in a specific library called Melissa_block.mdl**.

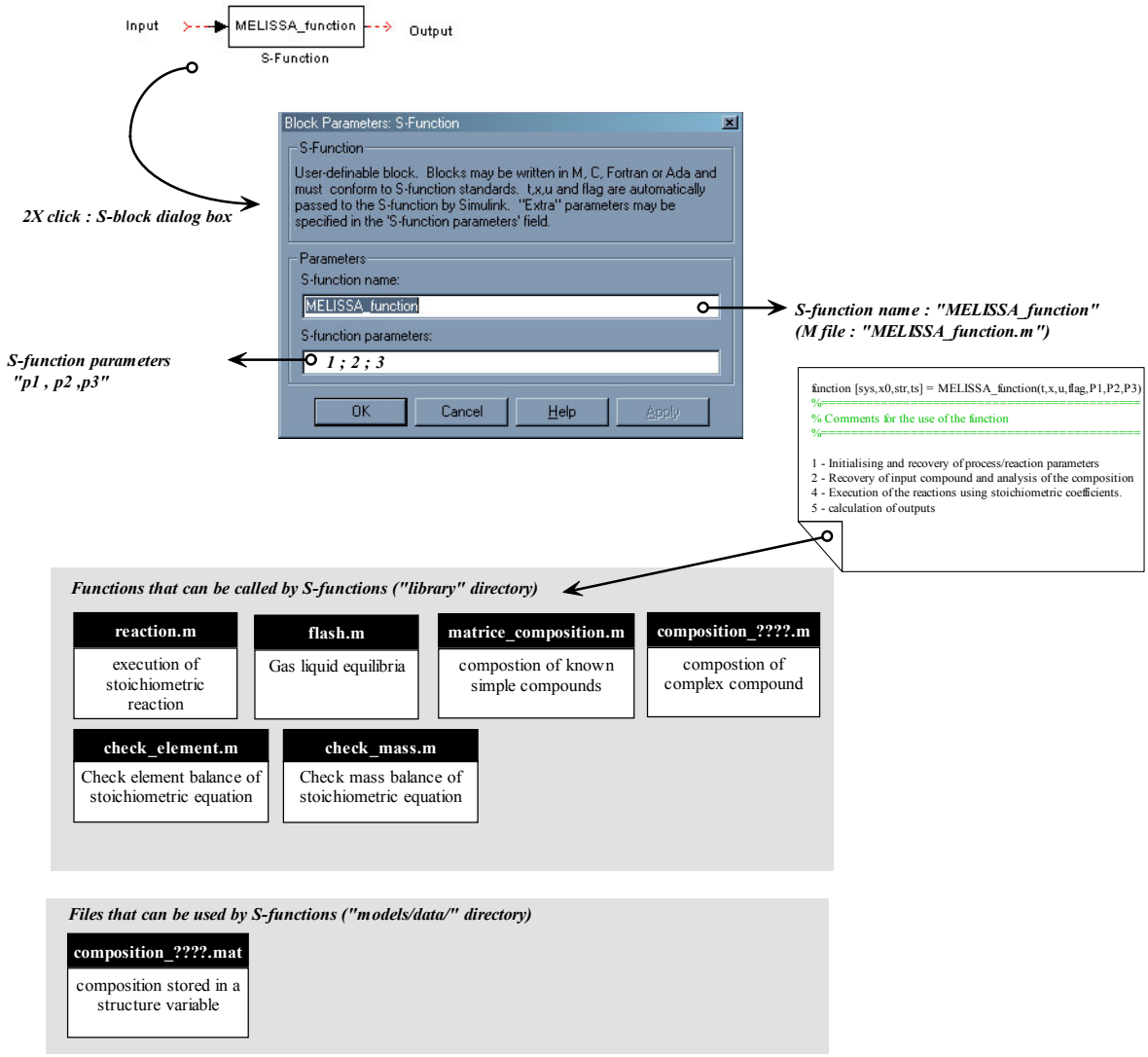

Figure 2.3 : Principles of S-Block for MELiSSA compartments

Linking S-blocks

The links between blocks consist in flows of matter. As the S-blocks (i.e. the process models) need to know what kind of matter it is, the flow are sorted for the whole loop and then inputs can be correctly recovered in S-functions. The list of compounds, their sorting in flow, and their elementary composition (when possible) are then fixed (Table 2.2). For several compounds, the elemental and macro-elemental (proteins, fat,…) composition cannot be determined "a priori". There is only 2 options for passing the composition information to the S-blocks : by links or by files. The second option is chosen as it is easiest to manage and reduce

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also the number of links between blocks. But it must be kept in mind that this option can probably not be conserved for a dynamic model of the loop. Then the variable composition of complex compound is exchanged between compartment model via ".MAT" files stored in the directory "/modeles/data/". These files contain a matlab variable stored into a "structure field" form.

Closing the loop

For closing the loop, it is necessary:

1 – To include sources and sinks at several points of the loop to avoid accumulation of compounds and to supply the loop in non recycled compounds

2 – To introduce constraints to fit requirements of a closed bioregenerative loop. This constraint concerns the liquid phase, the gas phase and the food for the crew. These constraints will be managed by "Management Unit" which are also built as S-Blocks. A fourth "Management Unit" is used for control of the recycling of organic matter in the loop.

Compounds list – (23 compounds list)	Name of compositions files for exchange [compound //created at]
1) water 2) NH3 + ionic forms 3) H2SO4 +ionic forms 4) H3PO4 + ionic forms 5) HNO3 + ionic forms 6) HNO2 + ionic forms 7) Urea 8) O2 9) CO2 + ionic forms 10) Acetic Acid 11) Propionic acid 12) Butyric Acid 13) Valeric Acid 14) Caproic Acid 15) N2 16) H2 17) CH4 18) Inert gas 19) Organic Matter 20) Nitrosomonas Biomass 21) Nitrobacter Biomass 22) Rhodobacter biomass 23) Spirulina Biomass	Composition_C4b_plante.mat [higher plant pool // C4b] Composition_C4b_waste.mat [higher plant wastes // C4b] Composition_nb.mat [nitrobacter biomass // C3] Composition_ns.mat [Nitrosomonas biomass // C3] Composition_OM_waste.mat [organic matter // mix from loop] Composition_onion.mat [onion //C4b] Composition_potato.mat [potato //C4b] Composition_rh_mat [rhodobacter biomass //C2] Composition_rice.mat [rice // C4b] Compostion_salad.mat [salad //C4b] Composition_soybean.mat [soybean // C4b] Composition_sp.mat [Spirulina biomass //C4a] Compostion_spinach.mat [spinach // C4b] Composition_tomato.mat [Tomato // C4b] Composition_wheat.mat [Wheat // C4b] Om_C1.mat [Organic matter // C1] **<u>Impotant</u> : These files are Matlab Format files. Variables are then directly store with their names and their values. The variables have a cell format.**

Table 2.2 : List (sorted) of compounds involved in the loop and list of files involved for exchanging information on compound composition. The "mat" files are stored in the directory "/modeles/data/" and are generated when simulation is running.

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2.2 Models of Compartments

Each model of the MELiSSA compartments for Simulink will be detailed here. In a first time, the layers of simulink subsystem blocks which define the compartment are described. Then the mass balance model and the associated S-function are detailed.

2.2.1 CREW

2.2.1.1 Description of the crew subsystem

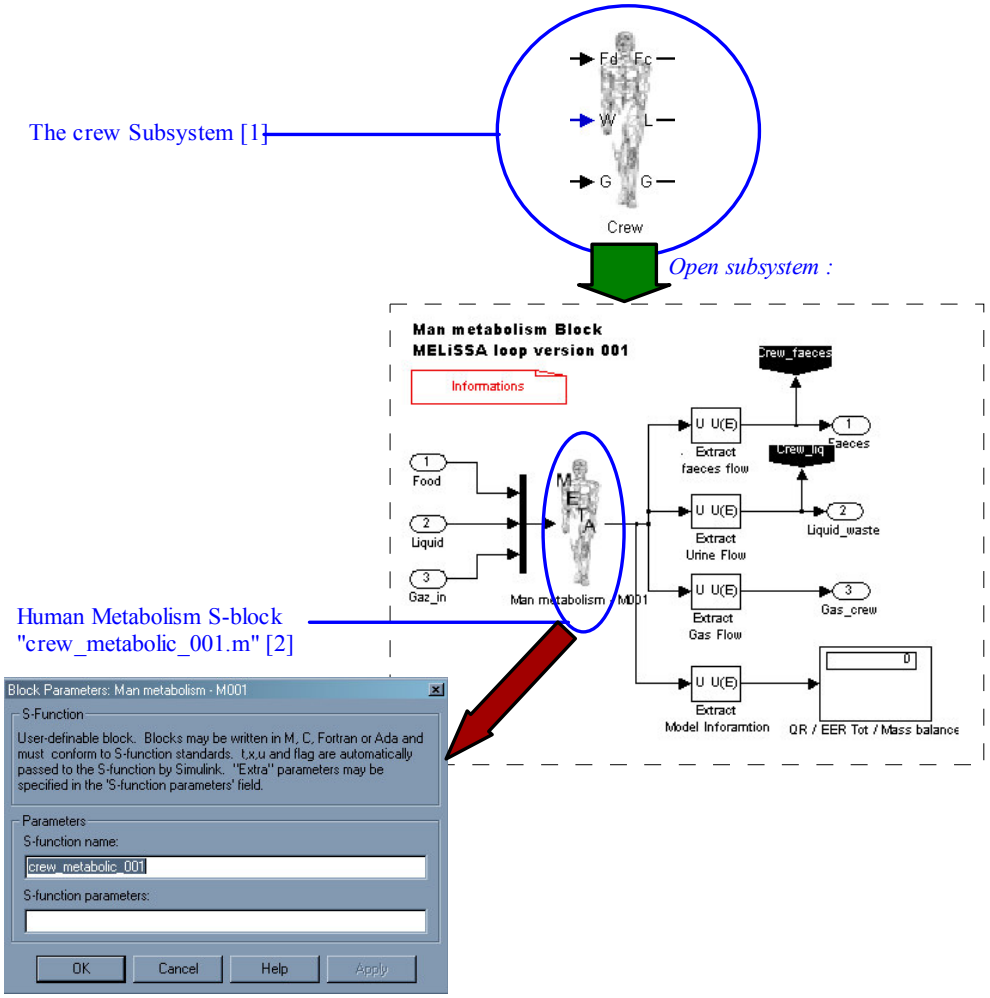

Figure 2.4 : The crew subsystem of the loop.

The layers of the crew compartment are presented in figure 2.4. The “crew subsystem” (Figure 2.4 [1]) has 3 inputs (Food , Liquid, Gas) and 3 outputs (Faeces , Urine , Gas). Liquid, Gas and Urine are flows built on the 23 compounds basis (Table 2.2). The flows Food and Faeces are

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specific flows which content is detailed in table 2.3. Inside the "crew subsystem" inputs flow are concatenated for the S-function block and the output of the blocks are splitted in order to produce the "crew subsystem" outputs. In this subsystem windows is recovered informations for the operation of the crew metabolic activity : QR (the respiratory quotient = CO_2/O_2) ; EER tot. (the crew Energy Expenditure Rate, in kcal/day) ; the mass balance on the calculations in the S-function.
In S-function block dialog box of "man metabolism M001", is given the name of the S-function: **crew_metabolic_m001**. There no parameters. The variables for the metabolism are directly given in the S-function.

Food Flow detail		Faeces flow detail
1) proteins (mass/day)	16) C_carbohyd	1)water faeces (mass/day)
2) C_proteins	17) H_carbohyd	2)faeces (mass/day)
3) H_proteins	18) O_carbohyd	3)C_faeces
4) O_proteins	19) N_carbohyd	4)H_faeces
5) N_proteins	20) S_carbohyd	5)O_faeces
6) S_proteins	21) P_carbohyd	6)N_faeces
7) P_proteins	22) fiber (mass/j)	7)S_faeces
8) lipids (mass/day)	23) C_fiber	8)P_faeces
9) C_lipids	24) H_fiber	9) % mass prot in faeces
10) H_lipids	25) O_fiber	10) % mass lip in faeces
11) O_lipids	26) N_fiber	11) % mass carb in faeces
12) N_lipids	27) S_fiber	12) % mass fiber in faeces
13) S_lipids	28) P_fiber	
14) P_lipids	29) water food (mass/day)	
15) carbohyd (mass/day))		

Table 2.3 : Details of specific flows of crew subsystem

2.2.1.2 Model of human metabolism (Version 0.0.1 /S-function crew_metabolic_001.m)

The **crew_metabolic_m001.m** matlab file is located in ./library directory. The function requires no more information other than the inputs and produces no result file.

The function solves 2 equations (Table 2.5) for which the stoichiometric coefficients are not fixed. In order to solve the equations several parameters are fixed. They are given in table 2.4, but can be changed in the function. This approach (Figure 2.5) allows having a variable food composition in the input.

Parameter **[Name in in crew_metabolic_m001.m]**	Value
Mass H2 produced / Mass Food consumed [**rdt_h2_food**]	0
Mass CH4 produced / Mass Food consumed **rdt_ch4_food**]	0
Mass Urea produced / Mass Food consumed [**rdt_uree_food**]	0.04
Fraction of Proteins not oxidised (i.e in Faeces) **[taux_residuel_prot]**	0.05
Fraction of Carbohydrate not oxidised (i.e in Faeces) **[taux_residuel_carb]**	0.01
Fraction of Fat not oxidised (i.e in Faeces) **[taux_residuel_lip]**	0.2
Fraction of fibre not oxidised (i.e in Faeces) **[taux_residuel_fib]**	1
Mass of water for persiparation **[eau_perspi]**	90% of input water

Table 2.4 : Parameters for the crew. They are fixed in the S-function

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$[CHONSP]Food + O2$ $\downarrow$ $CO2 + Urea + [CHONSP]Faeces + Water + H3PO4 + H2SO4 + NH3 + H2 + CH4$	Crew E-1
$LiquidWater \rightarrow PerspirationWater$	Crew E-2

Table 2.5 : Stoichiometric mass / Element balanced equations for the crew

The principle for solving Crew E-1 equation is summarised in figure 2.5. The solution for Crew E-2 equation is directly given by the parameter: mass of water for perspiration.

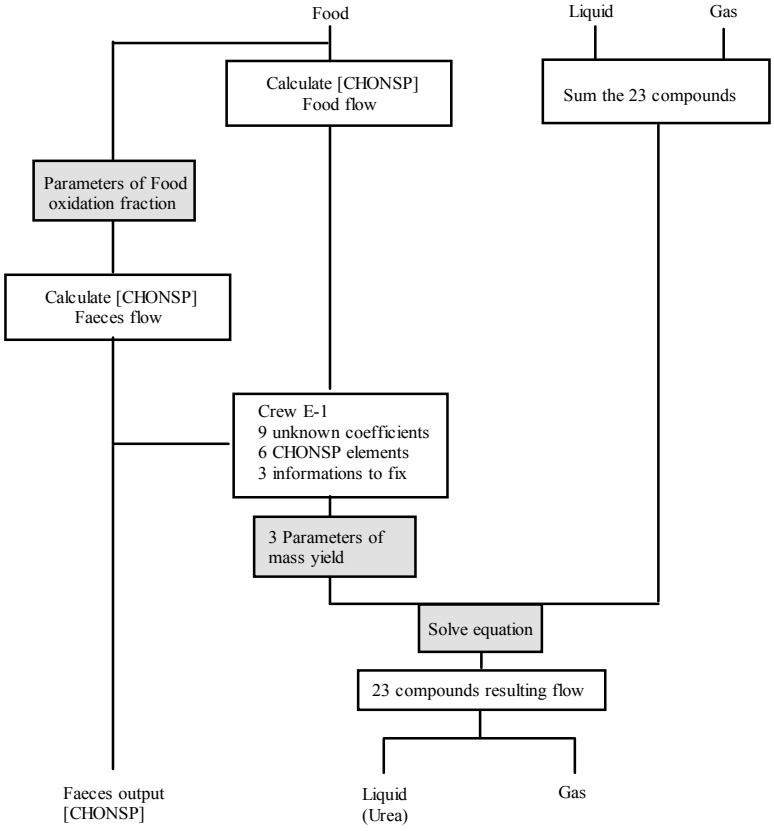

Figure 2.5 : Steps for solving Crew E-1

2.2.2 COMPARTMENT I

The first compartment is the trickiest MELiSSA compartment. The model presented here is not the final model. Moreover, the tests performed for the whole loop (report to chapter 3) indicate an unexpected behaviour of the compartment with this current model. The main critical points concerns the biomass production yields associated to the different step of anaerobic degradation.

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2.2.2.1 *Description of the C1 subsystem*

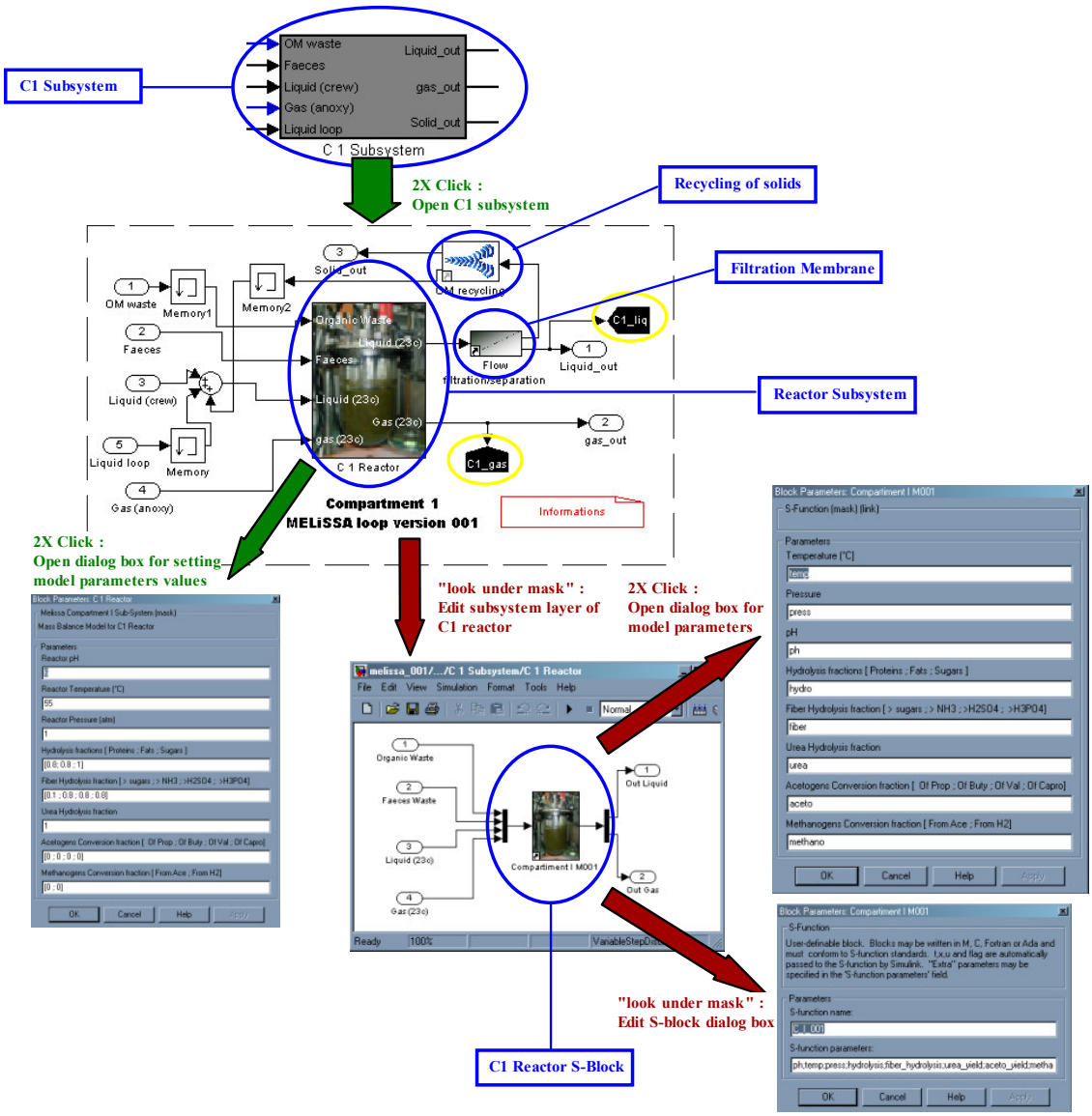

Figure 2.6 : C1 Subsystem. Details of subsystem layers. Red arrows ways are only used for development and building of the model. Green Arrows ways are the common operation for using the model and managing its parameters.

The compartment 1 subsystem is linked to the MELiSSA loop by 5 inputs and 3 outputs. The inputs are organic matter waste from the loop, Faeces from the crew, liquid form the crew (Urine), an anoxic gas flow and a liquid flow. The outputs are liquid, gas and solids corresponding to non recycled organic matter in the compartment. The liquid, gas and solid

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flow have the 23 compound format detailed in table 2.2. Faeces and input organic matter flow have the composition of the faeces flow of the crew subsystem, detailed in table 2.3.

The compartment 1 subsystem itself is built on the basis of the current general design for the compartment (TN 71.2). The reactor is fed with gas, liquid and organic matter. The liquid output of the reactor passes through a filtration membrane to separate solid (organic matter and biomass). A part of the solid is recycled to the reactor. This introduces an internal loop in the system. For technical reasons memory blocks were introduced in order to solve the loops, and these blocks mustn't be removed. Simulink sink blocks (black coloured and yellow circled) are used to measure the flow composition of outputs. These measurements will be further recovered after a simulation as results.
The 3 manageable elements of the C1 subsystem are: the **reactor**, the **filtration membrane** and the **solid recycling purge**. For each of them a dialog box allows to change several operating parameter and to set the reactor performances (Table 2.5). This is the normal use for managing the subsystem (report to chapter 3). Other changes in the design of the subsystem must be considered as a new model version for the complete loop and is not recommended excepted for advanced user of Matlab Simulink.

Reactor [Related equation]	Filtration Membrane	Purge
Reactor pH Reactor temperature Reactor Pressure Hydrolysis efficiencies for - Proteins [C1 E2-1] - Fats [C1 E2-2] - Sugars (carbohydrate) [C1 E2-3] Hydrolysis of Fibre - mass fraction hydrolysed into Sugar - N fraction hydrolysed into NH3 - P fraction hydrolysed into H3PO4 - S fraction hydrolysed into H2SO4 - Hydrolysis fraction of Urea into NH3 [C1 E1-1] Conversion Yield into acetic acid from: - Propionic ac., [C1 E3-1] - Butyric ac., [C1 E3-2] - Valeric ac., [C1 E3-3] - Caproic ac. [C1 E3-4] Conversion yield efficiency of acetic ac. into methane [C1 E4-1] Conversion yield efficiency of H2 into methane [C1 E4-2]	For each compound identified by its index (table 2.2) is given a separating capacity (between 0 and 1, 1 meaning the compound is retained in the first output flow). By default separating capacity is 0. Example : *Compound index*: **[10 ; 20]** *Separating capacity:* **[1 ; 0.5]**	This is a flow separation. The value given (between 0 and 1) gives the fraction of input for the first output flow, i.e. the fraction of solid recycled

Table 2.5 : List of modifiable parameters for C1 model in dialog boxes

For modifying the compartment model it may be necessary to modify also the C1 reactor S-block. It can be reached by "*looking under mask*" of the C1 reactor (right click on the block) in the C1 subsystem. The parameters for the S-function are given as matrix which names are defined in the S-block dialog box. The S-function parameter dialog box lists the name of the S-

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function (**C_I_001**) and the parameters passed to the function (names defined in the parameter dialog box).

2.2.2.2 Model of C1 reactor (Version 0.0.1 /S-function C_I_001.m)

The **C_I_001.m** matlab file is located in ./library directory. The S-function requires several parameters allowing to define the process efficiencies. It uses and creates also several data files located in /modele/data/. Even if it is given as parameter, the pH is not used at this time to calculate physico-chemical equilibria. Temperature and pressure are used only for the calculation of the water partial pressure; the other gas/liquid equilibria are fixed.

The function solves the equations for an anaerobic digestion (Table 2.6). The model for an anaerobic digestion process with autochthonous strains is not simple and the model for the compartment remains under study. The stoichiometric coefficients and the compositions of the macromolecules are defined in the program (function **C_1_001**). They can be changed, i.e. equations can be modified, and this will result in a new model for the compartment. The principle for modelling the Compartment 1 is summarised in figure 2.7.

The first step for solving the equations is to fix qualitatively **and** quantitavely the composition of the macromolecules (namely proteins, fat and carbohydrates) of the feed. Knowing a theoretical CHONSP mean composition for the macromolecules (Table 2.6) and their quantitative composition (i.e. mass) in the feed, a theoretical CHONSP composition for the feed is calculated and compared to the CHONSP composition of the feed in the input. Calculations were made in order to fit this CHONSP by using a variable fibre CHONSP composition and by changing if necessary the mass fractions of macromolecules.
The second step re-calculates the fibre part and composition, accordingly to its degradation into usable carbohydrate, ammonia, phosphate and sulphate. This degradation is fixed by parameters given in the reactor parameters dialog box (Table 2.5 and Figure 2.6).
With the third calculation step start the first stage of the classical anaerobic degradation. All the equations of anaerobic degradation (Table 2.6) are controlled by a degradation efficiency rate given in the reactor parameters dialog box (Table 2.5).
At the end, the non-degraded organic matter is added with the biomass. This whole is considered as “solid residue” and stored as compound number 19 in the 23-compounds list (Table 2.2). The composition of this “solid residue” as proteins, lipids, carbohydrates and fibre parts is stored in file **om_C1.mat** and file **composition_OMwaste.mat**. A part of this residue may be recycled in the reactor, and in such a case its degradability is taken as for the other organic substrates.
After the reactions, the gas/liquid thermodynamic equilibriums (composition of the gas and of the liquid) were calculated from the gas/liquid partition coefficients of each compound and the global composition of the mixture by the **flash** function.

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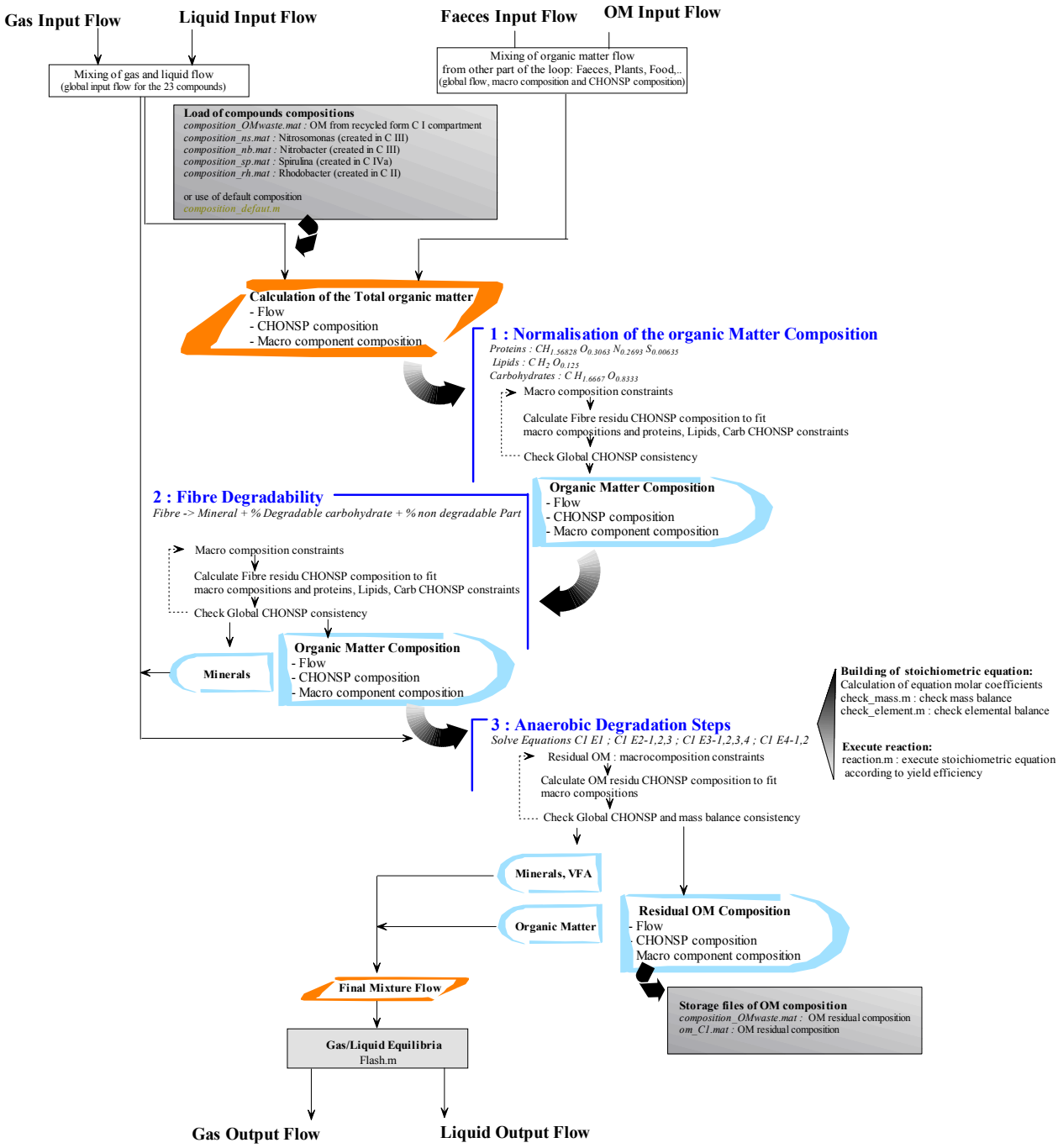

Figure 2.7 : Steps of calculations for C1_001 mass balance model.

Stoichiometric equation for C_1_001 model	Equation
$CH_4ON_2 + H_2O \rightarrow CO_2 + 2NH_3$	C1 E1

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$[CHONS]_{OM\_Prot} + 0.5539\,H_2O \Downarrow 0.0241[CHONSP]_{Bio\_AA} + 0.16373\,CH_3COOH + 0.0612\,C_2H_5COOH + 0.019\,C_3H_7COOH + 0.0177\,C_4H_9COOH + 0.01734\,C_5H_{11}COOH + 0.11816\,CO_2 + 0.1074\,H_2 + 0.2489NH_3$	C1 E2-1
$6.546\ [CHONSP]Carbo + 0.1091NH_3 + 0.6426 \longrightarrow 0.1091[CHONSP]_{Bio\_sugar} + 0.6667\text{Acetate} + 1.3333\text{Propionate} + 0.6667CO_2$	C1 E2-2
$0.95\ [CHON]_{lipids} + 0.05\,NH_3 + 0.68125\,H_2O \longrightarrow 0.05[CHONSP]_{Bio\_LCFA} + 0.83125\,H_2 + 0.35\,CH_3COOH$	C1 E2-3
$C_2H_5COOH + 1.85\,H_2O + 0.05\,NH_3 \longrightarrow 0.05[CHONSP]_{Bio\_HCFA} + CO_2 + 3\,H_2 + 0.875\,CH_3COOH$	C1 E3-1
$C_3H_7COOH + 1.85\,H_2O + 0.05\,NH_3 \longrightarrow 0.05[CHONSP]_{Bio\_HCFA} + 2\,H_2 + 1.875\,CH_3COOH$	C1 E3-2
$C_4H_9COOH + 3.85\,H_2O + 0.05\,NH_3 \longrightarrow 0.05[CHONSP]_{Bio\_HCFA} + CO_2 + 5\,H_2 + 1.875\,CH_3COOH$	C1 E3-3
$C_5H_{11}COOH + 3.85\,H_2O + 0.05\,NH_3 \longrightarrow 0.05[CHONSP]_{Bio\_HCFA} + 4\,H_2 + 2.875\,CH_3COOH$	C1 E3-4
$0.5\,CO_2 + 1.8909\,H_2 + 0.0109\,NH_3 \longrightarrow 0.0109\,[CHONSP]_{Bio\_Methano} + 0.4452\,CH_4 + 0.978\,H_2O$	C1 E4-1
$CH_3COOH + 0.022\,NH_3 \longrightarrow 0.022\,[CHONSP]_{Bio\_Aceto} + 0.945\,CO_2 + 0.945\,CH_4 + 0.066\,H_2O$	C1 E4-2

Table 2.6 : Anaerobic degradation equation solved in the C1 model. The equations C1 E2-1, C1 E2-2, C1 E2-3 apply for the degradable fraction of respectively proteins, carbohydrate and lipids. The theoretical compositions of macromolecules are:
$[CHONSP]_{OM\_roteins}=CH_{1.56828}O_{0.3063}N_{0.2693}S_{0.00635}$
Lipids : $[CHONSP]_{Lipids}=CH_2O_{0.125}$
Carbohydrates : $[CHONSP]_{OM\_carbo}=CH_{1.6667}O_{0.8333}$
Biomass : $[CHONSP]_{Bio}=C_5H_7O_2N$
Fibre/Non degraded residue : Composition calculated in program

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2.2.3 COMPARTMENT II

As the compartment is colonized by a single well-known strain, the steady-state mass balance model of the compartment is not really complex. But it must be kept in mind that the dynamic model that stills under development and is actually difficult to establish.

2.2.3.1 Description of the C2 subsystem

The compartment 2 subsystem is linked to the MELiSSA loop by 2 inputs and 4 outputs. The inputs are liquid and anoxic gas flow from compartment 1. The outputs are liquid, a gas flow to the next compartment, an anoxic gas flow recycled to the C1 compartment and solids corresponding to the dry biomass produced in the compartment. All flows have the 23 compound format detailed in table 2.2. The subsystem is composed of 3 units: the **C2 reactor**, a **filtration unit** for the biomass and a **gas flow divider** to recycle a part of the anoxic gas to C1 compartment. Operating conditions of these units are manageable using their dialog box (Table 2.8). If light is a parameter, it must be noticed that the current mass balance model didn't include the effect of light.

Reactor [Related equation]	Filtration system	Gas distribution system
Reactor pH Reactor temperature Reactor Pressure Reactor Ligth flux intensity Acetic ac. Assimilation yield [C2 E1] Propionic ac. Assimilation yield [C2 E2] Butyric ac. Assimilation yield [C2 E3] Valeric ac. Assimilation yield [C2 E4] Caproic ac. Assimilation yield [C2 E5]	For each compound identified by its index (table 2.2) is given a separating capacity (between 0 and 1, 1 meaning the compound is retained in the first output flow). By default separating capacity is 0. For the Rhodobacter biomass *Compound index*: **[22]** *Separating capacity* **[1]**	This is a flow separation. The value given (between 0 and 1) gives the fraction of input for the first output flow, i.e. the gas flow to C3

Table 2.7 : List of modifiable parameters for C2 model in the C2 reactor dialog box

	% mass (TN 23.3)	% mass without ash (a)	CHONSP
Protein	48.9	52.29	$CH_{1.5685}O_{0.3061}N_{0.2694}S_{0.0064}$
Carbohydrates	12.13	14.44*	$CH_{1.5405}O_{0.1892}$
Lipids	13.53	19.93**	$CH_{1.9223}O_{0.2153}P_{0.0263}$
DNA	3.73	4.01	$CH_{1.2585}O_{0.6205}N_{0.3961}P_{0.1034}$
RNA	8.40	9.03	$CH_{1.2295}O_{0.7256}P_{0.1043}$
PHB	1.30	** equivalent lip	-
Glycogen	5.00	* equivalent carb.	-
Ash	7.00	0	-

Table 2.8 : Rhodobacter biomass composition. The effect of light is not taken into account at this time. (a) is the composition used in composition_rh.m.

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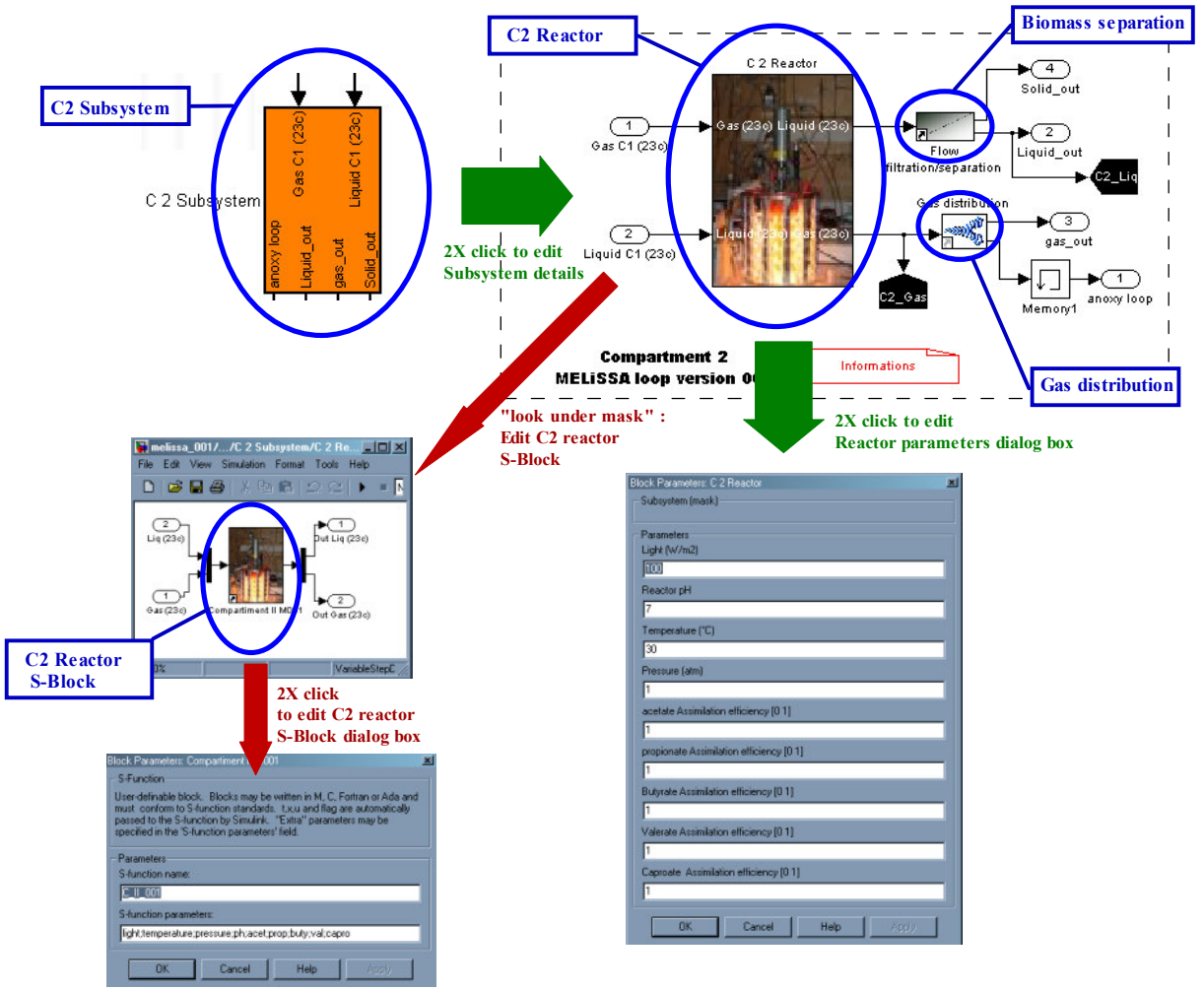

Figure 2.8: C2 Subsystem. Details of subsystem layers. Red arrows ways are only used for development and building of the model. Green Arrows ways are the common operation for using the model and managing its parameters.

2.2.3.2 Model of C2 reactor (Version 0.0.1 /S-function C_II_001.m)

The **C_II_001.m** matlab file is located in ./library directory. The S-function requires several parameters allowing to define the process efficiencies. The biomass composition (macromolecule mass percentage and composition) is taken from TN 23.3 (Table 2.8) and is calculated by the function composition_rh (composition_rh.m file). This composition is stored at each calculation step in **composition_rh.mat** data file located in /modele/data/ directory. Light and pH parameters are not used in this model version. Temperature and pressure are only used for calculation of the water partial pressure.

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The principle for modelling the Compartment 2 is summarised in figure 2.9. The function solves the 5 equations for the assimilation of VFA produced by the first compartment into biomass (Table 2.9). As it is not a dynamic model, the system of equations is solved sequentially from equation C2 E1 to C2 E5. This means that a limitation that don't appears for the first reaction (N limitation for example), may occur for the last one which then may be incomplete (i.e. caproic acid is not completely degraded).
Each equation is associated to a conversion yield for the main substrate (VFA) of the reaction (Table 2.8). This conversion yield gives the relative fraction of the compound converted in the reaction. It can be noticed that in table 2.9 the stoichiometric coefficients of the reactions are not indicated. If at this time the biomass composition is fixed, it is possible that the biomass changes with the light. Then instead of fixing a stoichiometric equation, it was chosen to recalculate at each time the stoichiometric coefficients (rebuild the reaction) in order to be able to take into account a variable composition of the biomass. To solve the equations presented in table 2.9 it is not necessary to give additional information on the reaction (6 compounds and 6 unknown coefficients).
After reactions, the gas and liquid flows were calculated by the **flash** function from the compound mixture.

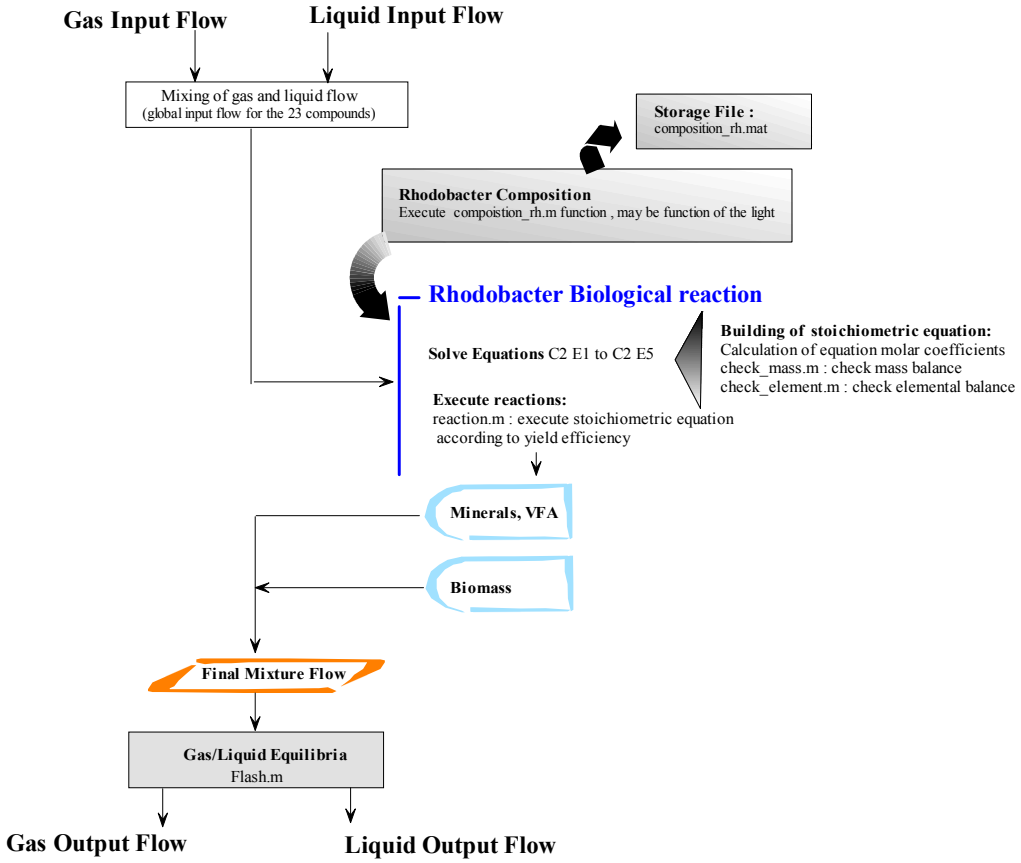

Figure 2.9 : Steps of calculations for C2_001 mass balance model

Stoichiometric equation for C_II_001 model	Equation

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1 Acetic ac + ? NH3 + ? H2SO4 + ?H3PO4 → ? $[CHONSP]_{Biomass\_Rh}$ + ? CO2 +? H2O	C2 E1
1 Propionic ac + ? NH3 + ? H2SO4 + ?H3PO4 → ? $[CHONSP]_{Biomass\_Rh}$ + ? CO2 +? H2O	C2 E2
1 Butyric ac + ? NH3 + ? H2SO4 + ?H3PO4 → ? $[CHONSP]_{Biomass\_Rh}$ + ? CO2 +? H2O	C2 E3
1 Valeric ac + ? NH3 + ? H2SO4 + ?H3PO4 → ? $[CHONSP]_{Biomass\_Rh}$ + ? CO2 +? H2O	C2 E4
1 Caproic ac + ? NH3 + ? H2SO4 + ?H3PO4 → ? $[CHONSP]_{Biomass\_Rh}$ + ? CO2 +? H2O	C2 E5

Table 2.9 : Compartment 2 mass balance equations . "?" are unknown stoichiometric coefficients that can be calculated if $[CHONSP]_{Biomass\_Rh}$ is known. The equations are solved in the S-function.

2.2.4 COMPARTMENT III

The third compartment is a co-culture of Nitrosomonas and Nitrobacter, caring respectively the oxidation of ammonia to nitrite and nitrite to nitrate. The difficulty for the mass balance modelling of these reactions is the coupling of the two reactions, which is obvious in a dynamic model but need to be fixed in a mass balance model.

2.2.4.1 Description of the C3 subsystem

The compartment 3 subsystem is linked to the MELiSSA loop by 3 inputs and 3 outputs. The inputs are a liquid flow from the previous compartment, an oxygenic gas flow (reactions need oxygen), and second liquid flow for supplying the compartment with nutrients form other part of the loop. The outputs are liquid, a gas flow to the next compartment, and solids corresponding to the dry biomass produced in the compartment. It can be noticed here that in fact the biomass would stays fixed in the reactor, but this will lead to a mass accumulation in the reactor and in the loop, what can give mass balance calculations difficult to analyse. In the future, it is probable that mass accumulation needs to be introduced in models. All flows have the 23 compound format detailed in table 2.2. The subsystem is composed of 2 units: the **C3 reactor** and a **filtration unit** for the biomass separation. Operating conditions of these units are manageable using their dialog box (Table 2.10).

Reactor [Related equation]	Filtration system
Reactor pH Reactor temperature Reactor Pressure NH3 assimilation yield [C3 E1] HNO2 assimilation yield [C3 E2]	For each compound identified by its index (table 2.2) is given a separating capacity (between 0 and 1, 1 meaning the compound is retained in the first output flow). By default separating capacity is 0. For the Nitrosomonas and Nitrobacter biomass *Compound index*: **[20 ; 21]** *Separating capacity* **[1 ; 1]**

Table 2.10 : List of modifiable parameters for C3 model in the C3 reactor dialog box

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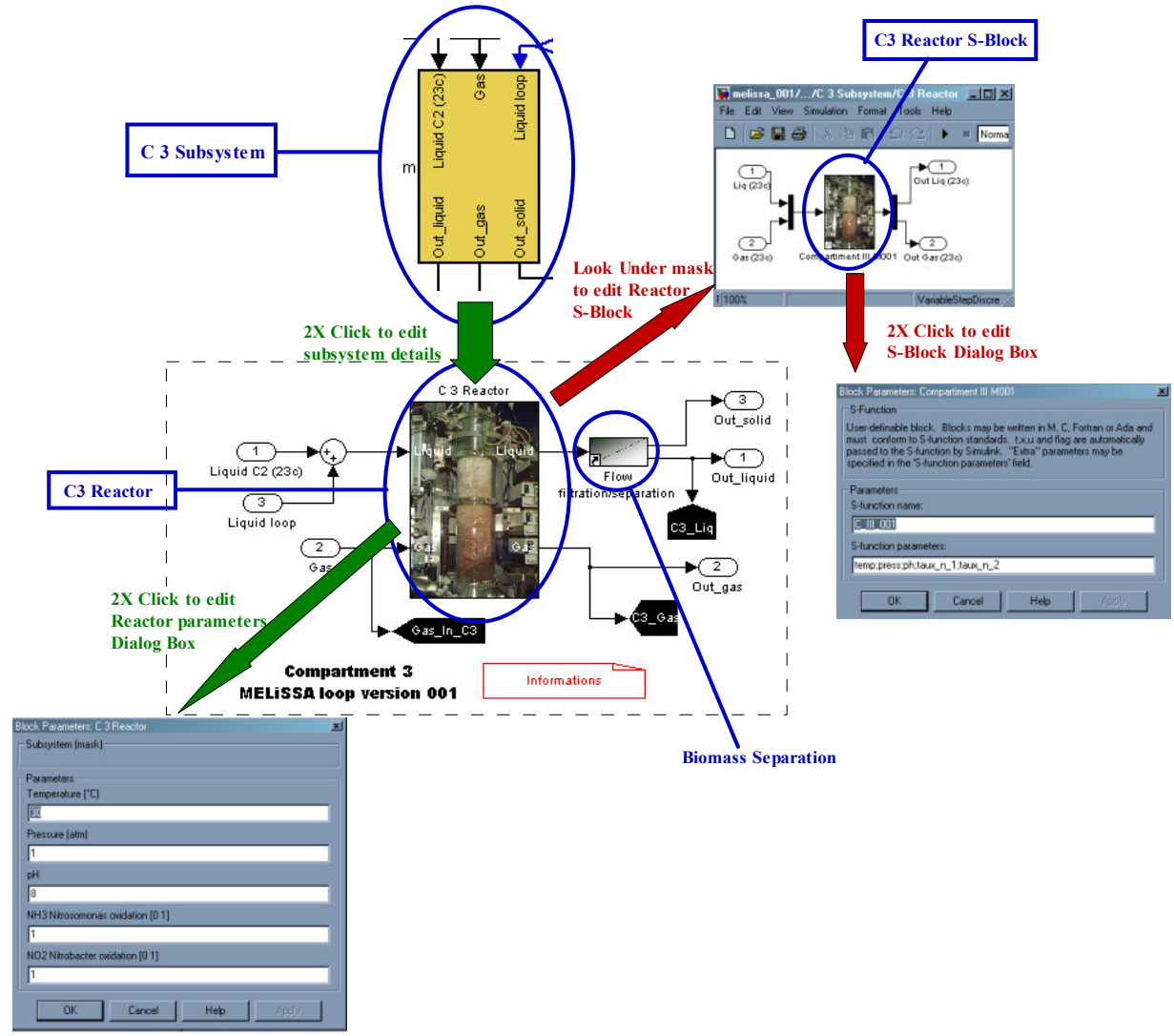

Figure 2.10 : C3 Subsystem. Details of subsystem layers. Red arrows ways are only used for development and building of the model. Green Arrows ways are the common operation for using the model and managing its parameters.

2.2.4.2 Model of C3 reactor (Version 0.0.1 /S-function C_III_001.m)

The **C_III_001.m** matlab file is located in ./library directory. The S-function requires several parameters to define the process efficiencies (Table 2.10). pH parameter is not used in this model version. Temperature and pressure are only used for calculation of the water partial pressure.

The biomass composition of the two strains (macromolecule mass percentage and composition) is taken identical to the composition of Rhodobacter (Table 2.8). This is not much more false than taking a "mean biomass composition ($C_5H_7O_2N$)". The compositions are respectively calculated by the function composition_ns (composition_ns.m file) for Nitrosomonas and composition_nb (composition_nb.m file) for Nitrobacter. These compositions are stored at each

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calculation step in **composition_ns.mat** and **compostion_nb.mat** data files located in /modele/data/ directory.

The principle for modelling the Compartment 3 is summarised in figure 2.11. The function solves the 2 equations for the nitrification (Table 2.11). The nitrification is more the result of the oxidation of ammonia (respectively nitrite) for energy maintenance metabolism of Nitrosomonas (respectively Nitrobacter) than the result of the growth of the micro-organisms. Then it was shown that the N-oxidation for maintenance is an important parameter in the building a global mass balance equation (TN 27.1). For this reason, for each strain is considered the anabolic growth equation and the maintenance equation. The two equations being coupled by maintenance yield, leading to a single equation (Table 2.11). The dynamic model developed on the basis of the Beefting equations is also built on this approach (TN 27.1). The maintenance yield is not considered as an operating process parameter but as a model constant. Thus the value is fixed directly in the function (but can be changed as for yields given in compartment 1).
As for the second compartment, the stoichiometric coefficient of the growth reaction are not fixed in the function, but calculated, as it was taken into account the possibility to change the biomass composition. To solve the equations presented in table 2.11 it is not necessary to give additional information, other than the maintenance yield, on the reaction if the biomass composition is known (6 compounds and 6 unknown coefficients).
When the two equations C3 E1 and C3 E2 were established in the S-function, they are coupled together in order to solve the nitrification in a single step. By this approach, the two nitrification equations are considered to occur simultaneously and not sequentially as it was done with the second compartment model. The coupling of the two reactions is based on the elimination of nitrite:

$$\text{Coupling} = \frac{HNO_2 \text{ stoichiometric coefficient in C3 E1}}{HNO_2 \text{ stoichiometric coefficient in C3 E2}} * HNO_2 \text{ elimination efficiency}$$

And the stoichiometric coefficients of the global equation are obtained by:

$$\text{Global stoichiometric coefficient} = \text{C3 E1 stoichiometric coefficient} + \text{Coupling} * \text{C3 E2 stoichiometric coefficient}$$

After the reaction, the gas and liquid flows were calculated by the **flash** function from the obtained compound mixture.

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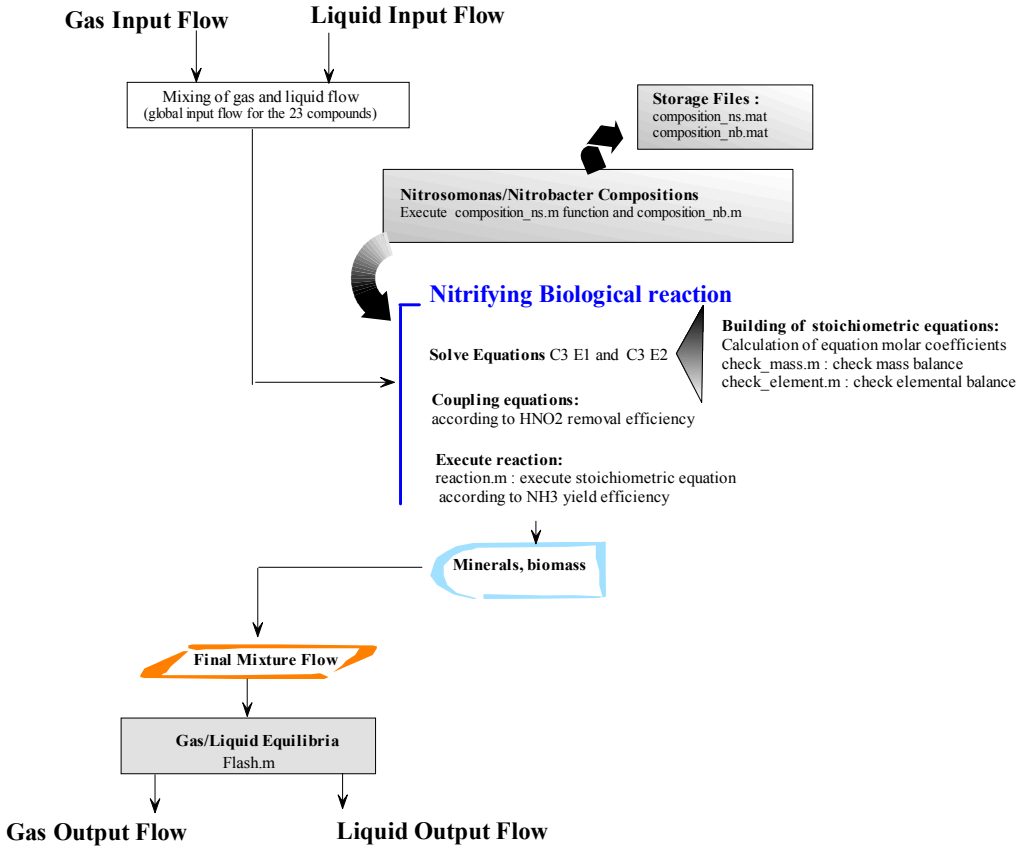

Figure 2.11 : Steps of calculations for C3_001 model

Stoichiometric equation for C_III_001 model	Equation **[S-Function parameter name]**
$"?"CO_2+"?"O_2+\left[\frac{3.6292}{1-Y_{NH3\_maint}}\right]NH_3+"?"H_2SO_4+"?"H_3PO_4 \Downarrow [CHONSP]_{Biomass\_Ns}+"?"H_2O+"?"HNO_2$	C3 E1 Y_{NH3_maint}=0.76 **[taux_maintenance_ns]**
$"?"CO_2+"?"O_2+\left[\frac{15.8398}{1-Y_{HNO2\_maint}}\right]HNO_2+"?"H_2SO_4+"?"H_3PO_4 \Downarrow [CHONSP]_{Biomass\_Nb}+"?"H_2O+"?"HNO_3$	C3 E2 Y_{HNO2_maint}=0.81 **[taux_maintenance_nb]**

Table 2.11: Compartment 3 mass balance equations. Y_{NH3_maint} is the fraction of NH3 oxidized for maintenance, and Y_{HNO2_maint} is the fraction of HNO2 oxidized for maintenance. The values given are those used in the current model (TN 27.1).

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2.2.5 COMPARTMENT IVA

Compartment IVa is the Spirulina (or photosynthetic) compartment of the loop. It is colonized by the cyanobacteria *Arthrospira platensis*. The composition of the biomass depends on the light intensity. The mass balance model previously developed is used (TN 17.3). There is only one stoichiometric equation for modelling the cyanobacteria activity which coefficients vary with the biomass composition (i.e. with the light).

2.2.5.1 Description of the C4a subsystem

The compartment 4a subsystem is linked to the MELiSSA loop by 2 inputs and 3 outputs (Figure 2.12). The inputs are liquid and gas flow from compartment 3. The outputs are liquid, a gas flow to the next compartment, and solids corresponding to the dry biomass produced in the compartment. All flows have the 23 compound format detailed in table 2.2. The first layer of the subsystem is composed of other 2 subsystems: the **C4a reactor subsystem** and a **HNO3 constraint subsystem.**

The objective of the constraint subsystem is to supply the bioreactor with HNO_3 (nitrate) which is used in the modelling as the key compound in the reaction (i.e. the reaction is based on the assimilation of nitrate with a defined efficiency). The supply of nitrate is drive by the request of a protein production by the Spirulina compartment (Figure 2.12). This request is calculated by the **Food Management Subsystem** of the loop. Then, the **productivity** of the compartment is control by the "proteins from Spirulina" in the Crew diet. It is important to notice that this approach already used in the previous version of the MELiSSA Loop model, is not the approach of the management of productivity (by light) by the control of atmosphere, as it is the case in the BioRat experiments. This choice has important consequences on the design of the loop. The model of the constraint subsystem itself only efficient if the operation of the loop doesn't conflict with the control of proteins production of Spirulina by addition of HNO_3. For example, operating the loop by wasting all the Spirulina biomass and trying to have Spirulina proteins in the diet failed. The current constraint model may also fail if the reaction is limited by another substrate. The model will not be detailed here but it may be improved.

The C4a reactor subsystem is composed of 2 units: the **C4a Reactor** and the **biomass separation** unit. Operating conditions of these units are manageable using their dialog box (Table 2.12).

Reactor [Related equation]	Filtration system
Reactor pH Reactor temperature Reactor Pressure Reactor Light flux intensity HNO3. Assimilation yield [C4a E1]	For each compound identified by its index (table 2.2) is given a separating capacity (between 0 and 1, 1 meaning the compound is retained in the first output flow). For the Spirulina biomass *Compound index*: **[23]** *Separating capacity* **[1]**

Table 2.12 : List of modifiable parameters for C4a model in the C4a reactor dialog box

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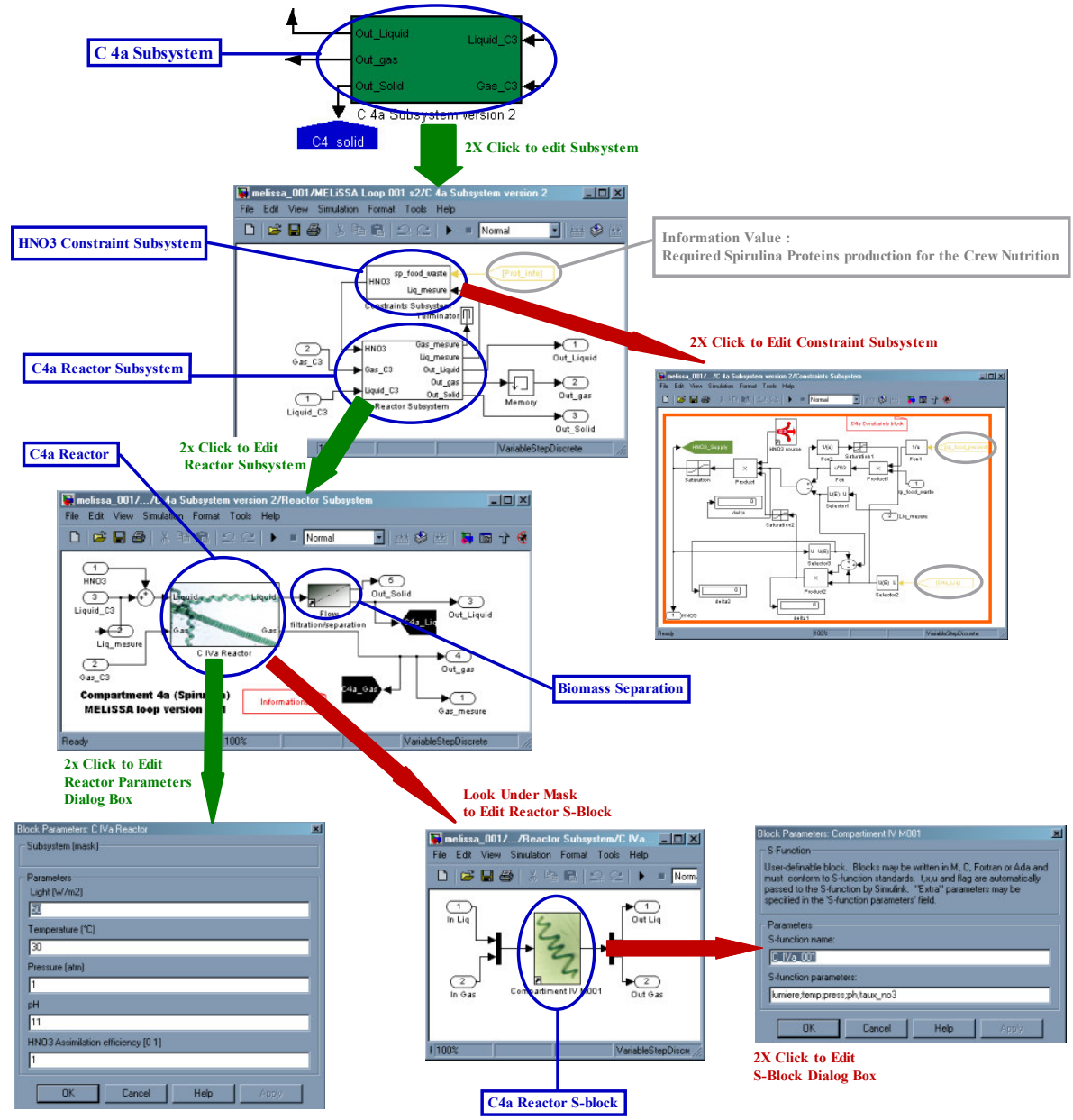

Figure 2.12 : : C4a Subsystem. Details of subsystem layers. Red arrows ways are only used for development and building of the model. Green Arrows ways are the common operation for using the model and managing its parameters. Gray colour underlines information from Management Units, used to setup the constraint Subsystem.

2.2.5.2 Model of C4a reactor (Version 0.0.1 /S-function C_IVa_001.m)

The **C_IVa_001.m** matlab file is located in ./library directory. The S-function requires several parameters allowing to define the process efficiencies (table 2.12). The biomass composition (macromolecule mass percentage and composition) is light dependent and is calculated by the function composition_sp (composition_sp.m file). The relation biomass composition/ light is

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taken from TN 17.3 (Table 2.13). This composition is stored at each calculation step in **composition_sp.mat** data file located in /modele/data/ directory. pH parameters is not used in this model version. Temperature and pressure are only used for calculation of the water partial pressure.

The principle for modelling the Compartment 4a is summarised in figure 2.13. The function solves the equation for the assimilation of HNO3 (Table 2.14) for which the coefficients are calculated as a function of the biomass composition, i.e. as a function of light. The reaction is carried out in order to assimilate HNO3 with a given yield efficiency (Table 2.12)
After the reaction, the gas and liquid flows were calculated by the **flash** function from the compound mixture.

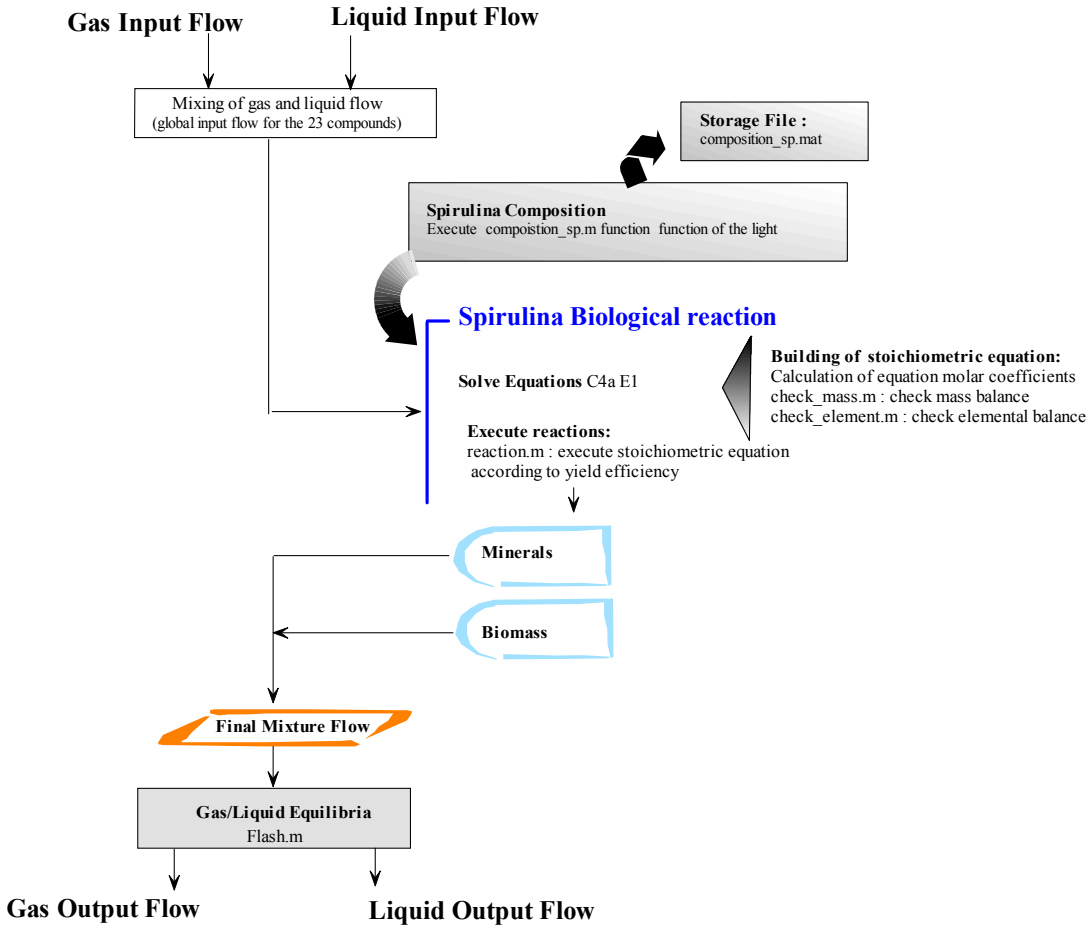

Figure 2.13 : Steps of calculations for C_IVa_001 model

	% mass (TN 17.3)	CHONSP
Protein	% mP=0,96 (-0,1067 Fo + 66,088)	$CH_{1,526}O_{0,327}N_{0,2496}$

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Lipides	% mF=9,6	$CH_{1,714}O_{0,204}$
Carbohydrates	% mC=0,96 (100 - % mP - % mF- % mE)	$CH_{1,670}O_{0,711}$
DNA	% mAN=0,04 (100 - % mE)	$CH_{1,273}O_{0,701}N_{0,393}$
Exopolysaccharid (Carbohydrate equivalent)	% mE=0,110 Fo + 9,028	$CH_{1,650}O_{0,950}$

Table 2.13 : Spirulina biomass composition. The effect of light is not taken into account at this time. The whole composition calculation is carried out in composition_sp.m. Fo is the light intensity (W/m^2)

Stoichiometric equation for C_IVa_001 model	Equation
1 CO2 + ? HNO3 + ? H2SO4 + ?H3PO4 → ? $[CHONSP]_{Biomass\_Sp}$ + ? O2 +? H2O	C4a E1

Table 2.14 : Compartment 4a mass balance equation. "?" are unknown stoichiometric coefficients that can be calculated if $[CHONSP]_{Biomass\_Sp}$ is known. The equation is solved in the S-function.

2.2.6 COMPARTMENT IVB

This compartment is the higher plant compartment of the loop. The model used is based upon the mass balance model previously detailed for the MELiSSA loop in the Technical Note 32.3. The higher plant chamber (or greenhouse) is composed of a set of 8 higher plants. It must be kept in mind that the greenhouse is not a bioreactor, and then can not be treated in the exact same way as the other MELiSSA compartment.

2.2.6.1 Description of the C4b subsystem

The compartment 4b subsystem is linked to the MELiSSA loop by 2 inputs and 4 outputs (Figure 2.14). The inputs are liquid and gas flow. The outputs are liquid and gas flow, and flows corresponding respectively to the harvested plants (useable for food) and their waste (i.e. roots, some leaves and stem) that cannot be use for food purposes. All liquid and gas flows have the 23 compound format detailed in table 2.2. The plants flows have a specific format detailed in table 2.15. A third input flow is used to link the compartment with the Food Management Unit. This input gives the information for the productivity objective of the greenhouse which is calculated by the Food Management Unit. This information acts as a constraint for the operating of the compartment.

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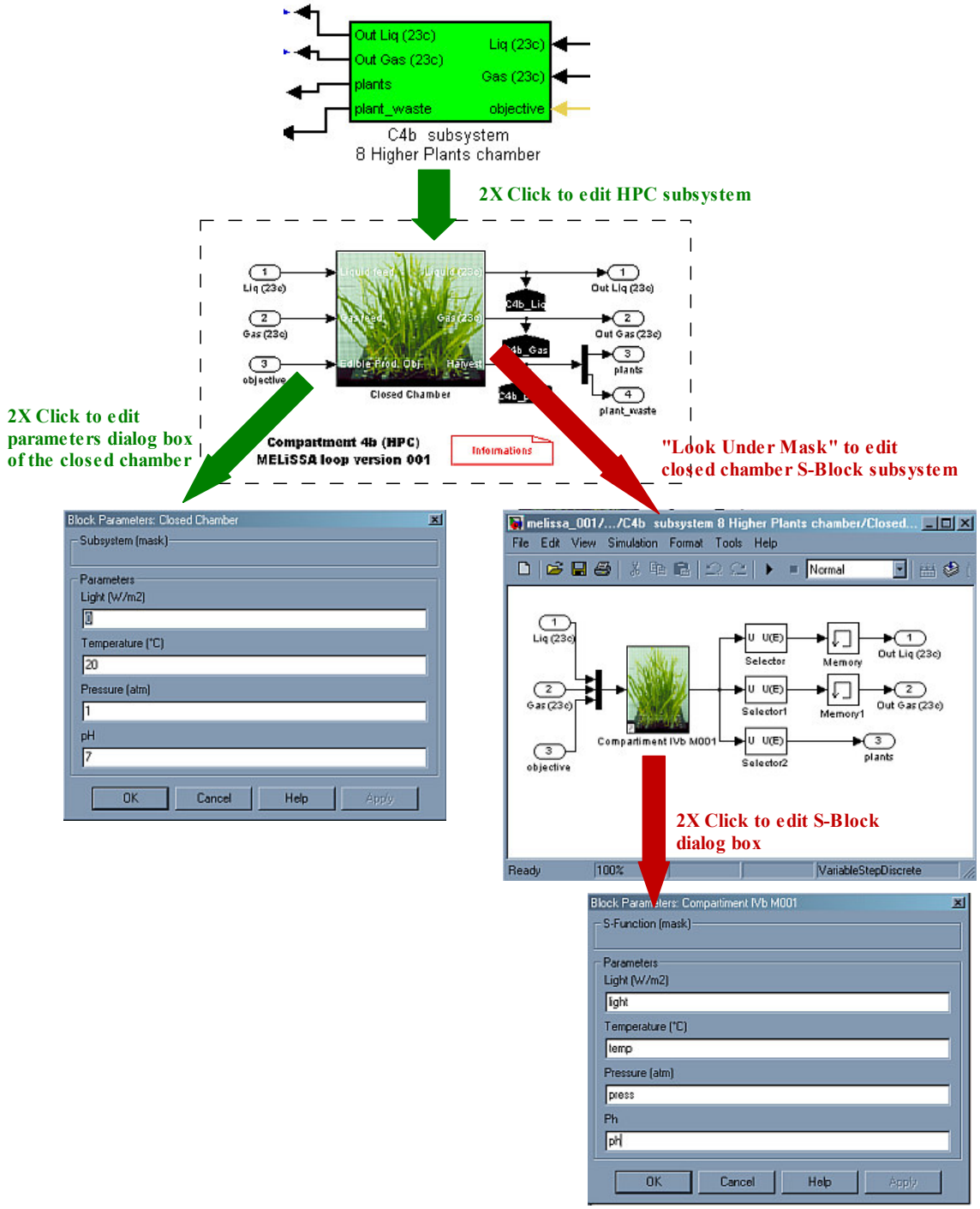

Figure 2.14 : : C4b Subsystem. Details of subsystem layers. Red arrows ways are only used for development and building of the model. Green Arrows ways are the common operation for using the model and managing its parameters. Gray colour underlines information/operating constraint from Management Units.

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At this time, the compartment subsystem is simple (Figure 2.14). It is only composed of the higher plant close chamber in which plants are growing. There are no pre or post operations. The current model of the higher plant chamber is also simple as it is only based on the mass balance growth equation of the plants. Even if some parameters can be set (Table 2.15), none of them are used in the model.

Closed Chamber parameters
pH
Temperature
Pressure
Light flux intensity

Table 2.15 : List of modifiable parameters for C4b model in the C4b dialog box In fact, none of the parameter is actually used.

2.2.6.2 Model of C4b greenhouse (Version 0.0.1 /S-function C_IVb_001.m)

The **C_IVb_001.m** matlab file is located in ./library directory. The S-function requires parameters (table 2.15) but doesn't use them. The parameters for managing the closed chamber and the crops are in the S-function itself. They are detailed in table 2.16.

Parameter **[Name in C_IVb_001.m]**	Value
Fraction of edible tomato in the edible production of the greenhouse [**crop(1).culture**]	0.008
Fraction of edible potato in the edible production of the greenhouse [**crop(2).culture**]	0.291
Fraction of edible wheat in the edible production of the greenhouse [**crop(3).culture**]	0.483
Fraction of edible rice in the edible production of the greenhouse **[crop(4).culture]**	0.161
Fraction of edible salad in the edible production of the greenhouse **[crop(5).culture]**	0.005
Fraction of edible soybean in the edible production of the greenhouse **[crop(6).culture]**	0.016
Fraction of edible onions in the edible production of the greenhouse **[crop(7).culture]**	0.016
Fraction of edible spinach in the edible production of the greenhouse **[crop(8).culture]**	0.016
Stoichiometric yield of N substrate g HNO3 / g NH3 for tomato **[Y_NN(1)]**	5 gHNO3 / g NH3
Stoichiometric yield of N substrate g HNO3 / g NH3 for potato **[Y_NN(2)]**	5 gHNO3 / g NH3
Stoichiometric yield of N substrate g HNO3 / g NH3 for wheat **[Y_NN(3)]**	5 gHNO3 / g NH3
Stoichiometric yield of N substrate g HNO3 / g NH3 for rice **[Y_NN(4)]**	5 gHNO3 / g NH3
Stoichiometric yield of N substrate g HNO3 / g NH3 for salad **[Y_NN(5)]**	5 gHNO3 / g NH3
Stoichiometric yield of N substrate g HNO3 / g NH3 for soybean **[Y_NN(6)]**	5 gHNO3 / g NH3
Stoichiometric yield of N substrate g HNO3 / g NH3 for onions **[Y_NN(7)]**	5 gHNO3 / g NH3
Stoichiometric yield of N substrate g HNO3 / g NH3 for spinach **[Y_NN(8)]**	5 gHNO3 / g NH3

Table 2.16 : Parameters for the definition of the greenhouse. They are fixed in the S-function

The plants composition (macromolecule mass percentage and composition) have been established for the pool of 8 plants in TN 32.3. For each plant a function was written in order to define this composition in the same way as for the biomasses. This function is called by the S-function modelling the closed chamber and when the composition is defined, the result is stored in a different file for each plant (Table 2.17).

Num.) plant	Function / File	Composition used to defined crops

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1) Tomato	Composition_tomato.m Composition_tomato.mat	**Proteins : 14.75 %** in dry edible [$CH_{1.46731}O_{0.46578}N_{0.23469}S_{0.000205}$] **Lipids : 14.75 %** in dry edible (composed of 22.84% of Lipids 1) Lipids 1 : [$CH_2O_{0.1231}$] Lipids 2 : [$CH_{1.81116}O_{0.1383}$] **Carbohydrates : 14.75 %** in dry edible [$CH_{1.8958}O_{0.9924}$] **Fibres : 14.75 %** in dry edible [$CH_{1.6560}O_{0.8280}$] **Waste : 955%** of dry edible [$CH_{1.43}O_{0.62}N_{0.017}S_{0.007}$] **Water content of Edible part : 93.6 %** of fresh mass **Water content of waste part : 50 %** of fresh mass Crop Yield : 18 d dry edible / m^2.day Transpiration Water : 5 kg / m^2 .day
2) Potatoes	Composition_potato.m Composition_potato.mat	**Proteins : 10.17 %** in dry edible [$CH_{1.50971}O_{0.38347}N_{0.25300}S_{0.000425}$] **Lipids : 0.55 %** in dry edible (composed of 22.84% of Lipids 1) Lipids 1 : [$CH_2O_{0.1214}$] Lipids 2 : [$CH_{1.74071}O_{0.11164}$] **Carbohydrates : 76.77 %** in dry edible [$CH_{1.6686}O_{0.8436}$] **Fibres : 12.51 %** in dry edible [$CH_{1.6513}O_{0.8257}$] **Waste : 49.96%** in dry edible [$CH_{1.43}O_{0.62}N_{0.017}S_{0.007}$] **Water content of Edible part : 79.5 %** of fresh mass **Water content of waste part : 50 %** of fresh mass Crop Yield : 33 d dry edible / m^2.day Transpiration Water : 5 kg / m^2 .day
3) Wheat	Composition_wheat.m Composition_wheat.mat	**Proteins : 13.8 %** in dry edible [$CH_{1.5}O_{0.359}N_{0.242}S_{0.007}$] **Lipids : 2.35 %** in dry edible (composed of 19.68% of Lipids 1) Lipids 1 : [$CH_2O_{0.1189124}$] Lipids 2 : [$CH_{1.8786}O_{0.11774}$] **Carbohydrates : 71.73 %** in dry edible [$CH_{1.6761}O_{08381}$] **Fibres : 12.12 %** in dry edible [$CH_{1.6667}O_{0.8333}$] **Waste : 152.50%** in dry edible [$CH_{1.43}O_{0.62}N_{0.017}S_{0.007}$] **Water content of Edible part : 13.44 %** of fresh mass **Water content of waste part : 12 %** of fresh mass Crop Yield : 33 d dry edible / m^2.day Transpiration Water : 2.9 kg / m^2 .day
4) Rice	Composition_rice.m Composition_rice.mat	**Proteins : 8.42 %** in dry edible [$CH_{1.53355}O_{0.35016}N_{0.25885}S_{0.00626}$] **Lipids : 2.57 %** in dry edible (composed of 29.9% of Lipids 1) Lipids 1 : [$CH_2O_{0.1231}$] Lipids 2 : [$CH_{1.81116}O_{0.1231}$] **Carbohydrates : 85.66 %** in dry edible [$CH_{1.8957}O_{0.99239}$] **Fibres : 3.35 %** in dry edible [$CH_{1.6667}O_{0.8333}$] **Waste : 119.77%** in dry edible [$CH_{1.43}O_{0.62}N_{0.017}S_{0.007}$] **Water content of Edible part : 13.26 %** of fresh mass **Water content of waste part : 15 %** of fresh mass Crop Yield : 4 d dry edible / m^2.day Transpiration Water : 5 kg / m^2 .day

Table 2.17a : Higher plants composition and characteristics. (Compiled from TN 32.3)

Num.) plant	Function / File	Composition used to defined crops
5) Salad	Composition_salad.m	**Proteins : 30.56 %** in dry edible [$CH_{1.64190}O_{0.19376}N_{0.24639}S_{0.00352}$]

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	Composition_salad.mat	**Lipids : 5.38 %** in dry edible (composed of 22.68% of Lipids 1) Lipids 1 : $[CH_2O_{0.12355}]$ Lipids 2 : $[CH_{1.725848}O_{0.111758}]$ **Carbohydrates : 26.89 %** in dry edible $[CH_{1.7962}O_{0.9919}]$ **Fibres : 37.1 %** in dry edible $[CH_{1.6537}O_{0.8268}]$ **Waste : 85.61%** in dry edible $[CH_{1.43}O_{0.62}N_{0.017}S_{0.007}]$ **Water content of Edible part : 95.27 %** of fresh mass **Water content of waste part : 80%** of fresh mass Crop Yield : 6 d dry edible / m^2.day Transpiration Water : 1.2 kg / m^2 .day
6) Soybean	Composition_soybean.m Composition_soybean.mat	**Proteins : 46.14 %** in dry edible $[CH_{1.53073}O_{0.34292}N_{0.25367}S_{0.00667}]$ **Lipids : 24.76 %** in dry edible (composed of 13.9% of Lipids 1) Lipids 1 : $[CH_2O_{0.1212}]$ Lipids 2 : $[CH_{1.83076}O_{0.11495}]$ **Carbohydrates : 8.34 %** in dry edible $[CH_{1.8822}O_{0.9411}]$ **Fibres : 20.76 %** in dry edible $[CH_{1.60}O_{0.80}]$ **Waste : 55.81%** in dry edible $[CH_{1.43}O_{0.62}N_{0.017}S_{0.007}]$ **Water content of Edible part : 10.42 %** of fresh mass **Water content of waste part : 50%** of fresh mass Crop Yield : 15 d dry edible / m^2.day Transpiration Water : 5 kg / m^2 .day
7) Onion	Composition_onions.m Composition_onions.mat	**Proteins : 12.09 %** in dry edible $[CH_{1.64586}O_{0.17818}N_{0.34576}S_{0.00448}]$ **Lipids : 2.42 %** in dry edible (composed of 47% of Lipids 1) Lipids 1 : $[CH_2O_{0.1210}]$ Lipids 2 : $[CH_{1.76406}O_{0.1111}]$ **Carbohydrates : 56 %** in dry edible $[CH_{1.8551}O_{0.9716}]$ **Fibres : 29.5 %** in dry edible $[CH_{1.6560}O_{0.8280}]$ **Waste : 157.87%** in dry edible $[CH_{1.43}O_{0.62}N_{0.017}S_{0.007}]$ **Water content of Edible part : 89.44 %** of fresh mass **Water content of waste part : 50%** of fresh mass Crop Yield : 22.5 d dry edible / m^2.day Transpiration Water : 5 kg / m^2 .day
8) Spinach	Composition_spinach.m Composition_spinach.mat	**Proteins : 47.82 %** in dry edible $[CH_{1.62780}O_{0.19299}N_{0.24837}S_{0.01169}]$ **Lipids : 5.69 %** in dry edible (composed of 14.61% of Lipids 1) Lipids 1 : $[CH_2O_{0.1244}]$ Lipids 2 : $[CH_{1.70827}O_{0.11226}]$ **Carbohydrates : 11.57 %** in dry edible $[CH_{1.6154}O_{0.9684}]$ **Fibres : 34.91 %** in dry edible $[CH_{1.6467}O_{0.8233}]$ **Waste : 157.55%** in dry edible $[CH_{1.43}O_{0.62}N_{0.017}S_{0.007}]$ **Water content of Edible part : 9756 %** of fresh mass **Water content of waste part : 80%** of fresh mass Crop Yield : 21 d dry edible / m^2.day Transpiration Water : 5 kg / m^2 .day

Table 2.17b : Higher plants composition and characteristics. (Compiled from TN 32.3)

The principle for modelling the Compartment 4b is summarised in figure 2.15.

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The plant composition (Table 2.17) is used to calculate the global CHONSP composition of each plant (edible part and non edible waste part). The stoichiometric equation for each plant (Table 2.18) can be solved using the ratio fixed between the 2 N-sources HNO3 and NH3 (Tbale 2.16). Once the equation for each plant established, a mass and element balance equation can be calculated for the complete greenhouse knowing the relative quantity of each plant in the greenhouse (Table 2.16). This final stoichiometric equation has the same form as the equation of each plant (Table 2.18), but in this equation the "plant" is a mix of the different plants of the greenhouse. As well the composition (macro composition and CHONSP compositions) of this "mix plant" are calculated using the composition of each single plant.

Stoichiometric equations for C_IVb_001 model	Equation
1 CO2 + ? HNO3 + ?NH3 + ? H2SO4 + ?H3PO4 → ? $[CHONSP]_{Plant}$ + ? O2 +? H2O	C4b E1-1 to E1-8

Table 2.18 : Compartment 4b mass balance equations. "?" are unknown stoichiometric coefficients that can be calculated if $[CHONSP]_{plant}$ is known. The equations are solved in the S-function.

With this final single equation, the mass balance reaction for the closed chamber can be executed as for the other biological compartment. The key for the reaction is the dry edible plant production by the chamber. This information comes from the Food Management unit and is one of the entries on the subsystem (Figure 2.14). This objective is used to calculate the theoretical yield efficiency for the CO2 assimilation in the reaction :

$$\text{CO2 Yield} = \frac{\text{CO2 Moles required to achieved edible production objective}}{\text{CO2 moles flow in inputs of the chamber}}$$

The moles of CO2 required to achieve the edible plant production can be calculated with the stoichiometric equation. The yield efficiency is in the range [0-1]. The reaction is calculated using this theoretical yield, but if another substrate is limiting in the reaction, the yield is reduced until complete exhaustion of the limiting substrate and then the objective production of edible plant can not be achieve.

After the reaction, the gas and liquid flows cannot be calculated by the **flash** function from the remaining compound as closed chamber is not a bioreactor. A strict separation of gas and liquid compound is done to create gas and liquid flow. Water is a special case as plants produce large amount of vaporized water by transpiration. It may be possible to use humidity parameter to manage the partial pressure of water but it requires to have a more dynamic approach especially for the gas flow rate in the chamber. Then for simplicity it was chosen to consider all the transpiration water to be in the gas flow at the chamber output without checking the humidity consistency of this calculation (i.e. this can lead to humidity > 100%). Note if water is limiting transpiration is limited and plant water content is reduced, but liquid phase can be dried.

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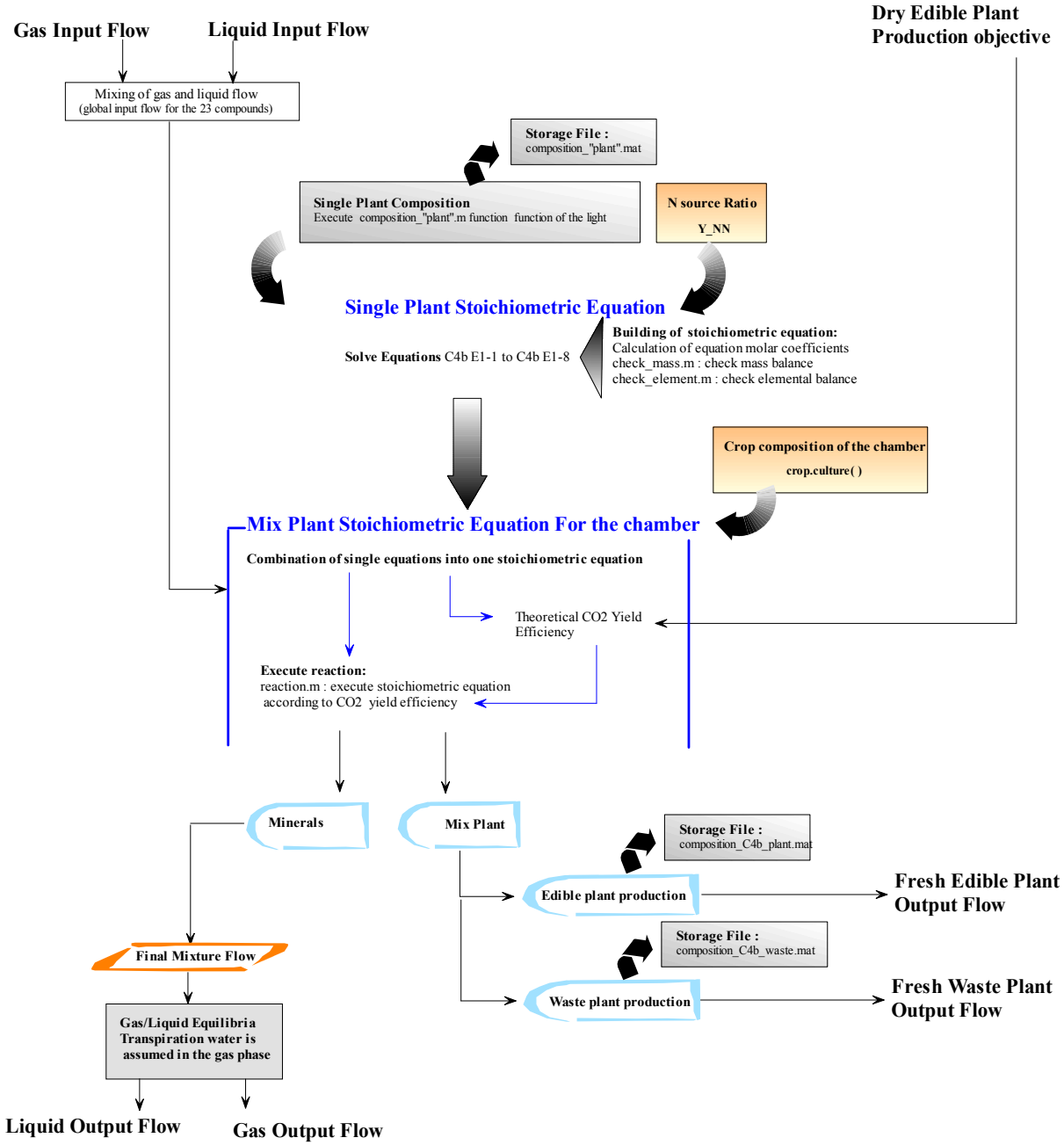

Figure 2.15 : Steps of calculations for C_IVb_001 model

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2.3 Models of Management Subsystems

The Management subsystems are introduced in the MELiSSA loop in order to control the different flow and to fix the operating constraints of the loop. These subsystems are used to manage the liquid, gas and solid (i.e. biomass, plant waste) flow.
The Food Management Unit is a special case. This subsystem fix the number of the crew and then by this way the size and the flow on the whole system. The operation of compartment 4b and compartment 4a are also directly fixed by this management unit.

2.3.1 GAS LOOP MANAMAGEMENT UNIT

2.3.1.1 Description of the subsystem

This subsystem (Figure 2.16) recovers the gas flow from the loop and the crew cabin, and produce the water condensate flow, the atmosphere gas flow for the crew and oxygenic gas flows to compartments C4a (Spirulina) and C3 (Nittrifying). The manageable parameters of the subsystem are resumed in table 2.19.

There are 2 objective for this unit :

1 - to create an atmosphere for the crew, which is defined in terms of flow, temperature and composition. This is done with the S-block (cabin_gas_mngt_001.m S-function) which create the atmosphere gas flow according to the recycled gas flow from the loop and the constraints (grey circles in figure 2.16). In order to maintain the flow and gas composition constraints external supply and/or sink are calculated (orange circled flow) corresponding to supply and sink to the MELiSSA loop itself. The gas mass flow rate is given in kg/day. It is important to notice that the value and unit given here affects all gas flow in the loop and must be consistent with the requirements of the complete crew. The gas composition constraints are fixed by giving gas fraction value for the 23 compounds (Table 2.2) in the constraints interface, expecting for water for which the value given is the relative humidity. Pressure (in atm) and temperature (°C) must also be given.

2 – to collect gas from the loop and redistribute gas to the loop. The gas from the cabin crew is divided into 3 flows: one for feeding the compartment 3, one for supplying the compartment 4a and one is the part of gas not sent to the loop. This last one is further added to the final gas flow coming from loop (after treatment in the different compartments). This resulting gas flow is used a recycled gas by the atmosphere management unit to create the atmosphere for the crew. The 3 gas flows are managed using dividers (circled in blue) in sequential step: first generating the gas flow for the compartment C3, further the remaining gas is divided to generate the gas flow for compartment C4. After the S-block grating the crew atmosphere, the condensate water is recovered from the supply/sink flow.

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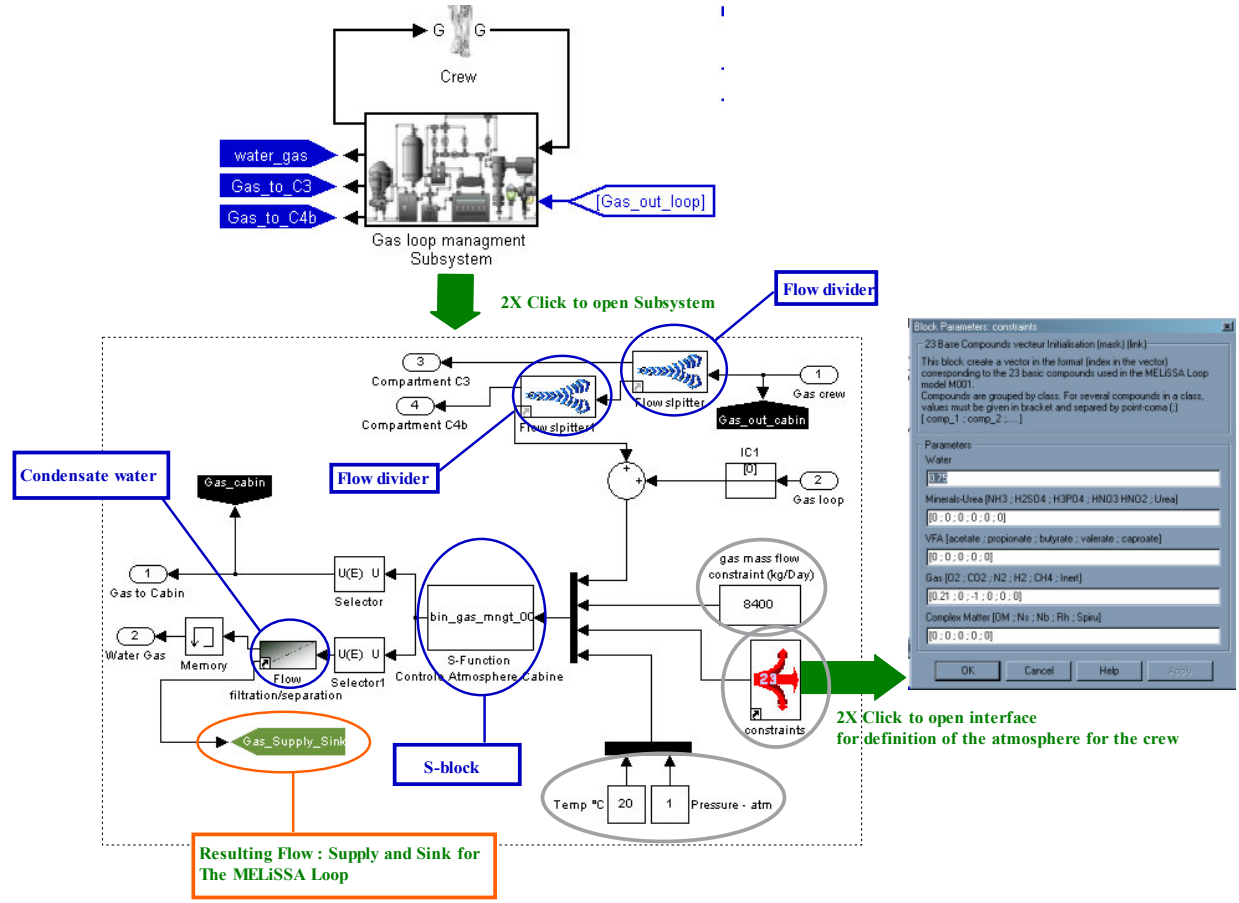

Figure 2.16 : Gas Management Subsystem. Details of subsystem layersGreen Arrows ways are the common operation for using the model and managing its parameters. Gray colour underlines constraint of the cabin atmosphere.

Crew cabin atmosphere	Gas flow management
Gas flow rate Gas temperature Gas pressure Gas composition - In relative humidity for water [0 to 1] - In gas fraction for the other 22 compounds. The gas fraction must be between 0 and 1. A negative value can be used. It means that the compound is not treated and all inputs remain in the final gas flow for the crew atmosphere.	**Flow separation.1** : The value given (between 0 and 1) gives the fraction of input for the first output flow, i.e. the gas flow to C3 **Flow separation.2** : The value given (between 0 and 1) gives the fraction of input for the first output flow, i.e. the gas flow to C4a **Water condensate** : (separation system for the water in the input flow *Compound index*: **[1]** *Separating capacity* **[1]** if completely condensate

Table 2.19 : List of manageable parameters/constraints for the Gas Management Subsystem.

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2.3.1.2 Model of Crew atmosphere control (Version 0.0.1 /S-function Cabin_gas_mngt_001.m)

The **Cabin_gas_mngt_001.m** matlab file is located in ./library directory. The S-function don't requires parameters, as all information are passed by inputs. The function itself is relatively simple. From the constraints for the crew atmosphere (Table 2.19) is created the gas flow for the crew. The complete system to solve is a set of 3 flows of 23 compounds, i.e. 69 variables. 23 of the variable are fixed as there are coming from the input flow. The gas composition constraints (i.e. a fixed gas fraction or the use of all the input to generate the crew atmosphere) fixes also 23 degree of freedom. The water gas fraction is calculated from the relative humidity accordingly to the water partial pressure calculated by the Antoine Law (TN 17.1). As there is no accumulation, mass balance equations for each compound fix 23 other degree of freedom. We obtain then a set of 69 for 69 variables. The system can be solved, but it can be noticed that in this case the information fixing the gas flow rate wasn't used to solve the system.

Thus 2 points must be checked in the calculations for the creation of crew atmosphere:

1 – Check the gas fractions consistency. If the sum of the gas fractions is greater than 1, the gas fraction of all compounds are normalized in order to have a sum equal to 1

2 – Check the degree of freedom. If all gas composition constraints are used, it is not possible to solve the 69*69 system **plus** the gas flow constraint (except with an optimization). Another way was chosen here, based on a **choice for N2** between a fixed gas fraction and a gas fraction adapted to fit the gas flow:

- For N2 gas fraction between 0 and 1 the gas fraction of N2 is used as a constraint to solve the system
- For N2 gas fraction <1, the gas flow rate is used as a constraint

The system 69*69 is solved in the S-function and outputs flows for the crew atmosphere and supply/sink are calculated.

2.3.2 LIQUID LOOP MANAGEMENT UNIT

This unit deals with the water and its minerals and gas dissolved compounds, namely HNO3, NH3,H2SO4, H3PO4, HNO2, CO2, O2, N2, H2. The subsystem recovers the liquid from the MELiSSA loop and the condensate water from the Gas Management Subsystem and distributes water to the crew for drinking, and to the MELiSSA loop at the level of compartment C1 and C3 (Figure 2.17).

For this subsystem it wasn't necessary to build an S-function. The constraints were applied for each compound using a constraint block built using a specification controller block (report to chapter 2.4). This subsystem fixes the liquid flow and composition (Table 2.20) before its recycling to the MELiSSA loop. This avoids accumulation/exhaustion of water and minerals listed in table 2.20 in the loop. As a consequence for each of the compound controlled is created in this subsystem a supply/sink flow. The minerals submitted to constraints are mainly substrate for the micro-organisms. As there is no other mineral supply on the loop (except

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HNO3 on the C4a compartment) it is necessary to fix a sufficient flow sufficient for the complete loop.

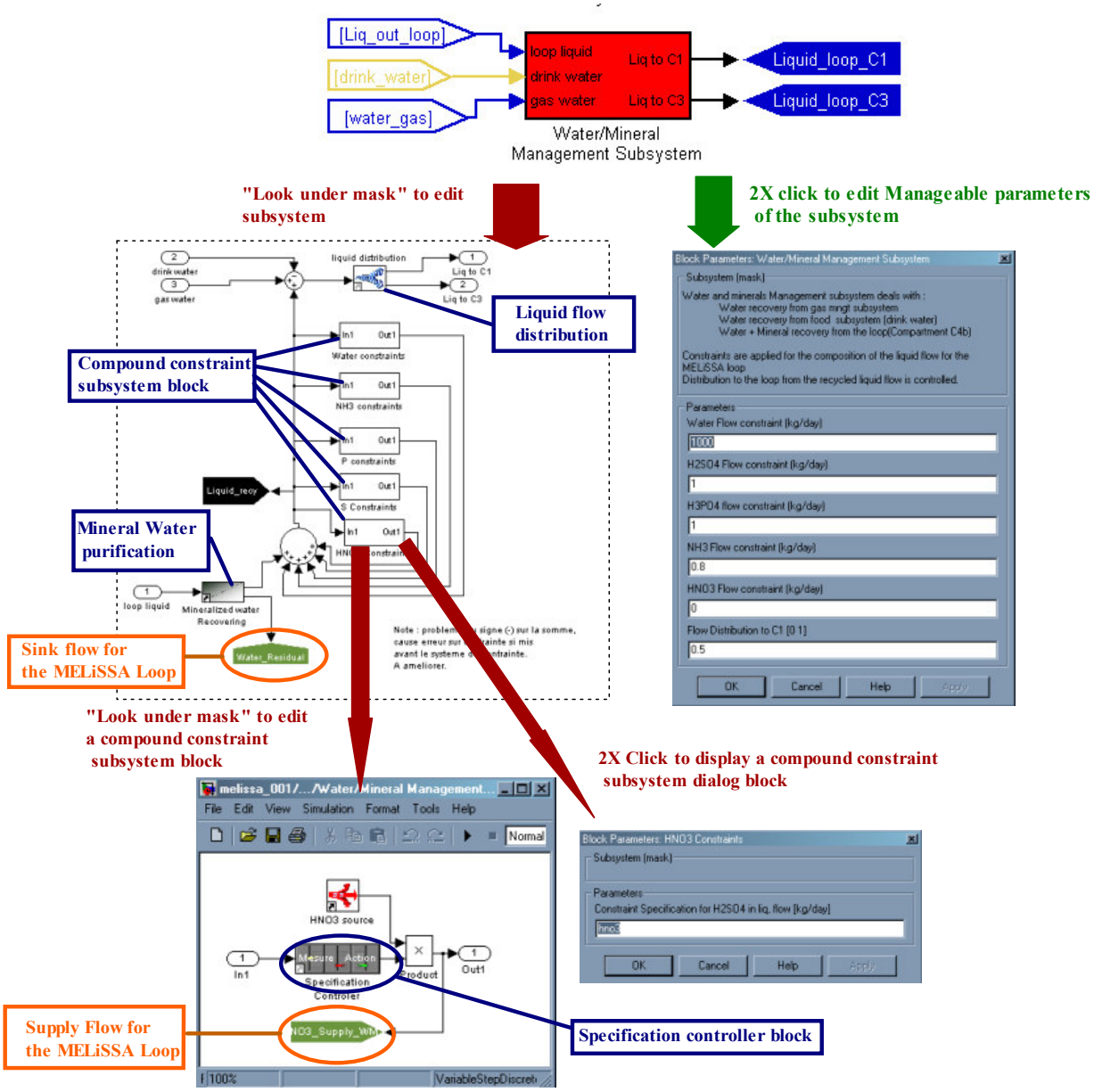

Figure 2.17 : Gas Management Subsystem. Details of subsystem layers. Green arrows ways are the common operation for using the model and managing its parameters, while red arrows are ways for modifying the subsystem.

Another important unit of the subsystem is the separation system called “mineral water purification” which **eliminates** from the recycled liquid loop the **organic matter** (Urea, Acetic Acid, Propionic acid, Butyric Acid, Valeric Acid, Caproic Acid, Organic Matter, Nitrosomonas Biomass, Nitrobacter Biomass, Rhodobacter biomass, Spirulina Biomass). This unit generates a sink flow for the

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loop called “water_residue”. It must be outlined that compounds that are recycled but not submitted to a constraint (Table 2.20) may be accumulated if the loop fails to operate correctly.

Fixed flow rate for the liquid recycled to the loop (in kg/day)	Supply/Sink flow associated to the constraint
Water	Water_supply
HNO3	HNO3_supply_WM
H2SO4	H2SO4_supply
H3PO4	H3PO4_supply
NH3	NH3_supply

Table 2.20 : List of manageable constraints for the Liquid Management Subsystem. These constraints are set through the dialog box interface (Figure 2.17).

2.3.3 FOOD MANAGEMENT UNIT

The food management (Figure 2.18) is a key unit for closing the loop as the constraints used here affect the operation of the C4a and C4b compartments. The subsystem is entirely based on the S-function “**food_crew_mngt_001.m**” located in ./library directory.
The subsystem receives the food from the loop (edible higher plants, Spirulina and Rhodobacter biomasses) and uses this food sources to fit the food constraints (Table 2.21). As the MELiSSA loop food sources may be insufficient, an external supply food source can be also used to fit the constraint. The mass flow for this supply is created by the S-function and appears inside the subsystem (Figure 2.18).

The food subsystem generates several flows :

- The food flow itself, for the crew, according to the food constraints. This flow has the food format detailed in table 2.3.
- The water drink flow (23 compounds format; Table 2.2)
- A liquid flow. This flow has the 23 compounds format (Table 2.2). It contains unused biomasses, and may contain water not used for the crew.
- A food supply flow. This flow has the food format detailed in table 2.3.)
- An organic waste flow. This is the edible plants wasted and not used in the food for the crew. This flow has the same format as the faeces flow detailed in the table 2.3 as they will be treated as organic waste
- In order to reduce waste and supply of food, the S-function calculates 2 objective values for operating the compartments C4a and C4b which are respectively a proteins production objective for the compartment C4a and an edible plant production by the greenhouse.

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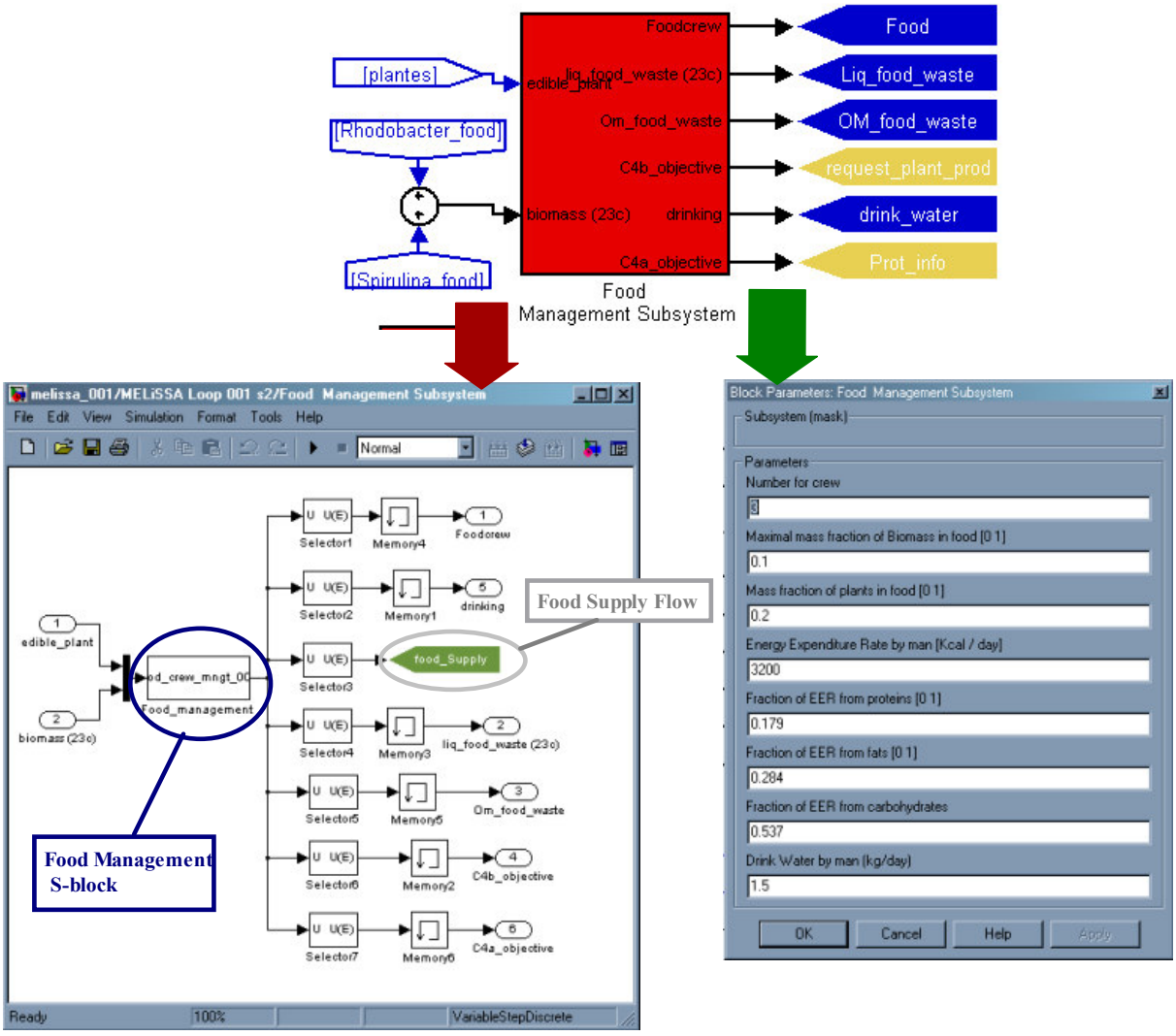

Figure 2.18 : Food Management Subsystem. Details of subsystem layers. Green arrows ways are the common operation for using the model and managing its parameters, while red arrows are ways for modifying the subsystem.

Crew information	Nutritionnal constraints
Number of the crew Drink water requirements (kg/ man.day) Energy Expenditure Rate (EER) (Kcal/man.day)	Maximal mass fraction of biomass in food Objective mass fraction of plants in food Fraction of EER from Proteins Fraction of EER from Fats Fraction of EER from Carbohydrates

Table 2.21 : List of manageable constraints for the Food Management Subsystem. These constraints are set through the dialog box interface (Figure 2.18).

The principle for modelling the Food Management S-function (**food_crew_mngt_001.m**) is summarised in figure 2.19. This function uses the biomasses and plants composition storage

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files in order to establish the nutritional value of the food from the MELiSSA loop and to compare them with the nutritional constraints.

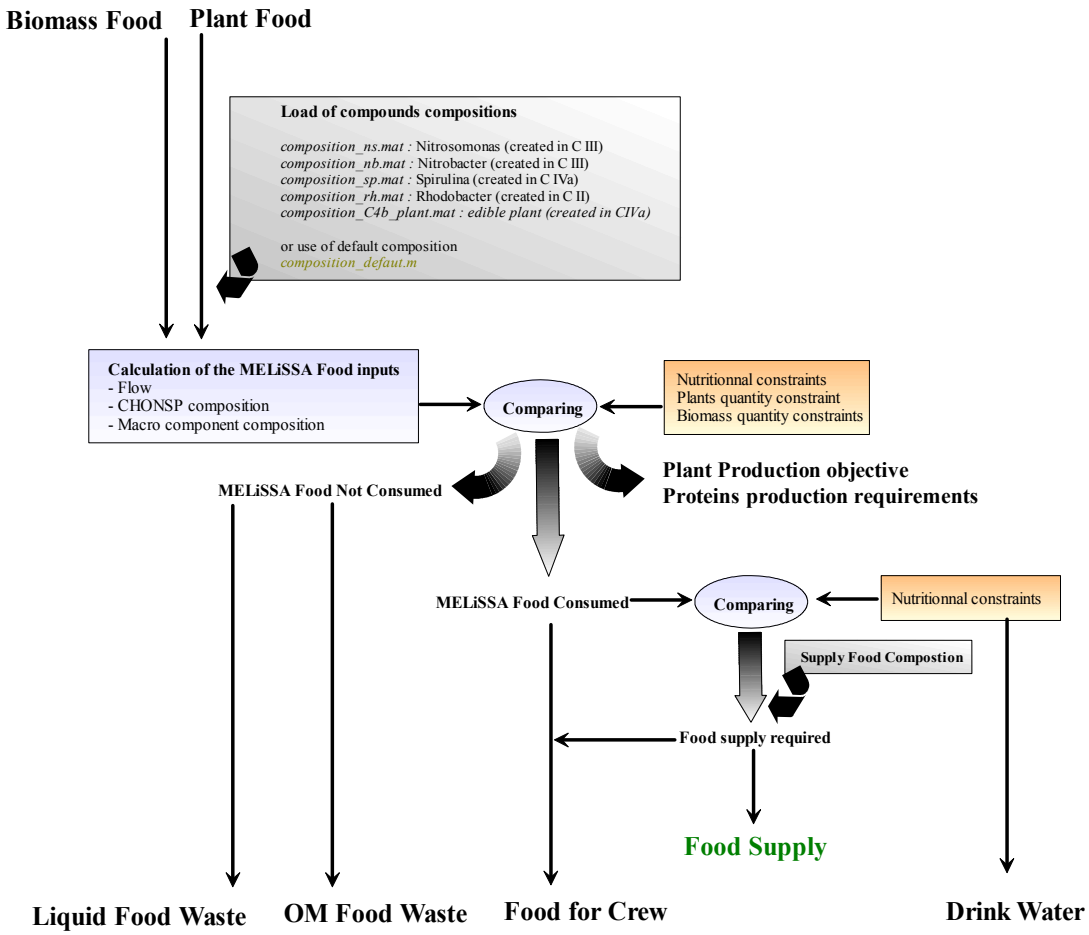

Figure 2.15 : Steps of calculations for The Food Management Function

2.3.4 BIOMASS DISTRIBUTION

The biomass distribution in the loop (namely the parameters X and Y in previous MELiSSA model) is a subsystem which apparently has not entries nor outputs. In fact input and output flow were masked inside the subsystem itself (Figure 2.16). With this subsystem is managed the distribution of the harvested biomass form compartment C2 and C4a.

In the dialog box can be set the parameters for :

- The fraction of Spirulina used for the food

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- The farction of Rhodobacter used for the food
- The fraction of the remaining biomass (i.e. not used for the food) which is recycled to the first compartment. The biomass not recycled to the compartment C1 and not used for the food are wasted out of the loop.

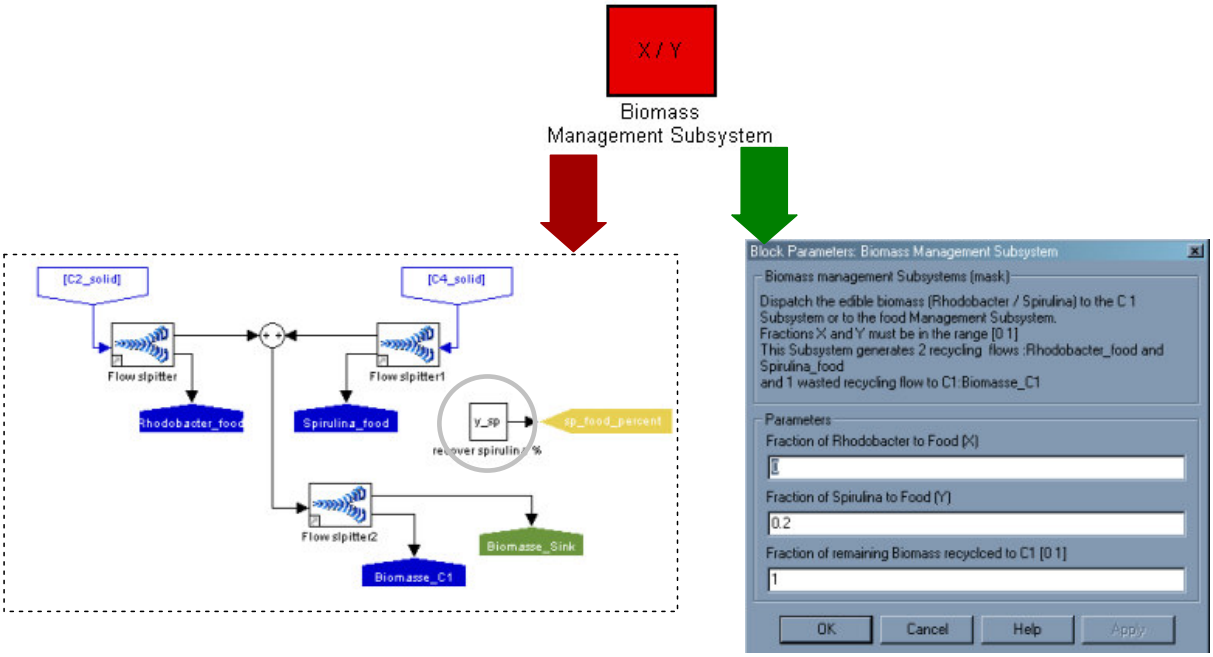

Figure 2.16 : Biomass Recycling Subsystem. Details of subsystem layers. Green arrows ways are the common operation for using the model and managing its parameters, while red arrows are ways for modifying the subsystem. “y_sp” is the fraction of Spirulina biomass used for food. This information is sent to the constraint subsystem for C4a compartment.

The subsystem is only composed of divider units. There is no S-function to describe the subsystem. The fraction of the Spirulina biomass used for the food is an information that is sent to the constrain subsystem of the compartment C4a in order to properly calculated the HNO3 supply to fit proteins production constraint.

2.3.5 ORGANIC WASTE DISTRIBUTION

This subsystem mixes the two organic waste flows from compartments C4b (plant waste) and Food management Unit (Food plant waste) and recycles a part of this mix to the first compartment.

Due to the specific format of the organic matter waste flows (Table 2.3) the mixing and the calculation of the composition of the mixed waste is done by an S-function

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(**OM_waste_001.m)** which is located in the ./library directory. The mix is further dispatched between the compartment C1 and out of the loop (Figure 2.17).

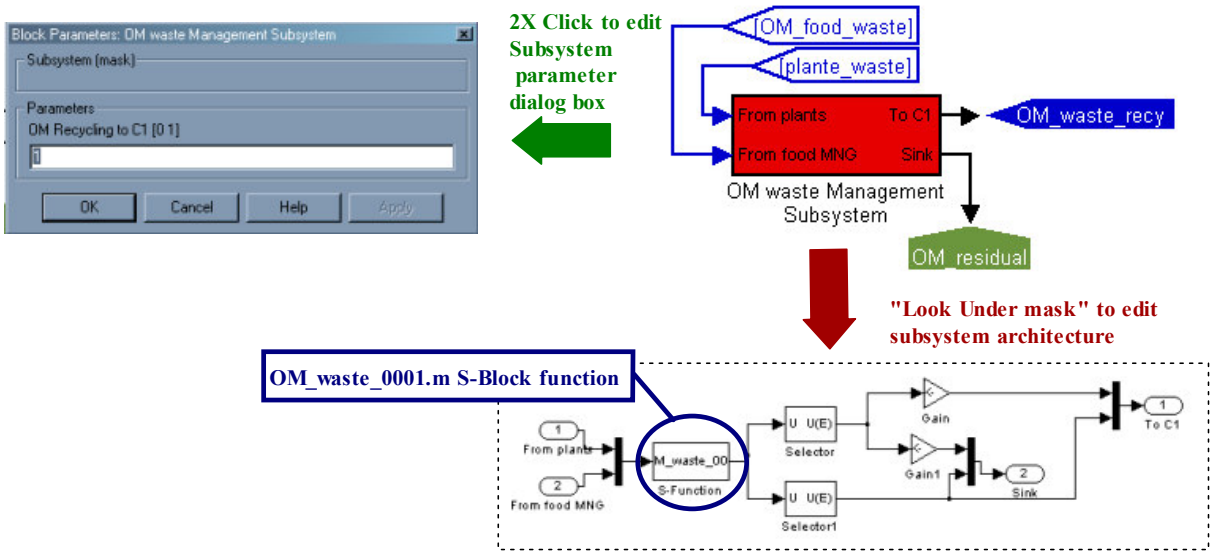
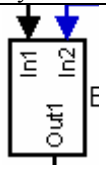


Figure 2.17 : Organic waste Recycling Subsystem. Details of subsystem layers. Green arrows ways are the common operation for using the model and managing its parameters, while red arrows are ways for modifying the subsystem.

2.4 Other "MELiSSA block" models

It was mentioned in the description of the main subsystems of the loop that several small specific S-block were built. There are briefly presented in the table 2.22 with their main principle and if exists their S-function, which is always located in the /library directory. The four units described here are the gas burner block, the flow divider block, the compound separation block and specification constraint block.

Block	Symbol	Functions	Operation
The gas burner		Burn (oxidation) of gas: Reactions are : H2 --> water Methane --> CO2 VFA --> CO2 NH3 --> HNO3	The two inputs flows are mixed and oxidation reactions are realised with an efficiency of 100% or according to limitations if they occur. The S-function associated is burner_001.m

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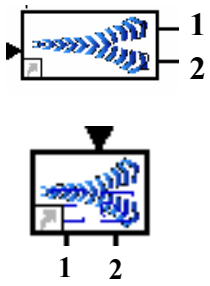
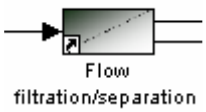
The flow divider		Split the input flow into two flows. The parameter given is a fraction of the input mass flow for the flow (1). The second flow (2) is the remaining of the input	The S-function associated to the block is **diviseur_001.m**. The parameter to gives is a fraction between 0 and 1 for the first output flow
Compound separation		It makes a selective separation of compounds in the 2 outputs flows. In the parameters dialog box are given the index retained in the first output flow with a separating fraction for each of them	The S-function associated to the block is **filtration_001.m**. Example of parameters Index of compound (see Table 2.2) : **[2 ; 8 ; 15]** Fractions of the input flow in the first output: 10 % of 2 ; 100% of 5 and 50% of 15 **[0.1; 1 ; 0.5]**
specification constraint		The input is the flow in which variables (compounds) are measured. The parameters of the blocks give the index of the compound measured, its objective value and the range of the action value. The actions must have an effect on the measured values.	The block is built from existing Simulink blocks.

Table 2.22 : Blocks build for the MELiSSA loop.

2.5 Model of the whole loop : MELiSSA Loop 0.0.1

The architecture described here is considered as model version 0.0.1 of the loop. Manipulations of the manageable parameters (chapter 3) are not considered as new version of the model. In the previous chapter where described the different subsystems used to form the MELiSSA loop. The loop is obtained linking the subsystems by flows. The model of the loop is formed by this linking of the different subsystems. The relation between subsystems can be changed, but the input/output flow format required by each subsystem must be respected.

Modification of the MELiSSA loop may occur in the future. The proposed incrementation of the model number is:

0.0.1 → 0.0.2 : small architecture modification and S-function correction
0.0.1 → 0.1.1 : architecture modification and new blocks
0.0.1 → 1.0.1 : New architecture, new blocks and important change in the loop operation strategy.

It is important here to keep in mind that in this model, the following strategy was used:

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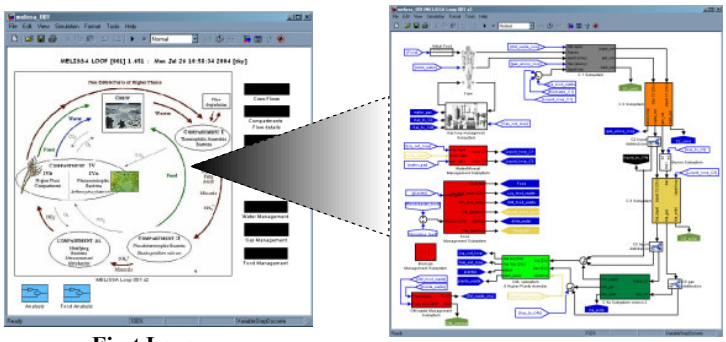
- Food is the main controller of the system. It fixes the operation of the C4b compartment (edible plant production objective) and also the operation of the C4a compartment (Maximum of proteins must come from the loop)
- Gas and water are controlled at the level of the recycling of the flows from the end of the loop (flows from compartment C4b and C4a) to the beginning of the loop (crew and compartment C1). This control is based on a controlled recycling flow in terms of flow rate and composition. These controls are made using sink/supply on the loop.

The choice of other strategies may require to develop new kinds of management subsystems.

The MELiSSA loop version 0.0.1 for Simulink is recorded as a Matlab/Simulink file : m**elissa_001.mdl**, located in the ./modele directory. The model must be started from this directory and this directory must be the current directory during a simulation. It is also required to add the MELiSSA folder and subfolder (report to 2.13) in the Matlab default path before starting **melissa_001.mdl.** Excepting files created in subsystems, the results of a simulation are not stored into results files. The results (flows details, recycling efficiencies) are displayed in the interface itself. In order to facilitate the use of the simulink model, the complete loop was built as a two layer system (Figure 2.18):

- The first layer is what appears when the program is started. With this layer results can be consulted but the loop cannot be managed (it is only a MELiSSA picture)
- The second layer is behind the MELiSSA subsystem picture. It is the real architecture of the loop with access to the MELiSSA subsystem and their manageable parameters.



First Layer **Second Layer**

Figure 2.18 : Two layers of the MEliSSA loop

2.5.1 FIRST LAYER: ANALYSIS OF RESULTS

This is the first interface that appears when the model is loaded (Figure 2.19). With this interface it is possible to run a simulation, to display the results (flow between MEliSSA subsystems) and to edit preliminary analysis (efficiencies) of the system. The management of the loop itself (parameters, links between subsystems,…) can be reached by opening the second layer which is behind the MEliSSA loop picture (Figure 2.18).

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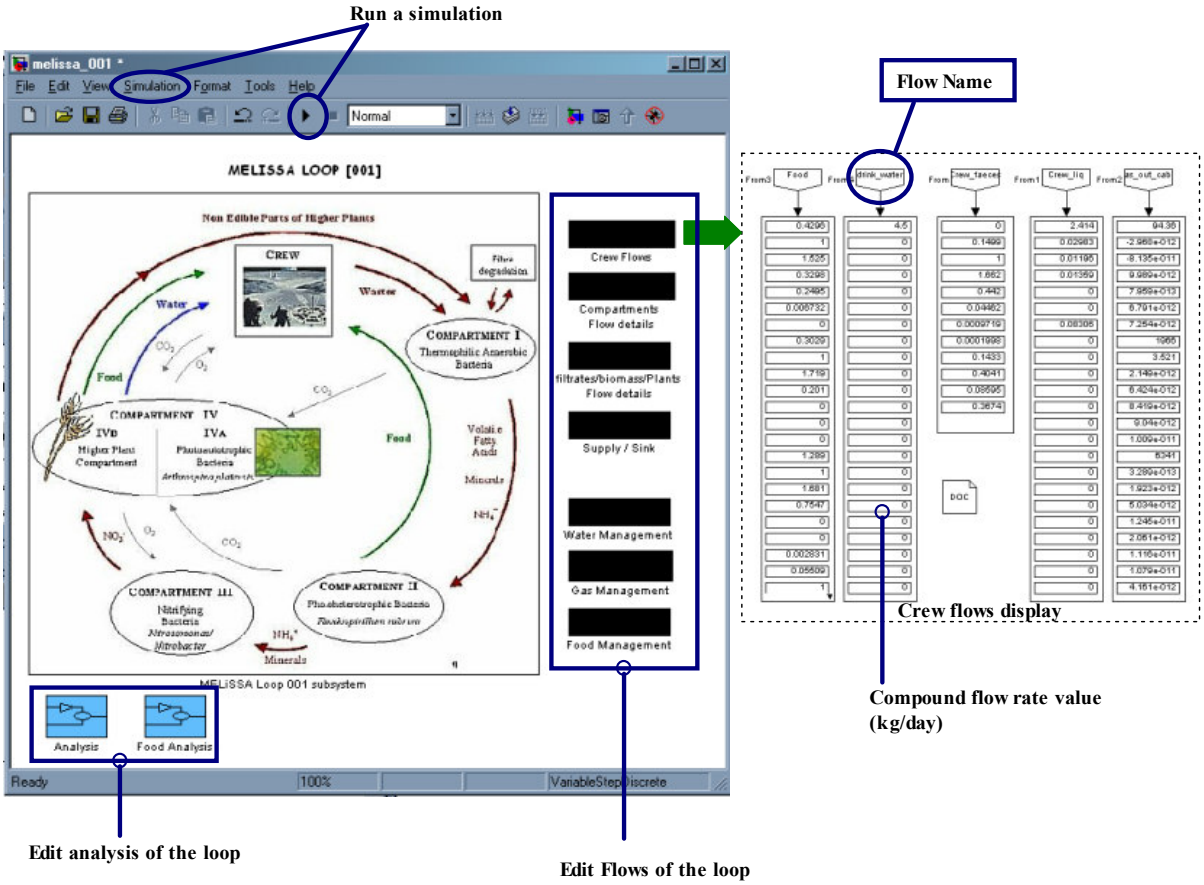

Figure 2.19 : MELiSSA_001 model. First layer.

2.5.1.1 Loop Simulation

The MELiSSA mass balance model simulation with Simulink can be done by clicking the simulation button or through the simulation menu. The parameters of the simulation (solver, diagnostic,…) can be managed with the simulation menu (see to Simulink manual). It is important here to remember that Simulink is in principle designed to perform dynamic simulations. This means simulation between a time t_0 and t. For mass balance modelling, i.e. steady state modelling, the time has no sense. In fact, two options were possible for computing the MELiSSA mass balance model :

1 – Simulation between **time** 0 and 0. This means that the Simulink solver tries to solve the system as a whole. This requires that the solver is able to solve all the loops as a single system. In principle it is feasible, but in practice it works only with small and simple loops.

2 – Simulation between **step** 0 and step X. In this approach the step for simulations are not time steps but calculation step. This approach is possible only is there is no time dependant equation in the complete model. This approach has the advantage to avoid trying to solve the solution of loop flow in a single step of calculation. By putting

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"memory blocks" in flows that create loops in the system we introduce something like "cut flow" and then loops are "opened" what make calculation easier in one step of calculation. The "cut flow" need to be initialised for the first step of calculation (most of the time initialised to 0), but for the second step of calculation, the value memorized is used instead of the initial condition value. After a certain step of calculations, we reach a convergence situation, i.e, the flows are constant over all the loop.

The second approach was used for the MELiSSA loop model (the first one has failed). For this reason it can be seen that "memory block" where introduced in the loop. Of course it is not recommended to modify the existing blocks in the model. In order to reach convergence 10 to 20 steps are at least required. By default the simulation is set to 40 steps.

At the end of a simulation results can be displayed (see below), and intermediates informations during calculations of subsystems are also displayed on the Matlab command line. These informations are comments written in the different S-functions.

2.5.1.2 Display of flows rates

A set of 7 black boxes are on the right of the windows (Figure 2.19). These boxes display the mains flow rates of the loop. The flow rates are in kg/day (default unit used for setting the flows in Management subsystems). Most of the flows have the 23 compounds format (Table 2.2), while some other have specific format (report to subsystems for detail of the flows format).

2.5.1.3 Display of analyses

A set of 2 boxes are at the bottom of the windows (Figure 2.19) displaying details on the system efficiencies. The calculation of the efficiencies is done combining, extracting values from various flows using Simulink blocks. The details of calculations can be seen by editing subsystems. The principles of the calculations of efficiencies will be detailed in chapter 3.

2.5.2 SECOND LAYER: LOOP MODEL AND PARAMETERS

This is the model of the loop (Figure 2.20). The loop is obtained by linking together the subsystems previously detailed. To improve clarity of the loop, all links are not directly done by a line to close the loop but flows are stored into a variable which is further used as input on another subsystem (dashed circle in figure 2.20). In addition to the susbsytems, 3 flows divider were introduced (gray circles – Figure 2.20) to manage the flows distribution within the loop.

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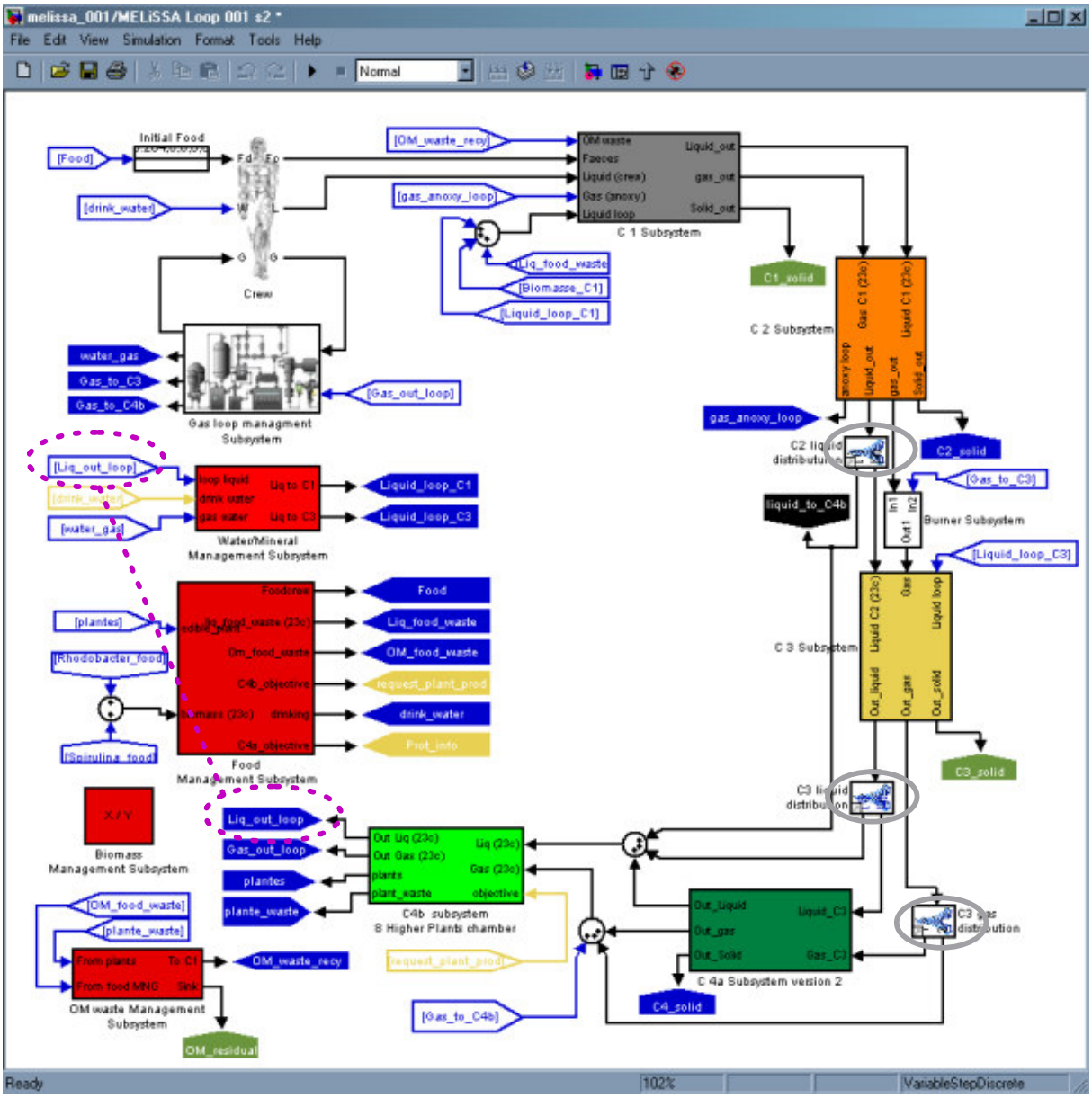

Figure 2.20 : MELiSA loop architecture model. Dashed circles indicate a flow passed between 2 subsystems by an intermediate variable (liq_out_loop).

The loop operating parameters can be managed directly through this window by editing each subsystem (report above) plus the 3 flow divider units. In order to simplify the understanding of the system, symbols and colours were used for each kind of flow or subsystem (table 2.23).

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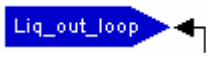
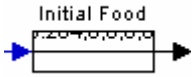
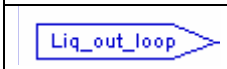
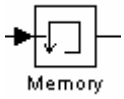
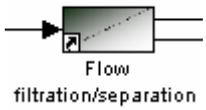
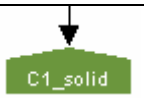
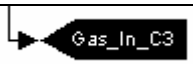
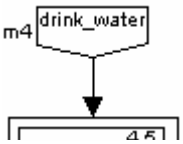
Symbol/colour	meaning	Symbol/colour	Meaning
	Store Flow for linking to another unit		Initial condition Block
	Use stored flow from another unit as input to the current unit		Memory Block
	Store information flow for use in another unit		Measure/Action Unit
	Use stored information flow from another unit as input to the current unit		Compound Separation Unit
	Store Flow as supply or sink for the loop		Flow Divider Unit
	Store Flow values (i.e. measure)		
	Display Flow values (i.e. measure)		Management Subsystem Compartment 4b (HPC) Compartment 4a (Spirulina) Compartment 3 Compartment 2 Compartment 1

Table 2.23 : Legends of the MELiSSA loop (Figure 2.20)

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3 USE OF THE MELISSA LOOP 0.0.1 SIMULINK MASS BALANCE MODEL

This chapter will detail how to use the MELiSSA loop mass balance model under Matlab Simulink. It can be readed in principle independently of the previous chapter but it is recommended to understand the models used.

3.1 Installation and required configuration

The model was developed and tested with Matlab® 6.5 R13 and Simulink 5.

A main directory (called here **melissa_sim**) must be created in which the files (Table 3.1) of the model must be placed accordingly to the directory hierarchy of Table 3.1.

File	Function	Location
alim_23c.bmp	Image for	./Melissa_sim /library
blue_divide.bmp	Image for divider_001 S-block	
burner_001.m	Gas oxidation(burner)	
C_1.bmp	Image for C1 reactor	
C_2.jpg	Image for C2 reactor	
C_3.bmp	Image for C3 reactor	
C_I_001.m	C1 compartment model	
C_II_001.m	C2 compartment model	
C_III_001.m	C3 compartment model	
C_IVa_001.m	C4 a (Spirulina) compartment model	
C_IVb_001.m	C4 b (HPC) compartment model	
cabin_gas_mngt_001.m	Gas Management control subsystem	
check_element.m	Check element balance of stoichiometries	
check_mass.m	Check mass balance of stoichiometries	
composition_defaut.m	Default composition for biomass	
composition_nb.m	Composition of Nitrobacter Biomass	
composition_ns.m	Composition of Nitrosomonas Biomass	
composition_onions.m	Composition of onions	
composition_potato.m	Composition of potato	
composition_rh.m	Composition of Rhodobacter Biomass	
composition_rice.m	Composition of rice	
composition_salad.m	Composition of salad	
composition_soybean.m	Composition of soybean	
composition_spinach.m	Composition of sinach	
composition_spiru.m	Composition of spirulina Biomass	
composition_tomato.m	Composition of tomato	
composition_wheat.m	Composition of wheat	
crew_metabolic_001.m	Crew metabolism model	
diviseur_001.m	Flow divider	
filtration.bmp	Image for separation/filtration S-block	

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filtration_001.m	Compound filtration/separation model	
flash.m	Gas/liquid thermodynamic equilibria calculation	
food_crew_mngt_001.m	Food Management control model	
man.bmp	Image for crew compartment	
man_meta.bmp	Image for crew metabolic S-block	
matrice_composition.m	CHONSP composition of known fixed compounds	
melissa.bmp	Image for the MELiSSA loop system	
melissa_block.mdl	**MELISSA Simulink library**	
OM_waste_001.m	Organic matter Management model	
plante.bmp	Image for C4b S-block	
reacteur.bmp	Image for C1 reactor	
reaction.m	Calcul of a stoichiometric reaction	
spiruline.bmp	Image for the C4a reacto	
spiruline2.bmp	Image for the C4a S-block	
tuning_control.jpeg	Image for the Measure/Constraint/Action S-block	
tuyaux.bmp	Image for the Gas Management subsystem	
Melissa_001.mdl	**MELISSA LOOP SIMULINK MODEL**	**./Melissa_sim /modeles**
Composition_ ?????.mat	Simulation resutls files (mainly composition of biomass and plants)	./Melissa_sim /modeles /data
composition_C4b_waste_defaut.mat	Default saved composition for plant waste	./Melissa_sim /modeles /default_data
composition_defaut.mat	Default saved biomass composition	
composition_C4b_plante_defaut.mat	Default saved plant composition	

Table 3.1 MELiSSA Model files

The main directory **../melissa_sim** and its subfolders must be added to the default path of the Matlab software. This can be done using the **addpath** command (report to Matlab documentation) or the "set path" menu in the graphical Matlab interface. You can not correctly open the MELiSSA model file until default path is not correctly defined

The Simulink file of the MELiSSA model is **melissa_001.mdl**. It is located in the **../melissa_sim/modeles/** directory which MUST BE the current directory of the matlab/simulink software when running a simulation. You can check the current directory with the command **pwd** on the matlab command line. If **./melissa_sim/modeles/** is not the current directory when a simulation is runnig an error message indicating that files in **../melissa_sim/modeles/data** directory can not be found should appear.

When the Matlab/Simulink environment and the MELiSSA model files are correctly configured, the model **melissa_001.mdl** can be opened.
The first window that appears (figure 3.1) gives access to box containing simulations results (flow rates and efficiencies) and to the box containing the MELiSSA loop model itself and its subsystem. You need to double click to open boxes. This windows is normally used for simulating the loop and analysing the results (report to chapter 3.3).
The MELiSSA loop is the second important windows. By opening this windows it is possible to acces all the subsystem of the MELiSSA loop (compartment and management units) and to their operating parameters (report to chapter 3.2).

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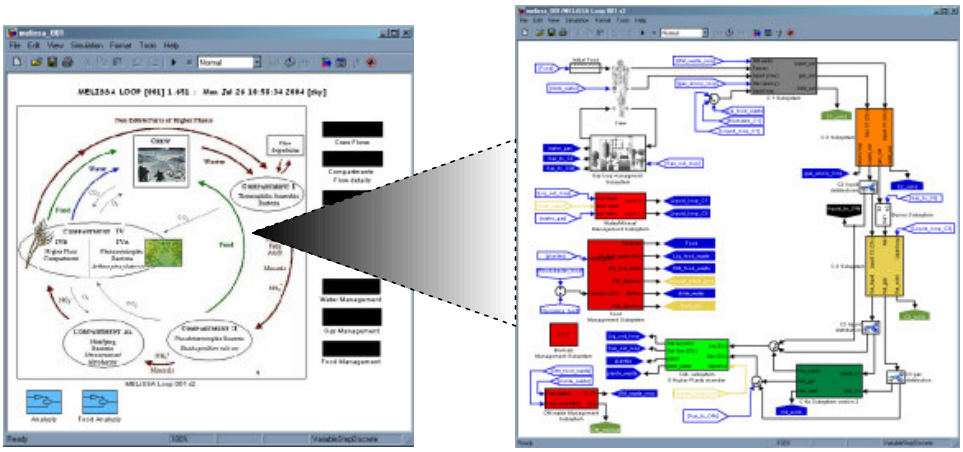

First Windows :
Loop system and access to results

Second Windows :
Loop detail and access to loop subsystems parameters

Figure 3.1 : Firsts MELiSSA windows. Report to table 2.23 for the legend of the loop.

3.2 Model parameters

It is obvious that parameters of the models are important as results of simulations can only be compared on the basis of these parameters. The sheet given in Annex, which reviews the main parameters, must be filled for each simulation. In the models there is two kinds of parameters: those which can be managed through the subsystems dialog boxes, and those fixed in the program code of the models.

3.2.1 PARAMETERS MANIPULATED BY INTERFACES

In the previous chapter, the access to the subsystems parameters dialog boxes was presented in figures. Subsystems and dialog boxes are opened by double clicking on them. Even if the parameters have been already listed and explained before for each subsystems, they will be resumed here in separate tables with a scheme to illustrate how to access to dialog box by green arrows, while yellow arrows indicates parameters that in principle don't need to be modified. It must be outlined that some parameters have low, and sometimes no influence as they are not currently included in models (this is the case of the pH for the reactors)

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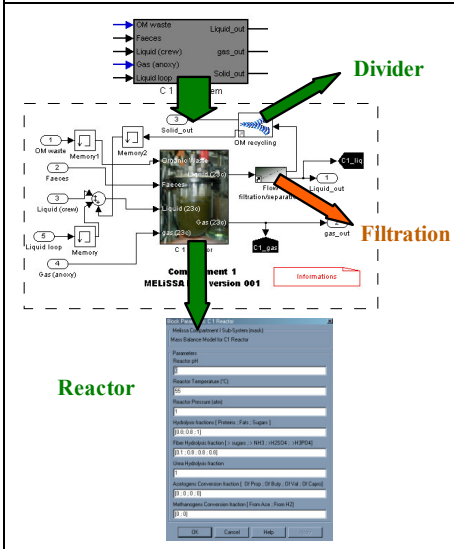
Crew		
Access	Parameter	Function
DON'T NEED TO BE OPENED	NO PARAMETERS DIALOG BOX	

Compartment I		
Access	Parameter	Function
	**Divider** One value between 0 and 1	Gives the fraction of recycled solid to the compartment (0=no recycling) The value 1 is not recommended (accumulation of matter in reactor)
	Filtration Compounds : [19; 20 ; 21 ; 22 ; 23] Separation : [1; 1; 1; 1 ; 1]	Filtration solid/liquid. In principle the default values don't need to be modified.
	Reactor Reactor pH Reactor temperature Reactor Pressure Hydrolysis efficiencies for - *Proteins [C1 E2-1]* - *Fats [C1 E2-2]* - *Carbohydrate [C1 E2-3]* Hydrolysis of Fibre - *Fiber frac. hydrolysed into Sugar* - *N frac. hydrolysed into NH3* - *P frac. hydrolysed into H3PO4* - *S frac. hydrolysed into H2SO4* - *Urea frac into NH3 [C1 E1-1]* Conv. yield into acetic acid from: - *Propionic ac., [C1 E3-1]* - *Butyric ac., [C1 E3-2]* - *Valeric ac., [C1 E3-3]* - *Caproic ac. [C1 E3-4]* Conv. yield of acetic ac. into methane [C1 E4-1] Conv. yield efficiency of H2 into methane [C1 E4-2]	Set the operating condition of the reactor and the efficiencies of the reactions (report to table 2.6). **Note** that efficiencies are given between 0 and 1. **Note** that due to the composition reconciliation it is not always possible to reach the 100% of efficiency for macro molecules hydrolysis.

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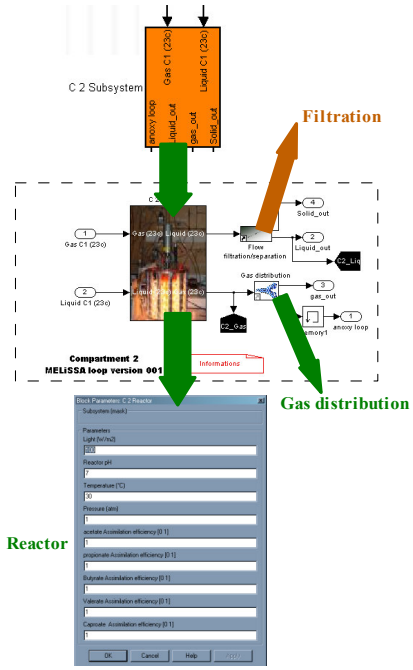
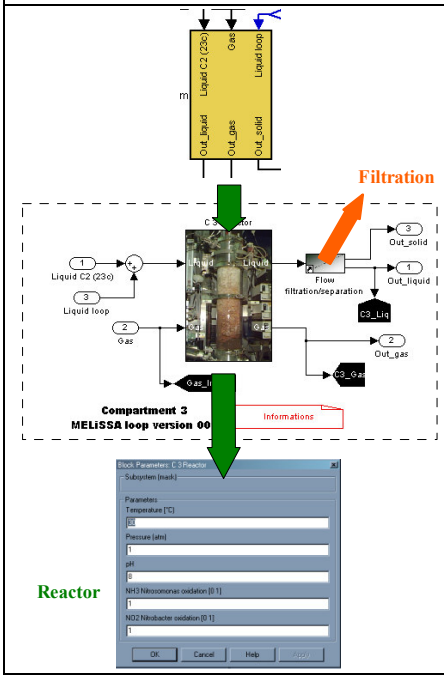
Compartment II		
Access	Parameter	Function
	**Divider (gas distribution)** One value between 0 and 1	Split the gas output from the reactor to the anoxygenic gas loop (CI and CII) and the flow to the C III compartment **Note** that value 0 (complete recycling to the anoxygenic gas loop is forbidden. This causes a gas accumulation loop.
	Filtration Compounds : [22] Separation : [1]	Filtration Biomass/liquid. In principle the default values don't need to be modified.
	Reactor Reactor pH Reactor temperature Reactor Pressure Reactor Ligth flux intensity Acetic ac. Assimilation yield [C2 E1] Prop. ac. Assimilation yield [C2 E2] Buty. ac. Assimilation yield [C2 E3] Val. ac. Assimilation yield [C2 E4] Capr. ac. Assimilation yield [C2 E5]	Set the operating condition of the reactor and the assimilation efficiencies of the reactions (report to table 2.9).

Compartment III		
Access	Parameter	Function
	**Filtration** Compounds : [20 ; 21] Separation : [1 ; 1]	Filtration Biomass/liquid. In principle the default values don't need to be modified.
	Reactor Reactor pH Reactor temperature Reactor Pressure NH3 assimilation yield [C3 E1] HNO2 assimilation yield [C3 E2]	Set the operating condition of the reactor and the assimilation efficiencies of the reactions (report to table 2.11).

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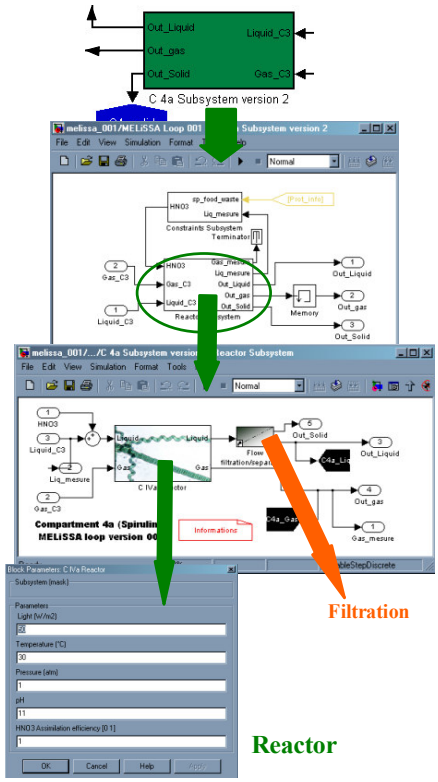
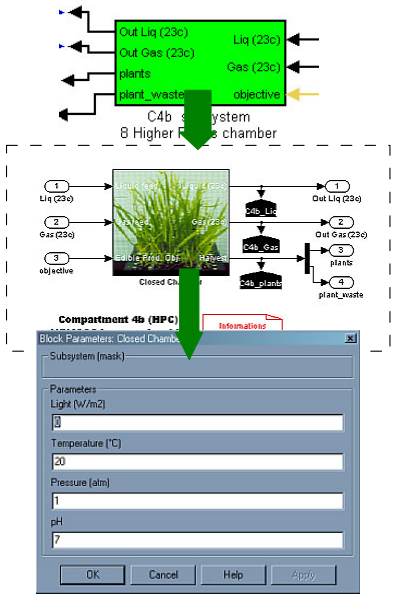
Compartment IVa (Spirulina)		
Access	Parameter	Function
	**Filtration** Compounds : [3] Separation : [1]	Filtration Biomass/liquid. In principle the default values don't need to be modified.
	Reactor Reactor pH Reactor temperature Reactor Pressure Light Intensity HNO3 assimilation yield [C4a E1]	Set the operating condition of the reactor and the assimilation efficiencies of the reactions (report to table 2.14). Note that the constraint subsystem may fail and lead to increase the supply of HNO3 (action is difficult to manage in a steady state system)

Compartment IVb (HPC)		
Access	Parameter	Function
	**Greenhouse/Closed Chamber** pH Temperature Reactor Pressure Light Intensity	Set the operating condition of the chamber Note that the in fact none of the parameters are used in the Higher plant model. All important parameters are fixed in the model program.

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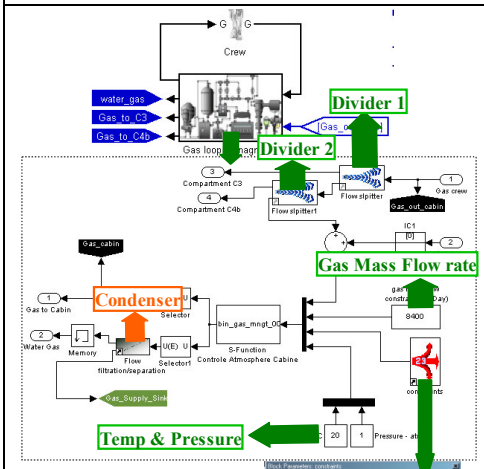
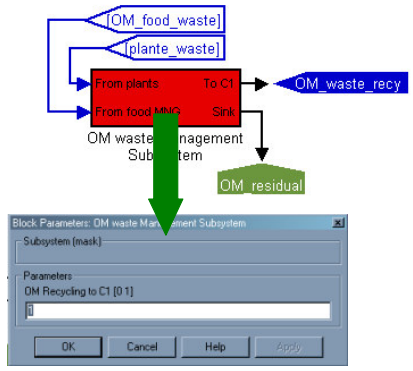
Gas management subsystem		
Access	Parameter	Function
 Composition constraints	**Gas Mass flow rate** A value in kg/day	Set the mass flow for atmosphere to the crew cabin
	Temp & Pressure In each box respectively the temperature of atmosphere (°C) and pressure (in atm)	
	Gas composition constraints *Water :* Relative humidity (between 0 and 1) *Other compounds :* gas molar fraction (between 0 and 1) **Or** value =-1 if the quantity of compound in entry is conserved in the output (i.e. no treatment)	Set the atmosphere composition constraints. **Note**: if N2 fraction is not set to -1, the N2 fraction forces the value of the gas flow rate to be changed (not recommended). **Note** : setting -1 for a compound (other than N2) can lead to its accumulation in the loop (no more in steady state)
	Divider 1 A value between 1 and 0	Give fraction of gas from the crew atmosphere sent to C3 subsystem
	Divider 2 A value between 1 and 0	Give fraction of remaining gas after dispatching to C3 sent to C4a subsystem
	Condense Compounds : [1] Separation : [1]**r**	Condensate gas water. In principle the default values don't need to be modified

Organic Matter management subsystem		
Access	Parameter	Function
	**Recycling to C1** A value between 1 and 0	Set the fraction of organic matter (plant wasted from HPC and food preparation) recycled to C1 subsystem

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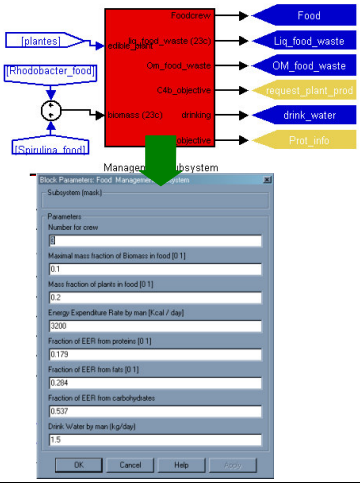
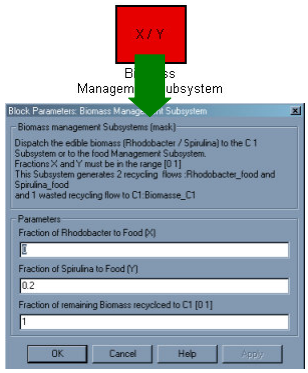
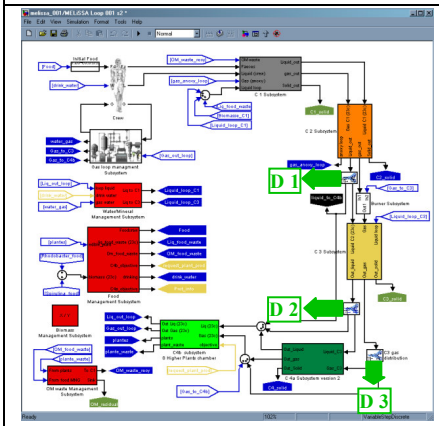
Food management subsystem		
Access	Parameter	Function
	Number of crew (>0) Biomass maximal mass fraction in the food : between 0 and 1 Plant objective mass fraction in food : between 0 and 1 Energy Expenditure Rate (EER) for one man (in kCal /day) EER repartition (fraction between 0 and 1) : Fraction from proteins Fraction from fats Fraction from carbohydrate Drink water for one man (kg/day)	Set the definition of the crew and of the food for the crew. **Note** : In fact EER is here the potential energy of food. The crew metabolism use only a part (about 94%) of the energy. For EER of 3200 kcal/day, this correspond to about 3000 kCal/day used by crew.

Edible Biomass management subsystem		
Access	Parameter	Function
	Fraction of produced Spirulina used for food preparation : between 0 and 1 Fraction of produced Rhodobacter used for food preparation preparation : between 0 and 1 Fraction of unused biomasses in food preparation that are recycled to C1 subsytem preparation : between 0 and 1	Set the distribution of the biomasses Spirulina and Rhodobacter inside the MELiSSA loop

Loop flow distribution options		
Access	Parameter	Function
	**Flow divider D 1** : value between 0 and 1	Liquid distribution from C2 to C3 and C4b (HPC). The flow to **C4b** is: **fraction*"entry flow from C2**"
	Flow divider D 2 : value between 0 and 1	Liquid distribution from C3 to C4a and C4b (HPC). The flow to **C4b** is: **fraction*"entry flow from C3**"
	Flow divider D 3 : value between 0 and 1	Gas distribution from C3 to C4a and C4b (HPC). The flow to **C4a** is: **fraction*"entry flow from C3**"

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3.2.2 PARAMETERS MANIPULATED IN MODELS MATLAB CODE

Some parameters are not accessible through the dialog boxes and can only be changed in the matlab code of the models. Changing these parameters must be exceptional and in principle it would be considered as new models version for the loop. Its is probable that in further developments of the MELiSSA loop models, dialog boxes will be created to manipulate these parameters. Three kinds of parameters may be interesting to manipulate :

- The parameters of the crew metabolism (Table 3.2) , and already presented in chapter 2.2.1
- The parameters for the Higher plant chamber composition and for the resolution of the plant stoichiometric equation (Table3.3), also presented in chapter 2.2.6
- The parameters for the Gas/Liquid equilibria (in each bioreactor model), namely the partition coefficients (Table3.4) , witch are at this time not temperature nor pH dependant. Improvement could be made on the basis of TN 23.1 and TN17.1.

Parameter **[Variable Name in in crew_metabolic_m001.m]**	Value
Mass H2 produced / Mass Food consumed [**rdt_h2_food**]	0
Mass CH4 produced / Mass Food consumed **rdt_ch4_food**]	0
Mass Urea produced / Mass Food consumed [**rdt_uree_food**]	0.04
Fraction of Proteins not oxidised (i.e in Faeces) **[taux_residuel_prot]**	0.05
Fraction of Carbohydrate not oxidised (i.e in Faeces) **[taux_residuel_carb]**	0.01
Fraction of Fat not oxidised (i.e in Faeces) **[taux_residuel_lip]**	0.2
Fraction of fibre not oxidised (i.e in Faeces) **[taux_residuel_fib]**	1
Mass of water for persiparation **[eau_perspi]**	90% of input water

Table 3.2 : Parameters for the crew. They are fixed in the S-function **crew_metabolic_m001.m**

Parameter **[Variable Name in C_IVb_001.m]**	Value
Fraction of edible tomato in the edible production of the greenhouse [**crop(1).culture**]	0.008
Fraction of edible potato in the edible production of the greenhouse [**crop(2).culture**]	0.291
Fraction of edible wheat in the edible production of the greenhouse [**crop(3).culture**]	0.483
Fraction of edible rice in the edible production of the greenhouse **[crop(4).culture]**	0.161
Fraction of edible salad in the edible production of the greenhouse **[crop(5).culture]**	0.005
Fraction of edible soybean in the edible production of the greenhouse **[crop(6).culture]**	0.016
Fraction of edible onions in the edible production of the greenhouse **[crop(7).culture]**	0.016
Fraction of edible spinach in the edible production of the greenhouse **[crop(8).culture]**	0.016
Stoichiometric yield of N substrate g HNO3 / g NH3 for tomato **[Y_NN(1)]**	5 gHNO3 / g NH3
Stoichiometric yield of N substrate g HNO3 / g NH3 for potato **[Y_NN(2)]**	5 gHNO3 / g NH3
Stoichiometric yield of N substrate g HNO3 / g NH3 for wheat **[Y_NN(3)]**	5 gHNO3 / g NH3
Stoichiometric yield of N substrate g HNO3 / g NH3 for rice **[Y_NN(4)]**	5 gHNO3 / g NH3
Stoichiometric yield of N substrate g HNO3 / g NH3 for salad **[Y_NN(5)]**	5 gHNO3 / g NH3
Stoichiometric yield of N substrate g HNO3 / g NH3 for soybean **[Y_NN(6)]**	5 gHNO3 / g NH3
Stoichiometric yield of N substrate g HNO3 / g NH3 for onions **[Y_NN(7)]**	5 gHNO3 / g NH3
Stoichiometric yield of N substrate g HNO3 / g NH3 for spinach **[Y_NN(8)]**	5 gHNO3 / g NH3

Table 3.3 : Parameters for the definition of the greenhouse. They are fixed in the S-function **C_IVb_001.m**

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Parameter **[Variable Name in S-functions]**	Value
Water gas Liquid partition coefficient **[ki(1)]**	Antoine Law : $\frac{\exp\left(18.3036-\frac{3816.44}{273.15+T(°C)-46.13}\right)}{760*P(atm)}$
O2 gas Liquid partition coefficient **[ki(8)]**	4200
CO2 gas Liquid partition coefficient **[ki(9)]**	2000
N2 gas Liquid partition coefficient **[ki(15)]**	10^{10}
H2 gas Liquid partition coefficient **[ki(16)]**	10^{10}
CH4 gas Liquid partition coefficient **[ki(17)]**	10^{10}
Inert gas gas Liquid partition coefficient **[ki(18)]**	10^{10}
Other compounds	0 (only in liquid phase)

Table 3.4 : Parameters for the gas/liquid partition coefficient of compounds. The same parameters are used in all bioreactors.

3.3 Simulations

3.3.1 RUNNING SIMULATION

Simulation can be started from any kind of the Matlab/Simulink MELiSSA loop model. Nevertheless it is preferable to start a simulation from the first windows (Figure 3.5) which gives also direct access to simulation results boxes. The simulation should reaches convergence for the steady in about 20 step of calculation. By default a simulation is done in 40 iterations step.

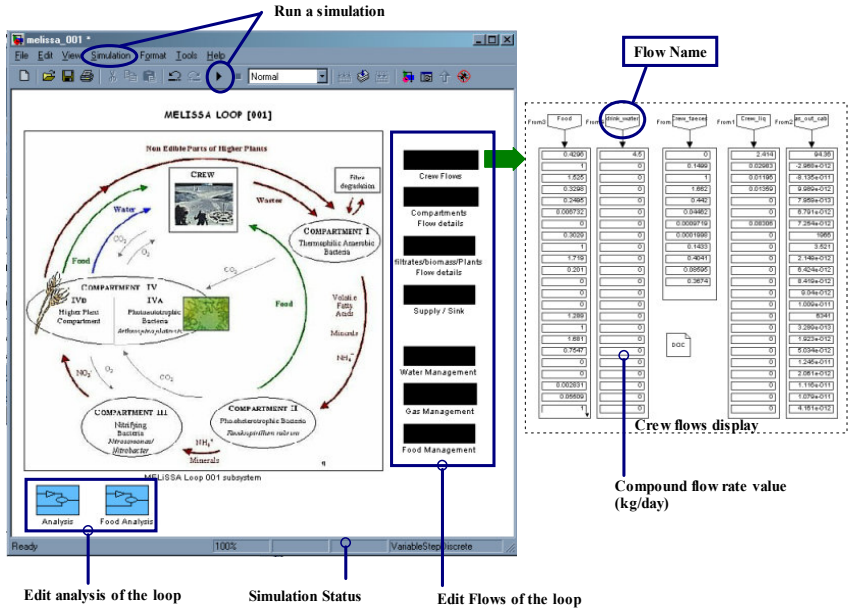

Figure 3.5 : MELiSSA_001 model. First layer.

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3.3.2 RESULTS AND ANALYSIS

A set of 7 black boxes on the right of the windows (Figure 3.5) displays the mains flows rates of the loop. The flow rates are in kg/day (default unit used for setting the flows in Management subsystems). Most of the flows have the 23 compounds format (Table 2.2), while some other (organic matter, plants, faeces flows) have specific format (report to subsystems for detail of the flows format).

Analysis of the loop is made by calculation of its recycling efficiencies and of the respect of the food constraints. The two blue boxes at the bottom of the window do these analyses. The calculi performed in analysis boxes are details in table 3.5

Loop Mass balance analysis	
Supply mass (kg/day.crew)	Sum of supply masses
Sink mass (kg/day.crew)	Sum of sink flows masses
Mass balance (kg/day.crew)	Supply - Sink
Relative mass balance	(Supply-Sink)/Sink
O2 analysis	
O2 recycling efficiency	(Consumed – Supply + Sink)/consumed
O2 consumption (kg/day.crew)	Sum of O2 consumed (crew+C3+burner)
CO2 analysis	
CO2 sink (kg/day.crew)	CO2 extracted/added in gas management subsystem
CO2 recycling efficiency	(produced - Out of loop after C4b)/produced
CO2 production (kg/day.crew)	CO2 produced in crew+C1+C2 compartments
N analysis	
Apparent N recycling	(N supplied + N in loop)/N supplied = N apparent
N distribution efficiency	N at out of loop after C4b / N in loop = efficiency
True N recycling efficiency	N apparent * (1 – efficiency)
S analysis	(S supplied + S in loop)/S supplied
P efficiency	(P supplied + P in loop)/P supplied
Food analysis (Fod management subsystem)	
Supply of prot; fat; carb; fiber (kg/day.crew)	Supply flow of Proteins , Fat , Carbohydrate and Fibre
Supply tot (kg/day.crew)	Total food supply mass
Supply, fraction of food	Food supply / Total dry mass of food consumed
Spirulina, fraction of food	Spirulina biomass used / Total dry mass of food consumed
Rhodocbacter, fraction of food	Rhodobacter used / Total dry mass of food consumed
Plant; fraction of food	Total plant mass used / Total dry mass of food consumed
Plant (kg/day.crew)	Total plant mass used (sum of plants)
Plant_obj :Fraction of plant objective reached	Plant mass consumed / Plant consumption objective
Sp : Spirulina in food (kg/day.crew)	Spirulina biomass used
Rh : Rhodobacter in food (kg/day.crew)	Rhodobacter biomass used

Table 3.5 : Loop efficiency calculi

In addition you must also report to the Matlab® command line in which are displayed the intermediate results for each subsystem of the loop. These information are displayed each time the subsystem model is called. The last informations displayed are those corresponding to the

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results of the simulation; An example is given in table 3.6. These information are useful to identify limitations in reaction and also checking the mass balance (mass_out-mass_in) on each subsystem (relative mass balance is $\frac{mass\_out - mass\_in}{mass\_in}$).

Information on the command line	Comment
Operating C I v. 0.0.1 ---------- Note : S and P elements > discrepency Orignal OM / standardised CHONSP Note : Problem in Fiber degradation for high content in waste recycling C 1 : Initial OM composition --------- Proteins : 0.43821 Lipids : 0.20213 Carbohydrates : 0.14231 C 1 : Computed OM composition Matching Standart CHONSP--------- Proteins : 0.43821 Lipids : 0.20213 Carbohydrates : 0.14231 Remaining : 0.21736 .....Composition correction factor : 1 C 1 : Computed OM composition With Fiber decomposition--------- While 2 correction 1 Proteins : 0.43821 Lipids : 0.20213 Carbohydrates : 0.14231 Non degradable: 0.21736 .....Total Hydrolysis correction factor : 1 While 3 : Final Residual OM correction 1 C 1 : Mass bal.=4.6744e-006// Mass Rel.=8.8595e-009// MS Rel.=-0.00067166 **Fin operation CI ----------**	Details the reconciliation procedure for the C1 model (report to 2.2.2)
Operating C II v. 0.0.1 ---------- Bilan Masse C II = 0 Relative masse balance=0 Reaction limited by other compound : 16... New key calculated : 0.99995 **Stop Operating C II v. 0.0.1 ----------**	Compound 16 is limiting in reaction. A new yield for the key compound is calculated
Operating C III v. 0.0.1 ---------- Bilan Masse C III = 7.276e-012 Relative masse balance=7.9156e-016 **Stop Operating C III v. 0.0.1 ----------**	
Operating C IVa v. 0.0.1 ---------- Bilan Masse C IVa = 0 Relative masse balance=0 **Stop Operating C IVa v. 0.0.1 ----------**	
Operating C IVb v. 0.0.1 ---------- Bilan Masse C IVb = 0 Relative masse balance=0 **Stop Operating C IVb v. 0.0.1 ----------**	
Operating Food Management Unit 0.0.1 ---------- Masse balance 6.6613e-016 relative : 8.9629e-017 **Stop Operating Food Management Unit 0.0.1 ----------**	

Table 3.6 : Details of the information displayed in the Matlab® command line.

The information for the crew compartment (QR, EER) are displayed when opening the crew subsystem.

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4 TESTS AND OBSERVATIONS

Simulations of the loop using the MELiSSA loop model were performed in order :

- To test the model itself
- To check the consistency of the behaviour of the loop with previous loop models
- To identify critical points and then the required improvements of the model or the model limitations

4.1 Tests

The tests performed and presented here are listed in tables 4.1a b,c,d and the parameters are given in table 4.2 (in the format of the data sheet given in annex). It can be noticed that the tests performed are :

- Simulations without the higher plant compartment, what is the configuration of the firsts MELiSSA loop configuration. These tests will allow to check the 2 behaviours observed in previous models : low N recycling and high atmosphere recycling / high N recycling and low atmosphere recycling. In this configuration, the matter flows never pass in the C4b subsystem by managing the 3 flow divider of the loop (Table 4.2).
- Simulations with a higher plant compartment producing 30% of the edible food.

The raw results of the tests (loop efficiencies) are given in annex.

Tests Series 1	Legend	
Test 1-1	Plant:0% Rh:0% Sp:100%	
Test 1-2	Plant:0% Rh:0% Sp:95%	For this serie of tests, the unused biomass in food and the organic residue of compartment 1 (biomass+non degraded matter) are dropped out of the loop and not recycled. The higher plant compartment is by-passed (i.e. loop without plant). There is no limitation in the biomass used in the food for the crew. The biomass is only limited by the amount of proteins required for the crew.
Test 1-3	Plant:0% Rh:0% Sp:90%	
Test 1-4	Plant:0% Rh:0% Sp:85%	
Test 1-5	Plant:0% Rh:0% Sp:80%	
Test 1-6	Plant:0% Rh:0% Sp:75%	
Test 1-7	Plant:0% Rh:0% Sp:70%	
Test 1-8	Plant:0% Rh:0% Sp:65%	
Test 1-9	Plant:0% Rh:0% Sp:60%	
Test 1-10	Plant:0% Rh:0% Sp:55%	
Test 1-11	Plant:0% Rh:0% Sp:50%	
Test 1-12	Plant:0% Rh:0% Sp:45%	In tests 1-1 to 1-21 the fraction of spirulina varies between 100% and 0% in order to observe the behaviour of the loop for N recycling and atmosphere recycling
Test 1-13	Plant:0% Rh:0% Sp:40%	
Test 1-14	Plant:0% Rh:0% Sp:35%	
Test 1-15	Plant:0% Rh:0% Sp:30%	
Test 1-16	Plant:0% Rh:0% Sp:25%	
Test 1-17	Plant:0% Rh:0% Sp:20%	In test 1-22 all the edible biomass produced by the loop is used in the food.
Test 1-18	Plant:0% Rh:0% Sp:15%	
Test 1-19	Plant:0% Rh:0% Sp:10%	
Test 1-20	Plant:0% Rh:0% Sp:5%	
Test 1-21	Plant:0% Rh:0% Sp:0%	
Test 1-22	Plant:0% Rh:100% Sp:100%	

Table 4.1a : details of the tests series 1

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Loop Model :			**Compartment C1**		
Name :	MELiSSA 001		C1 -> C1recycling waste :	0	(variables in some test)
C2 liquid distribution (to C3):	0 and 0,5 if C4b		PH :	6	
C3 liquid distribution (to C4b):	1 and 0,4 if C4b		Temperature :	55	°C
C3 gas distribution (to C4a) :	0 and 0,5 if C4b		Pressure :	1	atm
			Protein hydrolysis :	0,8	
Gas Management Subsystem			Fats hydrolysis :	0,8	
Gas flow :	8400	kg/day	Sugar hydrolysis :	1	
O2 fraction :	0,21		Fiber > sugar hydrolysis :	0,1	
CO2 fraction :	0		Fiber-N > NH3 hydrolysis :	0,8	
Temperature:	20	°C	Fiber-S > H2SO4 hydrolysis :	0,8	
Pressure:	1	atm	Fiber-P > H3PO4 hydrolysis :	0,8	
Flow fraction to C3 :	1		Urea hydrolysis :	1	
Flow fraction to C4b :	0		Propionate > Acetate Yield :	0	
			Butyrate > Acetate Yield :	0	
Water Management Subsystem :			Valerate > Acetate Yield :	0	
Water flow :	1000	kg/day	Caproate > Acetate Yield :	0	
NH3 :	0	kg/day	Acetate > methane Yield :	0	
H3PO4 :	1	kg/day	H2 > methane yield :	0	
H2SO4 :	1	kg/day			
Flow fraction to C1 :	0,7		**Compartment C2**		
			Gas anoxygenic loop recycling :	0,7	
Food Management Subsystem :			Light :	100	W/m2
Crew number :	3	man	PH :	7	
Limit fraction of biomass in food :	1		Temperature :	7	°C
Objective fraction of plants in food :	**0 or 0,3 if c4b**		Pressure :	30	atm
Energy Expenditure Rate (avialable from food) :	3200	kCal/man.day	Acetate assimilation Yield :	1	
EER fraction from proteins :	0,179		Propionate assimilation Yield :	1	
EER fraction form fats :	0,284		Butyrate assimilation Yield :	1	
EER fraction from carbohydrates :	0,537		Valerate assimilation Yield :	1	
Drinking water :	1,5	kg/man.day	Caproate assimilation Yield :	1	
Biomass Management Subsystem			**Compartment C3**		
Spirulina produced used in food :	**Variable**		PH :	8	
Rhodobacter produced used in food :	**Variable**		Temperature :	30	°C
Remaining biomass sent to C1 :	**0**	(variables in some test)	Pressure :	1	atm
			NH3 assimilation Yield :	1	
OM management Subsystem			NO2 assimilation Yield :	1	
fraction recycled to C1 :	0	(variables in some test)			
			Compartment C4a (version 2)		
			Light :	50	
			PH :	11	
			Temperature :	30	
			Pressure :	1	
			HNO3 assimilation Yield :	1	
			Control HNO3 output :	0	
			Control residual Sp, in food preparation :	0	
			Compartment C4b (useless)		
			Light :	0	
			PH :	7	
			Temperature :	30	
			Pressure :	1	
			Crop distribution fixed :		
			crop(1).culture=0.008; % tomato		
			crop(2).culture=0.291; % potato		
			crop(3).culture=0.483; % wheat		
			crop(4).culture=0.161; % rice		
			crop(5).culture=0.005; % Lettuce		
			crop(6).culture=0.016; % soybea,		
			crop(7).culture=0.016; % onions		
			crop(8).culture=0.016; % spinach		

Table 4.2 : Loop and subsystems parameters for the simulations

Tests Series 2	Legend	
Test 2-1	Plant:30% Rh:100% Sp:0%	The same configuration as tests 1 serie is used expecting that the higher plant compartment is used (the 3 flow dividers of the loop set to 0.5). Plants contributes to 30% of the food.
Test 2-2	Plant:30% Rh:100% Sp:100%	
Test 2-3	Plant:30% Rh:0% Sp: 0%	
Test 2-4	Plant:30% Rh:100% Sp:100%	

Table 4.1b : details of the tests series 2

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Tests Series 3	Legend	
Test 3-1 Test 3-2 Test 3-3	Plant:30% Rh:0% Sp:100% Recy 100% Plant:30% Rh:100% Sp:100% Recy 100% Plant:30% Rh:100% Sp: 0% Recy 100%	The same configuration as tests 2 serie is used. In addition 100% of the unused Spirulina and Rhodobacter biomasses and of the plant waste are recycled to Compartment 1

Table 4.1c : details of the tests serie 3

Tests Series 4	Legend	
Test 4-1	Plant:30% Rh:0% Sp:100% Recy 100% 50%C1	The same configuration as tests 3 serie is used. In addition 50% of the residue from compartment 1 is recycled to the compartment

Table 4.1d : details of the tests series 4

4.2 Tests results analyses

4.2.1 TESTS SERIES 1

The results are presented in figures 4.1 and 4.2. It can be seen that the 2 behaviours observed in previous models is also observed with the Simulink model :

- High N recycling with low atmosphere recycling
- Low N recycling with complete atmosphere recycling

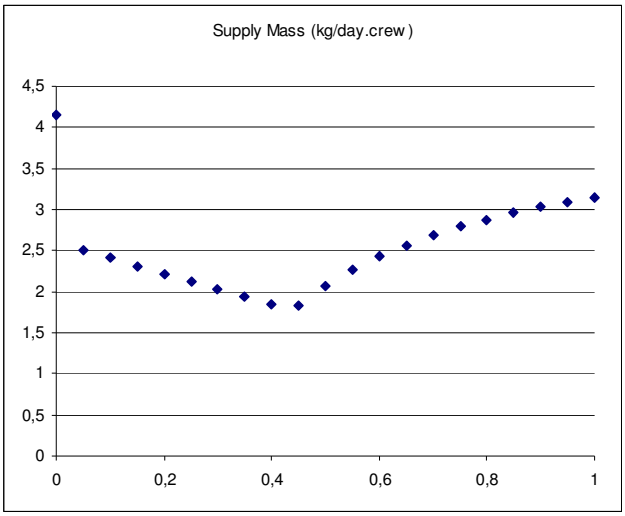

Figure 4.1 : Total supply mass as function of the fraction of produced spirulina used in food. (Tests 1-1 to 1-21)

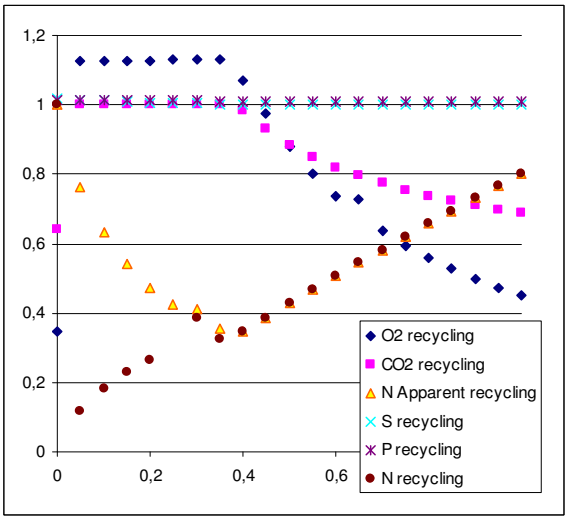

Figure 4.2 : Recycling efficiencies as function of the fraction of produced spirulina used in food. (Tests 1-1 to 1-21)

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In figure 4.2 it can be seen the discrepancy between the two methods for the calculation of the N recycling efficiency (Table 3.5). The two method gives the same results until a limitation (other than HNO3) occurs in the C4a (Spirulina) compartment. When a limitation occurs the method developed for the control of the compartment (based on addition of HNO3 to reach a production objective) failed. This affect the calculation of supply of HNO3 to the compartment and then the N recycling calculation as HNO3 is added while this addition is useless. This probably also affect the total supply mass calculated.

4.2.2 TESTS SERIES 2

Some results are compiled in figures 4.3 and 4.4. As attempted the addition of plant reduce the total supply mass (from 1000g man.day to 400g/man day) both because a decrease in the food supply and in O_2 supply (increase of atmosphere recycling). Biomass represents about 30 to 40% of the food as simulations are made without limit in the quantity of biomass in food. The addition of the higher plant compartment in the loop is difficult to manage as it works quite in parallel with the C4a compartment. Limitations may occur for the two compartments by changing only the biomass distribution. Moreover by construction there is in principle no HNO3 from the C4a compartment to the C4b compartment, and HNO3 limitation can occur. This is most a design problem of the loop and a C4a control strategy (C4a model) problem.

4.2.3 TEST SERIES 3,4

These tests were mainly for checking the effects of the recycling of organic matter (biomass, plant waste, C1 organic residues) to the C1 compartment. These test msut be carefully considered as the C1 model is complex and not fully validated. In principle we attempt to increase the efficiency of the loop by recycling to the C1 compartment.
If the N recycling increase, the total supply mass increase due to decrease of atmosphere recycling and plant production limitation by HNO3. More generally the effects of organic matter recycling to C1 will not be so obvious.

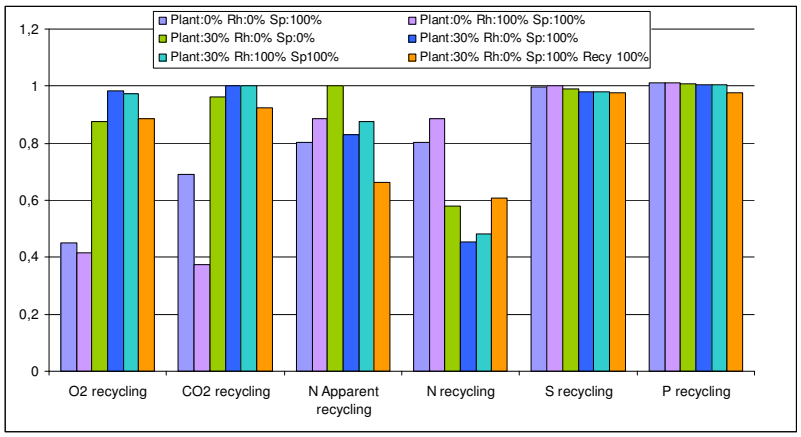

Figure 4.3 : Compilation of recycling efficiencies of tests performed for various operating conditions of the loop model.

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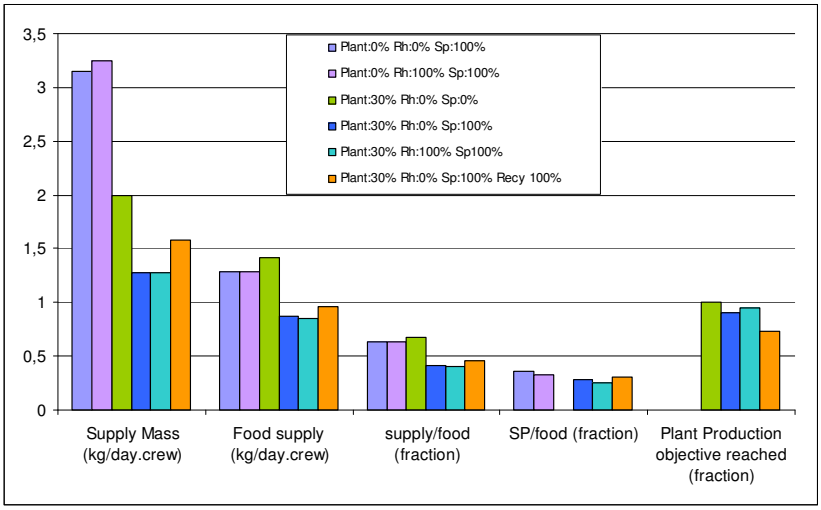

Figure 4.4 : Compilation of food and supply results of tests performed for various operating conditions of the loop model.

4.3 Main observations

The observations detailed here are some problems that were identified in the loop model. Other observation would be made in further simulations (other operating conditions) of the loop. The observations must help in improving the current MELiSSA loop model.

S and P recycling : The recycling of S and P may be > 1. It is probably due to the fact that S and P content of food supply are not taken into account. In principle it is impossible to have a recycling efficiency > 1 for an element (C, H, O, N, S ,P)

Mass balance on the loop : The relative mass balance varies from 10^{-5} % to 2%. At this time the problem of 2% relative mass balance on the loop is not solved. It seems linked to HNO_3 supply on the C4a compartment and problem of the control of this supply when other limitations occurs on the C4a compartment. It is possible that an accumulation occurs in the loop as during the simulation the relative mass balance seems increase with the number of calculation steps.

Limitation on C4a and C4b : This affects all efficiencies. These limitation may have various origin :

- Problem for N (NH3 and HON3) repartition in the loop.
- Inaccurate control procedure for the C4a compartment
- Insufficient CO_2 net production after compartment C1,C2 and C3.
- The design for coupling C4a and C4b may also be questionable.

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5 CONCLUSION

The complete MELiSSA loop was modelled for MatLab/Simulink. For modelling each compartment and each subsystem of the loop, S-blocks were built and associated to steady-state model describing compartments and subsystem on the basis of a mass-balance and an elements-balance. The MELiSSA loop by itself is the result of the linking of the subsystems together.

In principle the choice of Simulink was made as it is possible to do dynamic simulation by implementing dynamic model in S-blocks, in addition to the steady-state models. In practice it would be necessary to change the design of the loop for dynamic simulations, by removing the "memory" blocks and by adding "well configured "Initial Conditions" blocks.

Simulations of the loop were successfully made, even if preliminary tests have high-lightened several problems for some operating conditions. Most of the parameters of the loop can be easily managed using the graphical dialog boxes. Some parameters can be changed in the model code itself, but modification of the models must be carefully considered as it may lead to unexpected results.

In the perspective of the improvement of the current MELiSSA loop model, the attention would be focused :

- On the C1 model, as it represent a key compartment when recycling the organic matter
- On the loop design itself, especially the coupling between C4a/C4b/Food management system/Gas management system
- On the constraint strategy and model used at this time in the model, as most of the problems observed in test seem linked to it.

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ANNEX: DATA SHEET TEMPLATE FOR MELISSA LOOP MODEL PARAMETER

MELiSSA Loop Mass Balance Modeling with Matlab/Simulink

Loop Model :
Name : MELiSSA 001 -
C2 liquid distribution (to C3): -----
C3 liquid distribution (to C4b): -----
C3 gas distribution (to C4a) : -----

Gas Management Subsystem
Gas flow : ----- kg/day
O2 fraction : -----
CO2 fraction : -----
Temperature: ----- ℃
Pressure: ----- atm
Flow fraction to C3 : -----
Flow fraction to C4b : -----

Water Management Subsystem :
Water flow : ----- kg/day
NH3 : ----- kg/day
H3PO4 : ----- kg/day
H2SO4 : ----- kg/day
Flow fraction to C1 : -----

Food Management Subsystem :
Crew number : ----- man
Limit fraction of biomass in food : -----
Objective fraction of plants in food : -----
Energy Expenditure Rate (avialable from food) : ----- kCal/man.day
EER fraction from proteins : -----
EER fraction form fats : -----
EER fraction from carbohydrates : -----
Drinking water : ----- kg/man.day

Biomass Management Subsystem
Spirulina produced used in food : -----
Rhodobacter produced used in food : -----
Remaining biomass sent to C1 : -----

OM management Subsystem
fraction recycled to C1 : ----- (variables in some test)

Compartment C1
C1 -> C1recycling waste : ----- (divider = 1-va
PH : -----
Temperature : ----- ℃
Pressure : ----- atm
Protein hydrolysis : -----
Fats hydrolysis : -----
Sugar hydrolysis : -----
Fiber > sugar hydrolysis : -----
Fiber-N > NH3 hydrolysis : -----
Fiber-S > H2SO4 hydrolysis : -----
Fiber-P > H3PO4 hydrolysis : -----
Urea hydrolysis : -----
Propionate > Acetate Yield : -----
Butyrate > Acetate Yield : -----
Valerate > Acetate Yield : -----
Caproate > Acetate Yield : -----
Acetate > methane Yield : -----
H2 > methane yield : -----

Compartment C2
Gas anoxygenic loop recycling : -----
Light : ----- W/m2
PH : -----
Temperature : ----- ℃
Pressure : ----- atm
Acetate assimilation Yield : -----
Propionate assimilation Yield : -----
Butyrate assimilation Yield : -----
Valerate assimilation Yield : -----
Caproate assimilation Yield : -----

Compartment C3
PH : -----
Temperature : ----- ℃
Pressure : ----- atm
NH3 assimilation Yield : -----
NO2 assimilation Yield : -----

Compartment C4a (version 2)
Light : -----
PH : -----
Temperature : -----
Pressure : -----
HNO3 assimilation Yield : -----
Control HNO3 output : -----
Control residual Sp, in food preparation : -----

Compartment C4b (useless)
Light : -----
PH : -----
Temperature : -----
Pressure : -----
Crop distribution fixed :
crop(1).culture=0.008; % tomato
crop(2).culture=0.291; % potato
crop(3).culture=0.483; % wheat
crop(4).culture=0.161; % rice
crop(5).culture=0.005; % Lettuce
crop(6).culture=0.016; % soybea,
crop(7).culture=0.016; % onions
crop(8).culture=0.016; % spinach

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ANNEX: RAW RESULTS OF TESTS

	Plant in food	X (Rhodobacter)	Y(Spirulina)	Supply Mass (kg/day.crew)	Relative mass (absolute)	Relative mass (%)	O2 recycling	CO2 recycling	N Apparent recycling	N recycling	S recycling	P recycling	Food supply (kg/day.crew)	supply/food (fraction)	Plant/food (fraction)	Plant Production objective reached (fraction)	SP/food (fraction)	Rh/food	Remark
Plant:0% Rh:0% Sp:100%	0	0	1	3,153	2,00E-07	*0,00006306*	0,4509	0,6892	0,8015	0,8015	0,9989	1,011	1,29	0,6366	0	0	0,3634	0	
Plant:0% Rh:0% Sp:95%	0	0	0,95	3,096	2,00E-07	*0,00006192*	0,4735	0,6995	0,7661	0,7661	0,9989	1,011	1,29	0,6366	0	0	0,3634	0	
Plant:0% Rh:0% Sp:90%	0	0	0,9	3,032	2,09E-07	*6,33688E-05*	0,4987	0,711	0,7303	0,7303	0,9989	1,011	1,29	0,6366	0	0	0,3634	0	
Plant:0% Rh:0% Sp:85%	0	0	0,85	2,961	2,14E-07	*6,33654E-05*	0,5268	0,7239	0,6941	0,6941	0,9989	1,011	1,29	0,6366	0	0	0,3634	0	
Plant:0% Rh:0% Sp:80%	0	0	0,8	2,881	2,20E-07	*6,33791E-05*	0,5595	0,7383	0,6573	0,6573	0,9989	1,011	1,29	0,6366	0	0	0,3634	0	
Plant:0% Rh:0% Sp:75%	0	0	0,75	2,791	2,27E-07	*6,33557E-05*	0,5943	0,7547	0,6202	0,6202	0,9989	1,011	1,29	0,6366	0	0	0,3634	0	
Plant:0% Rh:0% Sp:70%	0	0	0,7	2,688	2,36E-07	*6,34099E-05*	0,6353	0,7734	0,5825	0,5825	0,9989	1,011	1,29	0,6366	0	0	0,3634	0	
Plant:0% Rh:0% Sp:65%	0	0	0,65	2,568	2,00E-07	*0,00005136*	0,7279	0,795	0,5444	0,5444	0,9988	1,011	1,29	0,6366	0	0	0,3634	0	
Plant:0% Rh:0% Sp:60%	0	0	0,6	2,429	2,60E-07	*0,000063154*	0,7378	0,8202	0,5057	0,5057	0,9989	1,011	1,29	0,6366	0	0	0,3634	0	
Plant:0% Rh:0% Sp:55%	0	0	0,55	2,265	2,80E-07	*6,33747E-05*	0,8029	0,8499	0,4666	0,4666	0,9989	1,011	1,29	0,6366	0	0	0,3634	0	
Plant:0% Rh:0% Sp:50%	0	0	0,5	2,068	3,00E-07	*0,00006204*	0,8812	0,8857	0,4269	0,4269	0,9989	1,011	1,29	0,6366	0	0	0,3634	0	
Plant:0% Rh:0% Sp:45%	0	0	0,45	1,827	3,47E-07	*6,33969E-05*	0,9768	0,9293	0,3868	0,3868	0,9989	1,011	1,29	0,6366	0	0	0,3634	0	
Plant:0% Rh:0% Sp:40%	0	0	0,4	1,839	3,44E-07	*6,32616E-05*	1,069	0,9839	0,3461	0,3461	0,9989	1,011	1,29	0,6366	0	0	0,3634	0	
Plant:0% Rh:0% Sp:35%	0	0	0,35	1,935	0,0008018	*0,1551483*	1,131	1	0,355	0,3255	1,001	1,011	1,361	0,6716	0	0	0,3284	0	CO2 limitation
Plant:0% Rh:0% Sp:30%	0	0	0,3	2,029	0,00179	*0,363191*	1,13	1	0,4101	0,3859	1,003	1,012	1,456	0,7186	0	0	0,2814	0	CO2 limitation
Plant:0% Rh:0% Sp:25%	0	0	0,25	2,124	0,00269	*0,571356*	1,129	1	0,4244		1,005	1,012	1,55	0,7656	0	0	0,2344	0	CO2 limitation
Plant:0% Rh:0% Sp:20%	0	0	0,2	2,219	0,00352	*0,781088*	1,128	1	0,474	0,2639	1,007	1,013	1,645	0,8125	0	0	0,1875	0	CO2 limitation
Plant:0% Rh:0% Sp:15%	0	0	0,15	2,313	0,00432	*0,999216*	1,127	1	0,5401	0,2304	1,01	1,013	1,739	0,8594	0	0	0,1406	0	CO2 limitation
Plant:0% Rh:0% Sp:10%	0	0	0,1	2,407	0,005	*1,2035*	1,126	1	0,6322	0,1838	1,012	1,014	1,833	0,9063	0	0	0,0936	0	CO2 limitation
Plant:0% Rh:0% Sp:5%	0	0	0,05	2,509	0,008448	*2,1196032*	1,125	1	0,7629	0,1158	1,014	1,014	1,927	0,9532	0	0	0,04683	0	CO2 limitation
Plant:0% Rh:0% Sp:0%	0	0	0	4,153	0,003912	*1,6246536*	0,3474	0,6429	1	1	1,017	1,014	2,021	1	0	0	0	0	
Plant:0% Rh:100% Sp:100%	0	1	1	3,246	0,000268	*0,0869928*	0,4135	0,3727	0,8875	0,8875	0,9998	1,013	1,292	0,6347	0	0	0,3312	0,03404	
Plant:30% Rh:100% Sp:0%	0,3	1	0	1,915	0,007388	*1,414802*	0,8855	0,9664	1	0,5671	0,991	1,008	1,355	0,6418	0,3254	1	0	0,069	
Plant:30% Rh:100% Sp100%	0,3	1	1	1,275	0,00215	*0,274125*	0,9734	1	0,876	0,4817	0,9796	1,006	0,8548	0,4049	0,3104	0,9539	0,5317	0,069	CO2 limiting (C4b)
Plant:30% Rh:0% Sp:0%	0,3	0	0	1,991	0,0073	*1,45343*	0,8767	0,9615	1	0,5778	0,9915	1,007	1,415	0,6736	0,3264	1	0	0	
Plant:30% Rh:0% Sp:100%	0,3	0	1	1,273	0,0014	*0,17822*	0,9845	1	0,8302	0,4524	0,9797	1,005	0,8749	0,4169	0,2966	0,9062	0,2865	0	CO2 limiting (C4b)
Plant:30% Rh:0% Sp:100% Recy 100%	0,3	0	1	1,585	0,000945	*0,1497825*	0,8856	0,9255	0,6627	0,6071	0,9775	0,9782	0,9563	0,4588	0,24	0,7285	0,3012	0	HNO3 Limiting on C4b
Plant:30% Rh:100% Sp:100% Recy 100%	0,3	1	1	1,128	0,004	*0,4512*	0,9442	0,9775	0,795	0,6306	0,9787	0,999	0,8373	0,3927	0,3221	1	0,1865	0,2103	
Plant:30% Rh:100% Sp:0% Recy 100%	0,3	1	0	1,826	0,0068	*1,24168*	0,7804	0,9044	1	0,9728	0,9856	0,9965	1,136	0,5301	0,302	0,9994	0	0,321	HNO3 Limiting on C4b
Plant:30% Rh:0% Sp:100% Recy 100% + 50%C1	0,3	0	1	1,999	0,0005	*0,09995*	0,7878	0,8713	0,6876	0,6491	0,9775	0,9658	1,021	0,4926	0,1943	0,586	0,313	0	HNO3 Limiting on C4b

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